Crystallography News

British Crystallographic Association

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22nd Congress of the IUCr in Madrid p6

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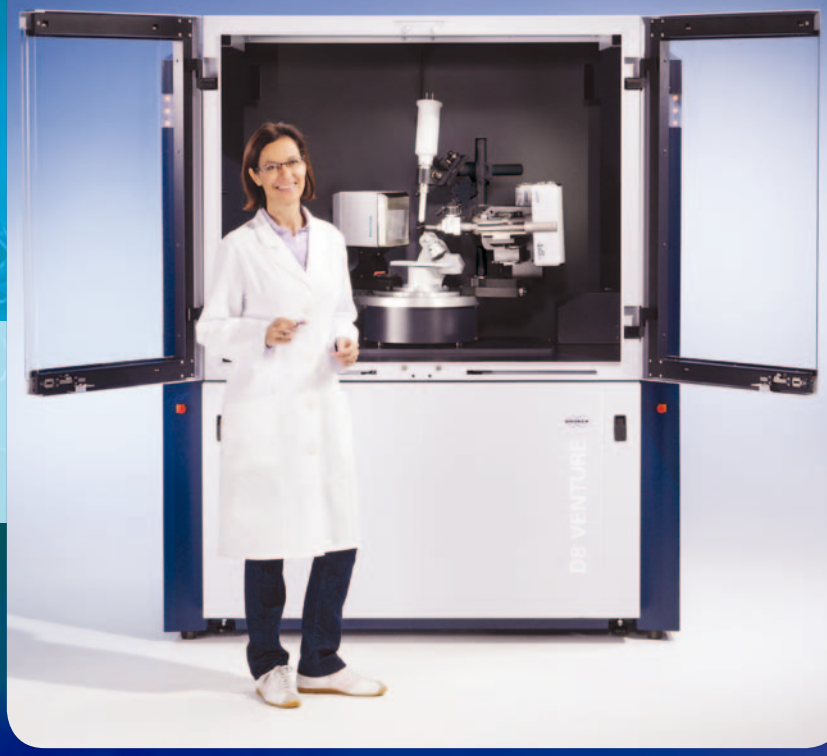

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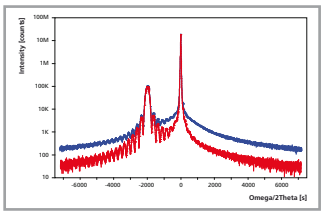

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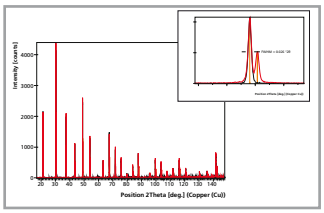

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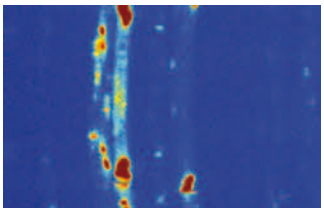

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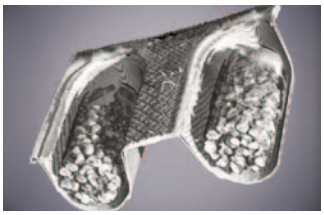

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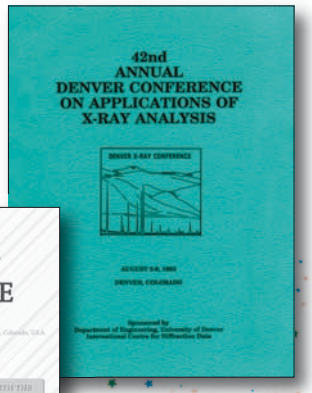

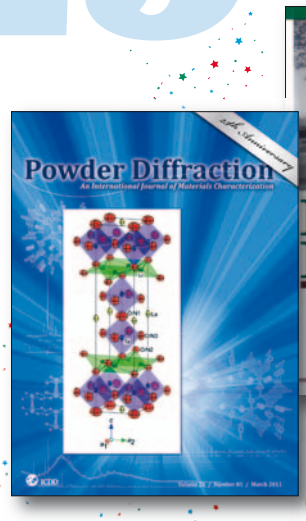

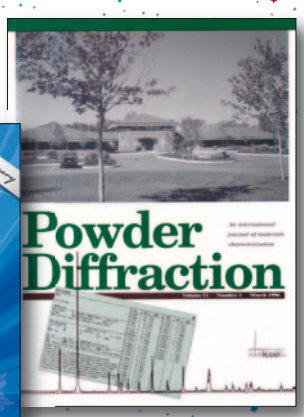

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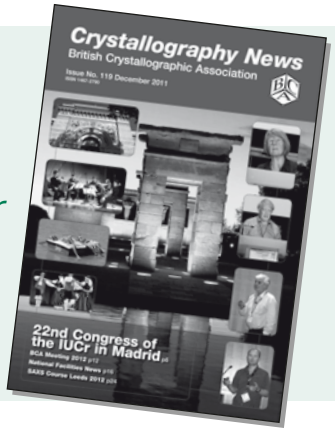

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From the Editor

THE RECENT Congress of the International Union of Crystallography (IUCr) in Madrid proved that our Spanish colleagues are not just brilliant crystallographers, they are brilliant meteorologists as well. Those of us who came a few days earlier had to contend with temperatures around 40° C.

Madrid was thronged with banner-waving young people taking part in a worldwide Catholic youth festival (JMJ) which included a papal visit. As I sweltered in my T-shirt and shorts, I felt sympathy for the poor Pope, who could hardly strip down to that extent. However, during the night before the Congress, a cold front came through with a brisk thunderstorm followed by a breeze that was no longer hot, just pleasantly warm. The cooling trend persisted and intensified throughout the Congress. The conference dinner was held outdoors in the lovely surroundings of the Botanical Garden of the Universidad Complutense de Madrid. The photo on page 10 of our President together with Brazilian friends conveys the happy atmosphere that prevailed, but one had to be tough to withstand temperatures that reached a low of 10° C. Though unprepared for such conditions, I managed to stay just about warm enough by putting on several layers of short-sleeved clothing topped with a summer-weight jacket. Unfortunately, hypothermia compelled several of the more skimpily clad ladies to leave this very pleasant event early. As for the conference itself, as usual it offered a feast of fascinating presentations. My account of the meeting can only provide a cross-section. The full set of abstracts will be made available online in a Supplement to Acta Crystallographica, volume A67. For a report with facts and figures and for a selection of pictures consult **www.iucr2011.madrid.es** . The Congress is also the setting for Council meetings of the IUCr and European Crystallographic Association (ECA), where important issues are decided. I am grateful to **Georgina Rosair** for briefing us about the significant decisions taken in Madrid.

The ECA Council decision of greatest importance to us was taken in Istanbul two years ago, when our bid to host the 2013 European Crystallographic Meeting narrowly prevailed over a competing bid from Greece. Under the circumstances one felt a tendency to regard Greek crystallographers as being in competition with us. Since then we have seen numerous reports in the general media about the devastating impact of the financial crisis on Greek society as a whole, but little about the effect on Greek science. More information is available in specialist media. According to a blog posted in January 2011 by **Anastasia Pappa** on **www.euroscience.org** Greek people love science but the government does not fund it sufficiently. Expenditure on science had decreased to less than 0.6% of GDP. The budget for universities was abruptly cut by 30%, and no fixed-term contracts for academic staff can be extended. A Guardian blog stated that an additional austerity package, passed in June 2011, cut public sector salaries by 15%. However, there is one (X-?) ray of hope. According to a Nature News item posted by **Alison Abbott** in May 2010, Greece had received an allocation of €1.5 billion in European Union structural funding to support research during the period 2007-2013 which had until then remained unspent. Any funds remaining at the end of 2013 would have to be returned to the EU. The then new general secretary for research and technology, **Achilleas Mitsos**, promised to spend the entire amount in roughly equal portions over the years to 2013, and to award these funds in response to peer-reviewed grant applications. We wish our Greek colleagues well as they confront the severe problems facing them.

The exciting international activity should not obscure the fact that an important SAXS workshop took place in the UK this summer. Reminding us that worthwhile structural information can be obtained from non-crystalline material, it deepened participants' knowledge of small-angle scattering. I am pleased to include a write-up by **Arwen Pearson** and a photo taken by Dr. **Edward Snell** from the Hauptman-Woodward Medical Research Institute in Buffalo, NY.

Winter is a peak time for biological crystallographers. The Group meeting on 'Supramolecular Assemblies' will be held at Diamond on December 14. In the New Year the ever-popular CCP4 workshop will take place from January 4-6 at the University of Warwick. To ensure adequate space for the large number of participants the Arts Centre is being used as the venue.

I conclude by mentioning the Big Event, the forthcoming BCA Spring Meeting at Warwick from April 16 to April 19. Under the general title 'Challenges in Crystallography' **Kirsten Christensen**, Chair, and the Programme Committee have crafted a very exciting series of sessions. Full details appear in this issue.

Carl Schwalbe

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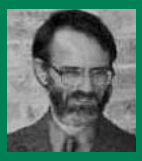

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(The dates in parentheses indicate the end of the term of office).

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

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

From the President

DEAR MEMBER

I am writing this letter on an Aegean aeroplane on my way to Athens to teach macromolecular crystal cryocooling techniques at an FP7-EU funded Workshop entitled 'Structure– & Computer– Aided Design Workshop: Bioactive Molecules & Materials' to be held at the National Hellenic Research Foundation. This morning the Greek Prime Minister, Mr. **George Papandreou** resigned, and negotiations are underway to form a coalition Greek Government to steer Greece through its current fiscal crisis. I hear and read of the dire employment and general depressed situation of the Greek people, and I am concerned for the future of the colleagues and students there with whom I am about to interact. Our Editor has addressed this issue in more detail in these pages.

This time last year in the UK we were ourselves trying to absorb and understand the likely effects of the Government's Comprehensive Spending Review and the Browne Report, both on the costs for future undergraduates at our Universities and on UK research efforts. Today we hear that due to recent changes in funding policy, many Universities during the next 3 weeks are likely to revise their April 2011 initial applications to charge the maximum (£9,000) per annum in student fees, and to reduce the amount they intend to charge. This is a positive step for our future undergraduates. On the research front we are becoming daily more 'REF aware' as Departments gather the information that will be required for the submissions, and I for one am grateful that Professor Sir **David Phillips**, the Head of the Oxford Laboratory of Molecular Biophysics when I moved there from Nuclear Physics in 1987, used to ask us every year for a list of talks we had given at meetings, in schools and to the public, conferences we had attended, interactions with the Press and for any other noteworthy news. Ever since then, I have kept a running log of all these activities, and this has proved to be a useful device when requests such as that for the 'REF narrative' come around.

The summer already seems a long time ago, but I very much enjoyed the IUCr Congress in Madrid, seeing many old friends and colleagues, and meeting new ones, as well as hearing some fascinating talks and with other BCA members, attending the evening Congress meetings to represent the UK. An account of the main decisions reached during the latter, written by the BCA Secretary, **Georgina Rosair**, can be found later in this issue. The Spanish crystallographers are to be congratulated for their superb organisation of the congress: the open air dinner for over 2000 people in the Universidad Complutense de Madrid Botanic Gardens and the subsequent dancing to a live band were especially memorable. To my delight I was approached by 4 glamorous looking students whom I did not recognise. They told me that they were from Brazil and that I had taught them all over the years at various Rapidata collection courses at Brookhaven (or 'Brookheaven' as my Mexican colleague, Enrique Rudiño-Piñera calls it!). There was a resulting photo shoot, and having then watched them dance, I decided I definitely needed, and would love to have, some dancing lessons from them!

I also attended the IUCr Commission on Journals for 2 days before the main congress in El Escorial, the location of a magnificent World Heritage Monastery built between 1563 and 1574 by Philip II, and which contains the remains of Spanish Kings and Queens in a crypt. We arrived in the town an hour after the Pope had left, and literally armies of JMJ youth from all over the world were crowding the streets and were much in evidence on the Madrid Metro system during the Congress. I found the Journals meetings really instructive and helpful for understanding the whole production process, and the role that the co-editors.have in expediting it.

As President I have the enjoyable task annually of inviting nominations for new Honorary Members of the BCA. Honorary Membership is the highest membership accolade of the BCA, and is awarded to a small number of colleagues who have contributed significantly both to crystallography and to the work of the BCA. Last year there were no new Honorary Members elected, in part since our dwindling membership numbers meant that we were in danger of having over 5% of all members being Honorary ones. However, I am happy to say that membership recruitment and retention efforts are now starting to bear fruit (although I fear that I am still winning the 'Member get a Member' competition) so that this eventuality is receding. Please send your nominations, together with a short (but not too short) supporting case, detailing how your candidate has contributed to crystallography and to the BCA, to me at **president@crystallography.org.uk** by 31st January, 2012. For information, a list of our 22 current Honorary Members is now available at **http://crystallography.org.uk/honorary-members** (thanks to **Richard Cooper** our WWW Master).

The 2012 Warwick Spring Meeting planning is now well underway, and details can be found later in this issue. I encourage all members to bring as many of their group as is feasible to the meeting, since it promises to be a stimulating event. The Young Crystallographers will again hold their pre-meeting event on Monday 16th April and the morning of Tuesday 17th April. After last year's very successful ceilidh, there will be a repeat at this year's Spring Meeting. At the AGM we will also be electing a new President who will take the helm for the 2013 ECM in Warwick and 2014

International Year of Crystallography.

I trust that the one-day autumn/winter Group meetings have been productive and well attended: unfortunately I could not attend any of them this year, not even that of the BSG. However, **Dave Allan**, our Vice-President, has been present at two of them on behalf of the BCA Council, and **John McGeehan** from Portsmouth University will do the same at the BSG one day meeting at Diamond on 14th December.

In preparation for the International Year of Crystallography, over the last 3 months each of the Groups within the BCA have nominated an Education representative who will be a contact person for the group and has a remit which was sent round by the Group Chairmen to group members by e-mail. I am happy to announce that these representatives are: **Airlie McCoy** (BSG), **Liana Vella-Zarb** (CCG), **Richard Morris** (IG), **Mike Glazer** (PCG), and **Robert Young** (YCG). I am most grateful to them for being willing to help the BCA in this way.

Lastly, I am pleased to say that we currently have only one member to whom e-mails now bounce, and I am hot on his track! My new name is **Elspeth Holmes**!

Wishing you all a Joyful Christmas and Peaceful 2012.

Elspeth

Puzzle Corner

'TIS the season to be jolly…

Recently I applied my fussy editor's eye to giving my son's PhD thesis in genetics a final check. I was struck by the whimsical names used for important genes such as Sonic Hedgehog. I have colleagues who are NMR specialists and apply techniques with whimsical acronyms such as COSY, NOESY, ROESY, HOHAHA and INEPT. (If you want to know what these acronyms mean, and many more besides, have a look at www.chem.ox.ac.uk/spectroscopy/nmr/acropage.htm .) Can readers think of similarly amusing names or acronyms used in crystallography, or are we just too sober-sided?

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Madrid Report

22nd Congress of the IUCr in Madrid

WHEN you have attended as many international meetings as I have, you have definite ideas about what to expect in an opening ceremony: some gentle classical music to soothe the stressed travellers upon arrival, some very formal speechifying by local worthies, some lively classical music to wake the audience up again, a smidgen of local folklore, and a prize-winner's lecture which is fascinating if you're active in that field and which you regard as an obstacle to eventual much-needed food and drink if you're not. However, the Madrid organisers provided us with several surprises. Yes, the classical music was lovely and the food was delicious, but early in the proceedings some muscular men in Roman garb bearing hefty tools appeared on stage. While we were told about the Roman quarries in Spain for *lapis specularis* (selenitic gypsum, which is transparent enough for use as window panes), the men processed a block of this substance into clear sheets as the Romans would have done. Those of us who were lucky enough to sit near the front could watch the proceedings directly, but a big screen above the stage provided a clear view from anywhere in the auditorium. Among the formal speeches was a bright, breezy and informal welcome by **Pilar Goya Laza**, the Vice-President of the Spanish Chemical Society. The winning, powerfully simple, logo design for the International Year of Crystallography was unveiled. Then we had not one but three Ewald Prize Lectures, given by **Eleanor Dodson**, **Carmelo Giacovazzo** and **George Sheldrick**. The common theme of their work was the development and dissemination of essential methods for doing structural crystallography. In less time than one lecturer would normally require, they gave lucid and entertaining accounts of developments in their fields with generous credit to colleagues.

Bright and early the next morning **Tom Steitz** brought us up to date with exciting developments in the exploitation of our hard-won knowledge of ribosome structure to discover new antibiotics. Next I selected, from a choice of 7, the microsymposium MS06 on crystal structure prediction. Inspired by the Cambridge Crystallographic Data Centre, blind tests of organic structure prediction have been running since 2000; but now the inorganic crystallographers have tried their hand. **Artem Oganov** effortlessly leapt from the earliest days of crystallography to the latest developments. The structure of zincblende (ZnS) was solved by the Braggs in 1913; and, starting from the known structure, density functional theory (DFT) gets the molar volume right to ±1-3%. For completely *ab initio* inorganic structure prediction the hybrid evolutionary algorithm USPEX has demonstrated its utility. The methodology and a variety of successful applications have recently been described in the article by A. R. Oganov, A. O. Lyakhov and M. Valle (2011), Accounts of Chemical Research, 44, 227-237. This approach was able to guide us through the weird world of high-pressure phenomena, where LiH_6 forms, becoming an excellent superconductor, and Na becomes transparent. Next, **Aurora Cruz-Cabeza** gave a comprehensive and impartial survey of recent advances in organic crystal structure prediction. The 2010 organic Blind Test included three familiar-looking target molecules; but to increase the challenge others had greater complexity, including a salt, an extremely flexible molecule and a polymorphic hydrate. Of the 15 participating research groups, four obtained and chose to submit correct predictions for at least one of the target structures, while a similar number found correct structure(s) but with too low a ranking to warrant submission. This was a computationally expensive venture: collectively 68 years of computing time was used, but every target was correctly predicted at least once. **Matthew Habgood** informed us about obstacles and progress in the difficult area of modeling and predicting disorder. Crystal structure prediction includes structure generation and stability calculation. To account for disorder one should use symmetry-adapted ensembles. In this way one creates a supercell, e.g. N = 16, where each site could be "red" or "blue". An example is the structure of eniluracil, in which different crystals exhibit different degrees of disorder, described by R. C. B. Copley et al. (2008) Crystal Growth & Design, 8, 3474-3481. Initial calculated results were discouraging: the free energy of the disordered structure compared to the ordered alternative was >3 kJ mol^{-1} higher. This discrepancy was attributed to the assumption of equally populated configurations. Some configurations created very high-energy close contacts between O atoms of adjacent molecules. Excluding them on the reasonable assumption that they would be avoided during crystal growth yielded a lattice free energy that was virtually identical for the disordered and ordered models. **Jacco van de Streek** gave an overview of the achievements of and recent improvements to dispersion-corrected density functional (DFT-D) methods for crystal-structure prediction, which have achieved much success in recent Blind Tests. DFT with plane waves was a big advance on its own, but it misses weak van der Waals interactions that are significant in most organic crystals. Rectifying this limitation by a dispersion correction has led to correct predictions for the "classical" Blind Test categories but less reliable energies for salts and hydrates. Help is on the way: the dispersion correction published in 2010 by Grimme et

al. is superior to previous ones, and improved density functionals have recently become available. A better set of reference data based on crystal structures below 30K has been created, along with improved software to use these data in parameter fitting. Despite the much improved performance, one must bear in mind that predictions still are at 0 K without consideration of entropy. Finally, **Rene de Gelder** extended the coverage to the combination of crystal structure prediction with other data. In an increasingly common situation moderate to high quality X-ray powder diffraction (XRPD) data are available for a new compound or new polymorph; but, possibly due to problems such as difficult indexing, low information content or preferred orientation, the structure cannot be determined. The program IsoQuestCSP takes predicted structures, generates XRPD descriptors and compares them with the experimental pattern. The Mercury Materials Module is used to identify the best rms fit. In the test case of nonpolar amino acids the correct structure is usually found, but seldom giving the best fit. Along with the aforementioned experimental difficulties the predicted structure may be deformed due to inadequacies in the force field. Anisotropic scaling gives much improved matches.

The powder diffraction theme continued in the afternoon with MS10, "Determination of Ab-Initio Crystal Structures from Powder Diffraction and their Applications in Pharmaceutical Industry". **Alastair Florence** began by presenting some impressive recent achievements of XRPD in structure determination: a hydrochlorothiazide methyl acetate solvate with 13 degrees of freedom; hydrochlorothiazide form II solved by simulated annealing followed by manual rotation to make the best hydrogen bonds, subsequently verified with single-crystal data; a disordered benzoate salt; cytenamide form II with Z' = 4 and 28 degrees of freedom; and chlorothiazide with 2 solvent molecules. **Chris Gilmore** addressed the situation where only low-resolution powder diffraction data are available. The charge flipping technique has achieved much success in structure determination; but it is believed to require complete data to atomic resolution. Chris proposed the alternative hypothesis that with lower-resolution data, e.g. to 2.0 Å, *Superflip* can still get the answer but does not know it. Generally convergence is not achieved even after 10,000 cycles and the figures of merit are ambiguous. However, sending the resulting phase sets to constrained entropy maximization improves them and provides a new ranking; maps are calculated for the top 24 solutions, filtered by histogram matching and examined. This procedure has successfully solved a number of structures from XRPD data. **Irene Margolaki** pushed XRPD to its ultimate challenge: microcrystalline proteins. With the aid of synchrotron data and the expertise of the ESRF team whale metmyoglobin has been successfully refined (subject to many restraints) and insulin data to 2.3 Å gave an electron density map clearly showing heavy atoms. **Hidehiro Uekusa** demonstrated the value of structure determination from powder X-ray diffraction data (SDPD) in the analysis of pseudo-polymorphic transition of pharmaceutical crystals. Many hydrates of drugs form single crystals that can undergo dehydration, but in the process they degrade to powders. The cephem antibiotic cephalexin is a particularly challenging example: it has five hydrated forms which are reversibly interchangeable by changes in relative humidity. Three of the pseudo-polymorphs were solved by SDPD, enabling the water molecules to be located and the structural changes upon hydration to be followed. Erythromycin and acrinol were also successfully studied.

While structure-based *drug* design is well established, **Peter Kwong** turned our attention to vaccine design. A vaccine against HIV-1 has been zealously sought, but success has not yet been achieved. Infected patients produce large quantities of antibodies, but most are ineffective, largely because cellular machinery covers most of the viral protein surface with glycan. In the early 1990s some rare or unnatural antibodies were found that do neutralize HIV, and their viral target sites were located. However, the main roadblock to elicitation of such antibodies seems to be maturation. In 2010 it became clear that affinity maturation only starts to work well in the final stages since affinity remains low until then. In 2011 the maturation process was delineated and immunogens to overcome the roadblock were created.

Microsymposium MS17 on "Synthons" featured an innovative combination of enzyme design, drug design and crystal engineering. **David Hilbert** introduced the programs *Rosetta Match* and *Rosetta Design* for the computational design of enzymes. An example of their functionality is the placement of opposite charges near the charged portion of a substrate and the identification of appropriate sequences of amino acids to supply them. The relevant genes can be prepared and put into micro-organisms. The resulting enzymes are likely to have only modest activity, but mutations in a process of directed evolution can raise the activity dramatically. In this way a catalyst for the non-natural retro-aldol reaction has been developed which provides a rate acceleration of 60 million. **Andreas Heine** described the use of highly soluble small molecular probes as a starting point for lead development. When they are crystallized with their target protein, their binding pockets can be identified. Then their affinity can be increased by successive modifications such as the use of linkers and the formation of salt links. Unusually for such an optimization process, by this approach it is possible for the ligand efficiency to increase as more groups are added. **Kumar Biradha** reminded us that the synthon concept originated in retrosynthetic analysis for organic synthesis. In the crystallographic context, networks such as honeycomb or diamondoid can be dissected. It is important to consider the probability of occurrence of particular recognition motifs; in the case of COOH groups these could be dimer *versus* catemer *versus* other interactions. In fact the COOH…pyridine interaction is one of the most reliable, occurring in 91% of relevant cases in the CSD. **Thomas Gelbrich** described the *XPac* dissimilarity index, published by Gelbrich & Hursthouse (2005), CrystEngComm, 7, 324, as a descriptor of isostructurality in series of closely related organic molecules. The test set

comprised 4,4'-benzenesulfonamido-2-pyridines bearing one substituent on the benzene ring and one on the pyridine ring. Matrix maps were created for the differences in distance parameters, angles and interplanar angles. If molecules are similar, they should have a significant number of points near (0,0), and average δ(ang) and δ(pl) values can be computed within the box they delineate. The resulting quantitative reference values agree with common sense, in that Br- and I-substituted derivatives are closely similar while H- and I- are not. The method is also useful for comparing a structure with itself in the Z' > 1 case, picking out local pseudo-symmetry. In the discussion which followed, it was established that acyclic molecules can also be subjected to such analysis, but only when their conformations are similar. A tutorial session the following afternoon was replete with examples that enhanced our understanding of *XPac*.

The list of speakers for MS53, "High-Throughput Crystallization and Polymorphic Search in Pharmaceuticals" consisted of some scientists from the pharmaceutical industry and many academics who work closely with the industry. Thus the discussion was highly relevant but not seriously hampered by commercial confidentiality. **Jukka Rantanen** took us through the stages from crystals of the drug to particles to powders to the final dosage forms. Prompted by the spectacular problem with ritonavir (Norvir), which changed to a less soluble polymorph two years after it was launched on the market, current practice is to screen for polymorphs as early as possible in drug development. Aided by molecular modeling, tables of descriptors have been prepared for common solvents, covering properties such as hydrogen bonding. Cluster analysis helps to create a set of test solvents for high-throughput crystallization that span the full range of properties. An important caveat remains: secondary manufacturing, which includes operations such as granulation, tableting, coating and/or freeze drying, could bring about polymorphic change. **Ingvar Ymén** described the fully automated screening system in use at AstraZeneca. Their "pet" is called PROTEUS and now covers 120 m^2. With two parallel benches it has a capacity of 380 parallel experiments. Under strict control of temperature, composition and time it can flexibly implement crystallization techniques such as antisolvent addition, cooling, evaporation to dryness, evaporation to a slurry, reaction and recrystallization from a slurry. **Doris Braun** posed the question "Does computational work help in solid form screening?" She rapidly convinced us that the answer is "yes". The test set of the isomeric 2,4- and 2,5-dihydroxybenzoic acids along with phoroglucinol (PhG) was subjected to a range of crystal growing techniques from solution, melt and vapour phases and variation of temperature and humidity. The experimental screen found a new polymorph, two new hydrates and five solvates for 2,4-DHB; two anhydrates and four solvates for 2,5-DHB; a new anhydrate and a new dehydrate for PhG along with two solvates. Computation of crystal energy landscapes found all five unsolvated structures at or near to the global minimum energy. The same is true for three hydrates. The computations picked out the reasons for problems such as proton disorder in OH groups. While even the combination of experimental and computational approaches cannot guarantee that no more metastable forms will be found, their agreement is strong evidence that the practically important forms will have been found. **Peter Wood** showed how the vast amount of knowledge embodied in the Cambridge Structural Database (CSD) can help to mitigate the risk inherent in the "polymorph time bomb." The late appearance of a new polymorph can be particularly distressing and costly, as happened with ritonavir and more recently with rotigotine. The Logit Hydrogen-bonding Propensity (LHP) method evaluates the propensity of a given hydrogen bond to form, based on frequency of appearance in the CSD. Participation, the number of hydrogen bonds per functional group, is another important factor. If a crystal structure has hydrogen bonds with low propensity, and alternative motifs with higher propensity are available, that is a clear warning that a new polymorph might appear. This was the case with ritonavir. However, omeprazole, which has 1 hydrogen bond donor group and 5 possible acceptors, exhibits one combination which is clearly the best. On the other hand, temozolomide, also with 1 donor and 5 acceptors, has polymorphs with differences in Z' and in the number of C=O accepting hydrogen bonds. Co-crystal formation can also be predicted by comparing the propensity of the hydrogen bonds in the "pure form" with the propensity in the co-crystal. After so much X-ray crystallography **David Kissick** reminded us that there are other useful techniques, specifically second order non-linear optical imaging of chiral crystals (SONICC). This technique requires a two-photon process that results in frequency doubling (IR in, visible light out) and is only feasible with chiral crystals (but not with unordered materials or most achiral salts) in an intense optical field. It offers high sensitivity, but not to optical scattering, and a very large dynamic range. The detection limit is a crystallinity of about 3 parts per thousand, and the smallest detectable crystal is about 90 nm across. The method was tested by comparing the recrystallization of griseofulvin from cryo-milled or melt-quenched sample, and it showed that the cryo-milled material still had some seed nuclei left.

The theme of hydrogen bonding returned in MS73. **Chick Wilson** offered us his tool-kit with the aims of first understanding hydrogen bonds and then using them as glue to make things. He and his group are looking at structural evolution, tuning hydrogen bonds and controlling self-assembly. An example of tuning is that variation of temperature controls proton disorder in the structure of p-dimethylaminobenzoic acid. Neutron powder diffraction from hydrogenous materials is challenging because of the strong background that arises, but sometimes there is no alternative, as in the beta-form of cisplatin which arises from a phase transition. Periodic density functional theory is a useful adjunct, as in co-crystals of nicotinamide and oxalic acid, where the oxalic acid can be "cis" or "trans". Currently the DFT geometry is very reliable for the isolated molecule but less so for the solid state. Using the tool-kit of the techniques mentioned above, Chick gave us applications to charge-assisted hydrogen bonds in DMAN + carboxylic acids, differing motifs depending on stoichiometry

in benzimidazole : 3-hydroxybenzoic acid co-crystals, and control of the crystal form in paracetamol. Next, **Piero Macchi** looked at strong hydrogen bonds in crystals under high pressure. A simulation of energy *versus* volume for ammonia showed that van der Waals interactions at 1 bar are pushed into the repulsive region of the potential curve at high pressure, promoting a new conformation or configuration. Alpha-oxalic acid dihydrate has the unequal C=O and C-O bond lengths that are indicative of a neutral molecule. However, neutron powder diffraction at 6 GPa shows that these bond lengths have become equal. Therefore a dianion has formed in an iso-symmetric phase transition. **Matteo Lusi** presented a distance-dependent neutron-normalized method for determining the position of hydrogen bonded hydrogen atoms. Because X-ray diffraction is sensitive to electrons and the electrons are not distributed symmetrically around the hydrogen nucleus, the need for a distance correction to locate the hydrogen nucleus is well known, and the standard procedure works well for most hydrogen atoms. However, although a plot of D-H distance *versus* D…A distance in D-H…A systems is horizontal over most of the range, it shows a definite upward kink at short D…A distances. Therefore, instead of normalizing to a constant D-H distance, it is better to fit a polynomial. A hydrogen calculator is available at **http://academic.sun.ac.za/barbour**. **Maya Tutugamiarso** presented pharmaceutical co-crystals as models for drug-receptor interactions, giving as an example nitrofurantoin with 2,6-diacetamidopyridine Further examples included 5-fluorocytosine with 6-aminoisocytosine, acyclovir, biuret and 6-acetamidouracil. **Carl Henrik Görbitz** found layered structures in all crystals of hydrophobic amino acids. The details differed: sometimes a hydrophilic bilayer of two sheets is found, and sometimes a hydrophobic bilayer. Solid-state phase transitions sometimes are reversible and sometimes irreversible (the crystal is damaged). The transition may change Z'. A martensitic transformation from alpha to beta is found at -80°C for amino acids that include 2-aminobutyric acid, norvaline and methionine. Despite a 7% change in molar volume this process is reversible. With norvaline there is partial occupancy of alternative A (straight) and B (bent) side chain conformations in the ratio 0.515:0.485. The slight excess of A can be explained: for adjacent molecules B next to B will not fit, while A next to A is a poor fit and A next to B is preferred. In a similar phenomenon conformational cascades might occur in proteins.

Near the end of the meeting MS83 presented teaching applications of crystal structure information. **Katherine Kantarjieff** described the evolution of cyber-enabled learning and practice starting from a data collection service in 1994, becoming remotely accessible since 1997, linked into the STARBURSTT consortium in 2005 and now a coordinated aggregate of software, hardware and human expertise. Studies have shown that students with remote access perform better at experiment design and troubleshooting while students sitting beside the equipment do better at theory and practice. We have now entered the Web 3.0 decade, adding integration and mobility of information to the connectivity available in Web 2.0. **Frank Allen** reminded us that chemistry textbooks use crystal structures rather sparingly, but public domain databases have provided new possibilities. The CSD offers over half a million structures. Importantly, it contains real data giving the opportunity for estimation of errors and variance. It can be used to exemplify and quantify concepts such as molecular shape, conformation and hydrogen bonding. The CSD teaching subset (chosen by **Greg Ferrence**) is freely available via the CCDC website, but it is worthwhile to use the full database to facilitate discoveries about chemistry and about the nature of data. For instance, a plot of Sb-Cl distances in ions with the formula $SbCl_6^{n-}$ gives a big central peak for Sb(V) and a smaller peak at longer distances for Sb(III). It includes another small peak at shorter distances due to the erroneous description of F as Cl! **Dean Johnson** put further emphasis on the importance of real data. Data-rich integrated exercises go beyond the presentation of idealized geometry, as in VSEPR, or average values of distances and angles disconnected from their sources. **Joseph Tanski** demonstrated that it is possible for many undergraduate students, if well guided in the treatment of data and in the writing of a journal-style lab report, to publish their results in carefully refereed journals like Acta Crystallographica. **Elena Boldyreva** showed, with infectious enthusiasm, that it is possible to generate a keen interest in crystals among chemists, materials scientists and children. Starting with real crystals and models and photographs, the concept of close packing is a natural next step. The change from graphene to graphite introduces polytypes. Correlation between structure and properties is illustrated by comparing the poorly compressible form I of paracetamol with the much better form II, where the layer structure provides slip planes that facilitate compression. The colour contrast between ruby and sapphire shows that even with similar structure, different impurities alter the optical properties.

There were many more interesting sessions which would exceed the space available here. However, the Cultural Evening deserves special mention. We were taken on a whirlwind tour of Spain by folklore-ballet dancers, who showed remarkable talents both at dancing and at quick changes from one regional costume to another. For each dance the big screen displayed a map of Spain with the region from which it came highlighted. Those of us who expected Mediterranean fire and passion were not disappointed, but other dances were stately and dignified. All were a feast for the eyes and ears.

Carl Schwalbe


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PILAR GOYA LAZA
RSEQ Vice-President
SINE LARSEN
IUCr President
SANTIAGO GARCÍA-GRANDA
President of the ECA


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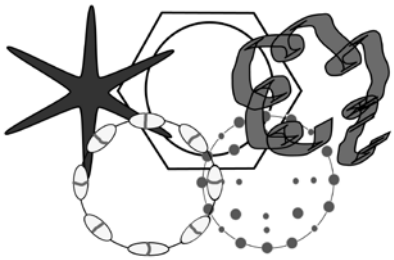
BCA Meeting 2012

BCA Annual Spring Meeting University of Warwick 16-19th April 2012 "Challenges in Crystallography"

IT is with great delight that I invite you to Warwick for the 2012 BCA Spring Meeting to be held from 16th to 19th April.

We all face challenges in our work and this is reflected in the program which is bursting with interesting sessions. The sessions cover topics including: 'Hydrogen Bonding', 'Multidimensional Materials', 'Phase Transitions', 'Protein Crystallisation', 'Membranes', 'Protein Crystallography in Drug Discovery' as well as sessions covering 'SAXS' and 'PAT-Online Processing'. Here, each session has a short description intended to give you a better taste of this year's program.



Designed by Helen Maynard-Casely.

In 2012, we also celebrate the Olympic Games to be held here in UK. With inspiration from the five Olympic rings, **Helen Maynard-Casely** has designed a logo that illustrates the overlap between the five groups of the BCA. In an attempt to bridge the current gap between MX and Small Molecule Crystallography **Arwen Pearson** and **Amber Thompson** are arranging a forum to shed light on topics where these two groups can learn from each other.

We are also having two award ceremonies: One is the BCA prize lecture in honour of Dr. **Frank Allen**, this year given by **Robin Taylor**. The second award ceremony comprises the CCG- and PCG- prize lectures including the IG prize to a young crystallographer.

This year we are trying something new and will have the Exhibitors Forum together with the Buffet Dinner and Poster session on Tuesday 17th April 2012 at 6:15 pm. As usual the Annual General Meeting of the BCA will take place on Wednesday 18th April 2012 at 6 pm.
Following last year's success, we will be Ceilidh dancing again after the conference dinner, so remember to bring your dance shoes!

I am looking forward to seeing you in Warwick in April.

Kirsten E. Christensen, Programme Chair.
Kirsten.Christensen@chem.ox.ac.uk

Registration and Abstract Submission
Meeting website:
http://crystallography.org.uk/spring-meeting-2012/
The registration is now open and the early bird deadline is **12th March 2012.**
The deadline for both oral and poster submission is on the **16th January 2012.**
This deadline cannot be postponed due to the tight schedule surrounding printing the abstract book.

Young Crystallographers Satellite Meeting

Monday 16th April

1.00-3.00 pm YC Session 1

YC Chemical Plenary
Speaker: **Kenneth Shankland** (Reading)
Downhill all the way: an optimisation view of crystal structures from powders

3.30-5.00 pm YC Session 2
YC Biological Plenary
Speaker: **Robin Owen** (Diamond Light Source)
Seeing the full picture: combining crystallography with tomography and spectroscopy at I24

5.30-7.00 pm YC Session 3
YCG AGM
Poster flash presentations

7.00-9.00 pm **Poster Session** with dinner and wine

Tuesday 17th April
9.00-10.30 am YC Session 4
Parkin Lecture
Nominations should be sent to **Anna Warren** (YCG Secretary/Treasurer)

10.30-11.15 am YC Session 5
Science Outreach

Abstract deadlines for the YC Satellite
Oral presentations and Posters:
16th January 2012

Abstracts can be submitted at:
http://crystallography.org.uk/spring-meeting-2012/

Meeting Highlights

Tuesday 17th April
12.15-1.00 pm **BSG Plenary**
Chair: **Elspeth Garman**
Speaker: Laurence Pearl (Sussex)
Title: TBC

Wednesday 18th April
9.00-9.45 am **IG Plenary**
Chair: **Judith Shackleton**
Speaker and title to be confirmed.

5.15-6.00 pm **The BCA Prize Lecture**
in honour of Dr **Frank Allen**
Speaker: Dr **Robin Taylor** (Taylor Cheminformatics Software)

Thursday 19th April
9.00-9.45 am **PCG Plenary**
Chair: **Ivana Evans**
Professor **Branton Campbell** (Brigham Young University)
Symmetry modes: Nature's favoured description of structural distortions

Wednesday 18th April
10.00-11.45 am **Young Scientist Award Ceremony**
Award of CCG CCDC Young Scientist Prize, the PCG PANalytical Thesis Prize and the Young Crystallographers Industrial Group Prize Lecture will be announced and presented at the meeting.

Scientific Programme

Tuesday 17th April
1.30-3.00 pm Session 1
Multidimensional Materials
(Joint PCG and CCG Session)
This session will cover the use of crystallographic and imaging methods to understand the structure and properties of low-dimensional materials: zero-dimensional clusters, nanotubes, layered materials and frameworks.
Chair: **Andrew Goodwin**
Mark Weller (Southampton)
Valeria Nicolosi (Oxford)
Jeremy Sloan (Warwick)

Proteases in Disease
(BSG Session)
The session is themed around protease structure, mechanisms of proteolysis and understanding the regulation of complex processes such as blood coagulation and innate immunity.
Chair: **James Huntington**
Vilmos Fulop (Warwick)
Oligopeptidases in peptide processing memory disorders and pathogen virulence
Piet Gros (Utrecht, Nederlands)
Proteases in complement and innate immunity
James Huntington (Cambridge)
Thrombin structure and dynamics

3.30-5 pm Session 2
Piecing Together the Puzzle – Multidimensional Approaches
(Joint CCG, YCG and PCG Session)
This session will cover investigations where a number of techniques are required in order to see the full picture. Sometimes we are so focussed on diffraction that we fail to see the added value of viewing the problem from a different angle. This session will show the benefits and extra information one can obtain by using a multi-dimensional approach.
Chairs: **Iain Oswald** and **Anna Warren**
Lynne Thomas (Bath)
Beyond the structure: investigating physical properties in molecular materials
Andrew Goodwin (Oxford)
Frameworks, Flexibility and Frustration

Protein Crystallography in Drug Discovery: Binding Sites in the Spotlight
(BSG Session)
The session will cover aspects of protein crystallography in a drug discovery setting, including issues arising during ligand fitting, as well as new structure-guided inhibitor design possibilities opened up with the structure elucidation of G-Protein Coupled Receptor structures.
Chair: **Robert Van Montfort**
Judit Debreczeni (Structural Genomics Consortium)
Practical considerations in ligand substructure validation
Andy Dore (Heptares Therapeutics)
Structure Based Drug Design for the human A2a G-Protein Coupled Receptor

Interdisciplinary Forum

5.15-6.16 pm Forum
Bridging the Gap Between MX and Small Molecule Crystallography
Introduced by **Arwen Pearson** and **Amber Thompson**
As small molecules get larger, the challenges they pose increasingly approach those associated with macromolecular crystallography. However, with the

divergence of the two fields, we now talk different languages as well as have different scientific backgrounds. This forum is intended to help breakdown these barriers through the medium of questions with a panel of experts. Possible questions for discussion include, “What is Rfree?”; “How do you judge data quality?”; “How do you prevent solvent loss?” and “What do you do to prevent radiation damage?”. The session is short and intended to promote discussion; if successful it could be a prototype for a longer event next year, so suggestions and feedback are greatly encouraged.
Chair: **Kirsten E. Christensen**

Wednesday 18th April

1.30-3.00 pm Session 4

H-bonding: From Water to Supermolecules I
(Joint PCG and CCG Session)
The session will give an overview of recent theoretical and experimental studies on the condensed phases of water. Specific topics will range from supercooled water and the nucleation of ice at surfaces to stacking disorder in ice.
Chair: **Christoph Salzman**
Benjamin Murray (Leeds)
The structure of ice crystallised from supercooled water
Angelos Michaelides (UCL)
Ice nucleation at surfaces

Hot Structures and Hot Methods
(BSG Session)
This session consists of talks selected from abstracts reflecting late breaking topics, reports of new structures and updates on new methods.
Chair: **Jon Cooper**

SAXS
(Joint IG and BSG Session)
The technique of Small Angle X-ray Scattering, in particular biological SAXS, has become increa-singly popular in recent years, complementing high resolution structural studies by crystallography, NMR and electron microscopy. Sensitive to length scales in the nanometre range, SAXS can be applied to a wide range of different types of samples including polymers, lipids, nanoparticles, proteins and biomaterials. This session will highlight some recent advances in the field.
Chair: **Elizabeth Shotten**
Clair Baldock (Manchester)
Combining SAXS and biophysical techniques to investigate the nanostructure of extracellular matrix proteins
Nick Terrill (Diamond Light Source)
Small Angle Scattering - The last resort of the desperate?

3.30-5.00 pm Session 5

H-bonding: From Water to Supermolecules II
(Joint CCG and PCG Session)
This session focuses on the Crystal Engineering aspects of the hydrogen bond. Intermolecular interactions mediated by hydrogen are frequently structure-defining in organic and metal-organic structures from hydrates, polymorphs and co-crystals right through to highly complex supra-molecular systems. The session will touch on the importance of the hydrogen bond in analysis, design and prediction of small molecule crystal structures.
Chair: **Peter Wood**
Doris E. Braun (UCL)
Contrasting organic hydrate structures generated in silico to in vitro
Laszlo Fabian (UEA)
Cocrystal design: interactions and properties

Crystallography and Cancer
(BSG Session)
High throughput structural biology approaches can play a pivotal role in the target validation, hit identification, hit-to-lead and lead-optimisation phases of drug discovery. In this session, two pioneers of these approaches will discuss high value and high throughput approaches to unlocking the potential of anti-kinase and anti-chaperone drug targets.
Chair: **Jane Endicott**
Chris Murray (Astex Therapeutics, Cambridge)
The application of fragment-based drug design to drug targets in oncology
Stefan Knapp (Structural Genomics Consortium, Oxford)
Strategies for the structure guided design of selective kinase inhibitors

Process Analytical Technology (PAT) for Online Monitoring of Material Quality in Manufacture
(IG Session)
Industrial group session covering the application of PAT for monitoring and controlling the quality of a product during manufacture, as used in the Pharmaceutical and Aggregate/ Cement industries.
Chair: **Brett Cooper**
Ali Saleemi (Loughborough)
The role of PAT in crystallisation process monitoring and control

Thursday 19th April

10.15-11.45 am Session 6

Phase Transitions: Distortion Mode Analysis
(Joint PCG and CCG Session)
The session will connect the fundamentals with the topical materials research and provides the basis for a state-of-the-art diffraction data analysis approach.
Chair: **Ivana Evans**
Speakers and titles: TBC

Membrane Protein Crystallography
(BSG Session)
Protein crystallographic analysis of membrane proteins is critical to understanding structure-function relationships and important to understand-ding disease processes and for the development of new medicines. Only a small subset of independent structures of integral membrane proteins have been reported so far and in this session the technological challenges and recent breakthroughs of research in this important area are explored.
Chair: **Jonas Emsley**

So Iwata (Imperial College)
Structural studies of integral membrane proteins
Andrew Leslie (Cambridge)
Crystallography of G-protein coupled receptors

Coatings
(IG Session)
Coats of many colours: Probing and understanding surfaces and the coatings interacting with them, is a science that continues to grow as technology becomes more specifically focused on this interesting environment. This session will present lectures from speakers picked across a number of industrial sectors, showing how these surfaces and coatings are important to each and the techniques used to understand the associated challenges.
Chair: **Judith Shackleton**
Speakers and titles: TBC

12.00-1.30 pm Session 7
Protein Crystallisation:
Magic Versus Logic
(BSG Session)
This session will focus on non standard methods for obtaining and optimising macro-molecular crystals using "logic" (i.e. chemical and physicochemical prior knowledge, crystallisation diagno-stic techniques and further means) to counter-balance the "magic" ingredient which many regard as essential for producing diffracting crystals.
Chair: **Naomi Chayen**
Terese Bergfors (Uppsala, Sweden)
Highways, biways and detours: the IspD story
Emmanuel Saridakis (Demokritos, Greece)
Discovering crystallisation conditions using Dual Polarization Interferometry

Phase Transitions II:
Transformations in the Solid State
(Joint CCG, IG and PCG Session)
This session is concerned with the transformation of one crystalline form into another as a result of a stimulus such as a change in temperature. The primary tool to monitor such processes is the monitoring of structure before and after transition by diffraction-based techniques. However the field is now increasingly turning to other techniques to probe the kinetics, dynamics and mechanisms of these transitions and complementary techniques such as Calorimetry, Solid State NMR and computational-based calculations are now being employed to further our understanding of these complex processes. The session will draw on all these complementary approaches in presentations outlining examples from different areas of academia and particularly pharmaceutical relevance.
Chairs: **Simon Coles** and **Cheryl Doherty**
Kenneth Harris (Cardiff)
Structural and dynamic aspects of phase transitions in solid inclusion compounds

Young Crystallographers Satellite Meeting

THE next Young Crystallographers Satellite Meeting (YC2012) will take place prior to the main BCA Spring Meeting from 1 pm on Monday 16th April until 11.15 am on Tuesday 17th April at the University of Warwick.
Following the established format there will be three sessions of oral presentations - a superb opportunity for Young Crystallographers to present and discuss their work in a friendly and relaxed environment. More senior crystallographers are of course welcome to attend, but difficult questions should be kept to a minimum. The poster session will commence on Monday evening together with the buffet dinner and drinks.
This year there will be two plenary lectures, with a chemical and biological theme. The second Parkin lecture will also be awarded to a Young Crystallographer who will then present their work at this satellite.
The Parkin Lecture has been established as the prize lecture of the YCG in recognition of the outstanding contributions of the late Dr **Andrew Parkin** to the YCG of the BCA.
The candidate should be a Young Crystallographer (undergraduate or graduate student or a crystallographer within five years of graduation), who has been recognised for outstanding contributions to any of the following:

- Promoting science
- Raising public awareness of science
- Teaching crystallography/science
- Originality in outreach and teaching activities.

If you think you know of a Young Crystallographer who has excelled in any of these areas then why not nominate him or her for the Parkin Lecture!
The rules for the Parkin Lecture, details regarding the nomination process and nomination form can be found under the prizes section on the YCG website (**http://ycg.crystallography.org.uk/prizes/**). The nomination form should be sent to the YCG Secretary **Anna Warren** (**Anna.Warren@diamond.ac.uk**) no later than 15th January 2012.
At the main meeting there will also be a joint session with the CCG and PCG entitled "Piecing Together the Puzzle – Multidimensional Approaches." This will give Young Crystallographers the opportunity to present their work at the Spring Meeting.
Dinner and registration for the YC2012 will be free for those attending the whole Spring Meeting. There is the option to only attend the YC2012 and not the main meeting, but a fee will be charged. There are a limited number of bursaries available and applications have to be made online on the BCA webpage.
The deadline for abstracts to be considered for oral presentations and posters is 16th January 2012.
Submissions should be made via the main meeting abstract submission webpage using the template available there. The AGM will again include elections to fill the YCG Committee vacancies, which will be advertised nearer the time. For more information about the YCG have a look on the YCG website (**http://ycg.crystallography.org.uk/**).

YCG Committee

National Facilities News

IN the previous issue of Crystallography News we looked at the development of neutron scattering facilities at the Rutherford Appleton Laboratory and the inauguration of the ISIS spallation neutron source. We will now turn our attention to some of the instruments at ISIS which are, perhaps, of most direct interest to the crystallographic community.

Although it was among the original suite of instruments at ISIS, it was not until 1989, approximately five years after ISIS generated its first neutrons, that POLARIS was converted from its original role as a development facility for neutron polarising filter devices to full time use as a powder diffractometer. The instrument was adapted to meet the steadily increasing user demand for neutron powder-diffraction facilities. Its potential quickly became apparent in a variety of scientific themes and, despite a rather modest initial detector complement of 42 ^{3}He tubes arranged into 3 discrete banks, it demonstrated the importance of using epithermal neutrons to collect diffraction data to very short d-spacings (high Q values), allowing reliable refinement of site occupancies and thermal vibration parameters in disordered crystal structures such as ionic conductors. It also highlighted how the fixed scattering geometry at a pulsed neutron source could be used to develop specialised sample environment equipment. For example, POLARIS was employed in the early development of the highly successful Paris-Edinburgh pressure cell programme, which eventually led to the construction of the dedicated PEARL instrument, and it was also used to measure residual stress distributions within engineering components, leading to the construction of ENGIN and subsequently ENGIN X. The advances in the scope of research that could be conducted on POLARIS led to a concomitant and rapid increase in the over-subscription for beamtime on the instrument. ISIS responded by increasing the POLARIS detector complement, in the period 1992 to 1994, to reduce data collection times and, hence, increase both the experiment throughput and the range of studies that could be undertaken. In late 1996 POLARIS was moved from beamline South 1 (S1) to beamline North 7 (N7) on TS1 to make room for the MAPS instrument which, due to its large secondary flight path and wide scattering angle range, required an “end” beam port. This placed POLARIS roughly diametrically opposite its original location. For all practical purposes, the incident neutron fluxes on N7 and S1 are the same, since the two beamlines view opposite sides of the same water moderator and the poison-depth geometry within the moderator is symmetrical – maintaining high flux, particularly at shorter neutron wavelengths. However N7 was an unused beam port, providing a “blank canvas” on which to design the new instrument and allowing the design to be optimised from the ground up. Significantly, improvements in shielding and the incident beamline collimation resulted in an order of magnitude reduction in levels of background scattering, which was further enhanced by the provision of a nimonic chopper a year or so later. The nimonic chopper stops the very high energy (fastest) neutrons produced by the spallation process and, although these neutrons are of little use for a diffraction experiment, they can be slowed down and scattered by components at the sample position so that they give rise to an enhanced background in the detectors. The background suppression offered by the nimonic chopper is particularly important whenever bulky sample environment is used, such as cryostats and pressure cells. The provision of a much more open sample enclosure, also, permitted an almost unhindered access to the sample position, vital for some in situ studies. Following this move, POLARIS remained largely unchanged, supporting a high throughput of experiments over a diverse range of scientific disciplines (physics, chemistry, materials science, the Earth sciences, etc) until its recent upgrade to further improve its capabilities.

The current upgrade of POLARIS was funded by a Facilities Development grant from the STFC in 2007, with subsequent additional contributions from Swedish and Spanish collaborators. Its aim is to provide POLARIS with a modern high-solid-angle detector and improved beam collimation to fully exploit the excellent characteristics of the ISIS source. The detectors are replaced with modules accommodating the latest ZnS scintillator technology which, with their improved efficiency and the accompanying large increase in the solid-angle of detector coverage, will lead to a very significant increase in count rate (approximately ×20 at low angles) coupled with enhancements in δd/d resolution (down to ~0.3% at backscattering). The collimation of the incident beam has also been improved to allow the beam size to be adjusted more readily so that it can be tailored for each experiment, thereby reducing parasitic scattering from around the sample position. To improve the collimation of the diffracted beams, a radial collimator will be installed so that full advantage can be gained from the instrument’s fixed diffraction geometry to further reduce background scattering picked up in the detectors - especially background

generated from complex sample environment equipment. To perform the upgrade work, POLARIS was removed from user operation in August 2010, with final installation of the instrument due in November 2011 and resumption of the user programme planned for early 2012.

A range of furnaces and cryostats will be available for use on the upgraded POLARIS diffractometer, offering sample temperatures in the range from 1.5 K to 1000°C. For conventional room temperature measurements, a 20 position automatic sample changer may be used to minimise the effort required and time taken to change a sample, and which also allows the unattended data collection over a prolonged period, e.g. through the night. The cryostats and furnaces can also be used with specialised sample sticks to allow, for example, the measurement of electrical properties simultaneously with diffraction data, whilst gas flow cells to subject samples to variable partial pressures of oxygen or humidity are also available. The diffractometer can also support high-pressure studies, including the Paris-Edinburgh cell. For samples requiring only a more limited pressure range up to 5.5 kbar there is a gas pressure cell made from a null-scattering TiZr alloy, which can offer access to longer d-spacings due to its less restricted diffraction geometry.

The powder diffraction programme on POLARIS was originally managed by **Steve Hull**, who joined ISIS in 1988 at about the same time as the instrument changed its role to become a dedicated diffractometer. A couple of years later, in November 1990, **Ron Smith** was recruited as a beamline scientist on Polaris and they have both steered it through its development, its move from beamline S1 to beamline N7 and are currently overseeing the final stages of its rebuild and upgrade.

The single-crystal diffractometer, SXD, is situated on beamline S3 on TS1 and, like POLARIS, it receives neutrons from a water moderator. The development of SXD has been very much an evolutionary process with each stage being primarily driven by improvements in detector technology. In contrast to detectors for time-resolved neutron powder-diffraction, a detector for single-crystal diffraction must not only have a large active area, to increase the solid-angle coverage around the sample, but it must also have a high spatial resolution, to accurately resolve the scattering vectors of reflections. It must also be capable of counting quickly, with extremely short dead-times, to cope with the locally intense single-crystal Bragg peaks. Therefore, good pixel resolution, a fast count rate, linearity of response and excellent response stability are all required for a large-area position-sensitive-detector (PSD) suitable for single-crystal diffraction. When SXD was first made available to users an Anger camera was installed which fulfilled these criteria. At its heart was a hexagonal array of 45 photomultiplier tubes which were bonded to a layered optical element. This was composed of a sandwich of a thin external reflective layer, a thin Li-glass scintillator of 2 mm thickness and a 40 mm thick glass light dispersing layer. An air-gap of 0.1 mm was set up between the scintillating layer and the dispersing layer so that the total internal reflection at the gap restricts the cone of transmitted light to ~45°. The centroid position of a neutron striking the scintillator could be derived from the comparison of signals from the six tubes surrounding the tube directly beneath the scintillation centre, as these are the only tubes affected by the light cone from an event, thanks to the air-gap. Despite the relatively small number of PM tubes, this technique gave a very good positional resolution of 2-3 mm given that the PM tubes themselves had dimensions of 60 mm across the flats. The camera had an active area of 300 mm × 300 mm which was divided into 128 × 128 pixels. Naturally a third dimension was also provided electronically via the time-of-flight of the neutron causing the event. Installed on the instrument, the detector subtended an angle of ~60° in both the horizontal and vertical positions.

The Anger camera was eventually replaced in 1989 with an early version of a new class of ZnS scintillator PSDs. The first detector of this type was built as a prototype to develop the concept of using fibre-optic cables to encode the pixel positions. It was composed of a square array of 256 pixels, each with 5 mm × 5 mm dimensions, arranged on a ceramic grid. The position of each pixel was encoded onto a set 32 photomutliplier tubes with one group of 16 tubes recording the x-coordinate position on the detector surface with the remaining group of 16 tubes recording the y-coordinate. Each pixel was encoded to its corresponding x and y photomultiplier tube via a pair of fibre-optic cables and the position of an event, in terms of pixel position, was located when a light-pulse was simultaneously recorded on one photomultiplier tube from the x coordinate group and one photomultiplier tube from the y coordinate group. The scintillator material was a single, continuous, piece of ~0.4 mm thick ^{6}Li-doped ZnS plastic, supported just above the pixels, which provided an overall active area of 80 mm × 80 mm. This material is robust, linear, has low noise, and has a very short deadtime. It has the added advantage that with a careful tuning of the discriminator level it can be made extremely insensitive to γ rays. The detector type that is currently in use was introduced in 1992 from the development of this first ZnS PSD. They consist of a square array of 4096 3 mm × 3 mm pixel elements with only a very thin Gd_2CO_3 coated metal grid separating the optic fibres required for each pixel from its neighbours. The total active area is 192 × 192 mm – which is a significant improvement over the prototype. In this detector each pixel has four fibre optic cables encoding its position and the four-way coincidence requires only 32 photomultipler tubes, again separated into two groups of

16, to discriminate an event into a unique location in the 64 × 64 grid of pixels. In this detector the grid (pixel) locations are encoded into 8 strips in the horizontal (X) and 8 strips in the vertical (Y) with each strip subdivided into 8 rows (x) or 8 columns (y) of pixels. The pixel locations are then uniquely encoded by grouping the 16 photomultiplier tubes for the horizontal direction into two sets of 8 tubes for the X and x coordinates and performing a similar grouping of the 16 vertical photomultiplier tubes for Y and y. A neutron is located on the detector surface when a simultaneous event is recorded in each of the 4 sets of 8 photomultiplier tubes to give the coordinate in terms of (X1 8,x1 8; Y1 8,y1 8). By encoding the pixel coordinates in this way the number of photomultiplier tubes was kept the same as the prototype, which provides savings both in the cost of the electronics and the space required to house the detector. The fibre optic bundles do, however, become much more complex and 16384 individual cables are required.

A second of these detectors was installed on the instrument in early 1995 and a third was added in June 1998 following a move of the shared eVS/ SXD blockhouse wall the year before to provide more space for the left detector bank. Perhaps the most significant upgrade to SXD, however, came in the period from November 1999 when **David Keen** was responsible for a three-year EPSRC funded project to increase the complement of detectors to 11 so that the solid angle coverage around the sample was increased to an approximate hemisphere - though due to the gaps between the detectors the coverage is approximately 50% of the potential solid angle in a full hemisphere. The commissioning of all detector banks was completed by September 2001 and SXD has remained largely unmodified since then. This period of stability has allowed **Matthias Gutmann**, who took over from **David Keen** as the SXD instrument scientist, to fully revise the software for the diffractometer and automate the sample goniometer. A goniometer is required as sample reorientations are still necessary both to maximise geometrical coverage of the diffraction volume and to increase the number of reflections lying within the d-spacing envelope of the instrument.

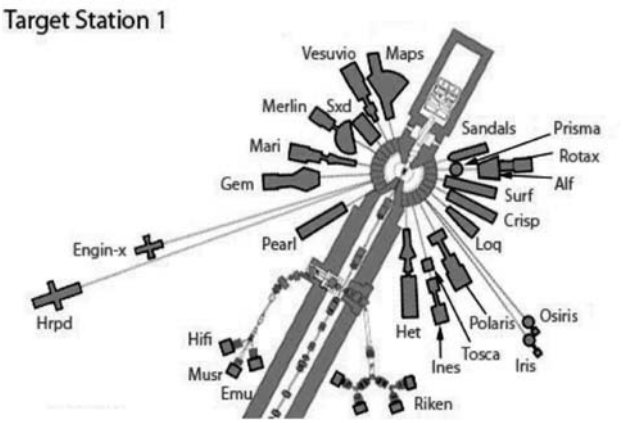
The SXD sample tank can accommodate a variety of cryostats and furnaces which allow sample temperatures in the range from 300 mK (using the Orange cryostat with ^{3}He insert) to 1133 K. The instrument also supports a top-loading He refrigerator which can be operated in the 4 K to 320 K temperature range and has interchangeable centre-sticks that support a 5 kbar He gas pressure-cell, a cell that enables samples to be contained in a high electric field and a stick that allows fully motorized sample re-orientation.

The SXD diffractometer has been managed by a number of scientists during its period of operation. It was initially supported by **Bruce Forsyth** and **Mike Johnson** who subsequently handed responsibility to **Chick Wilson**.

Chick oversaw the transformation of the instrument through its various upgrades to the period of its current full complement of detectors. As already mentioned, **David Keen** was instrument scientist during the time of its most recent upgrade and, when David took up an Advanced Research Fellowship at Oxford and subsequently moved on to GEM and the LMX instrument project on TS2, **Matthias Gutmann** took over. Matthias is currently responsible for the instrument and he was assisted for a time by **Aziz Daoud-Aladine** who has now moved on to HRPD.

In the next issue of Crystallography News we will acquaint ourselves with GEM and PEARL and catch up on recent developments on both instruments. We will also look at developments on HRPD, which was among the first suite of instruments made available to users of ISIS and has seen over 20 years of service. I would like to express my thanks to **Steve Hull**, **Ron Smith**, **David Keen**, **Matthias Gutmann** and **Nigel Rhodes** for their help in preparing this article and for providing some of the photographs and images.

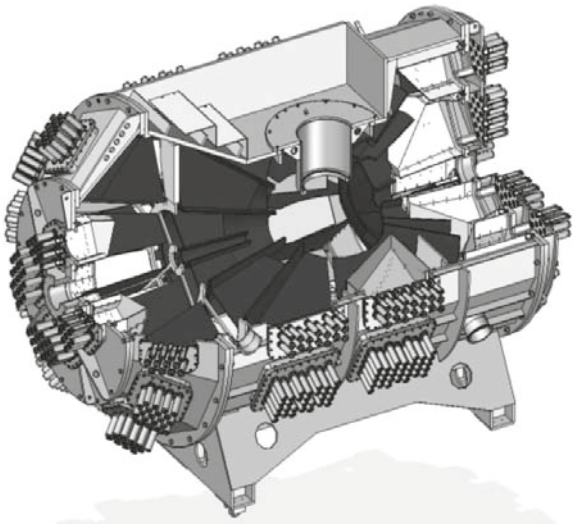
Dave Allan

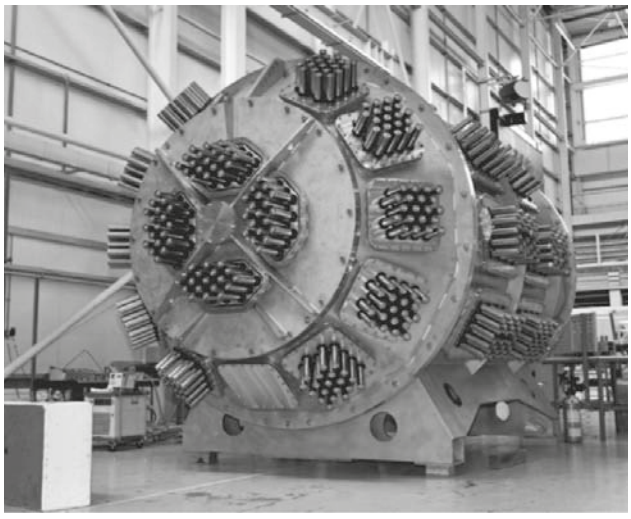


The current complement of instruments on Target Station 1 at ISIS.

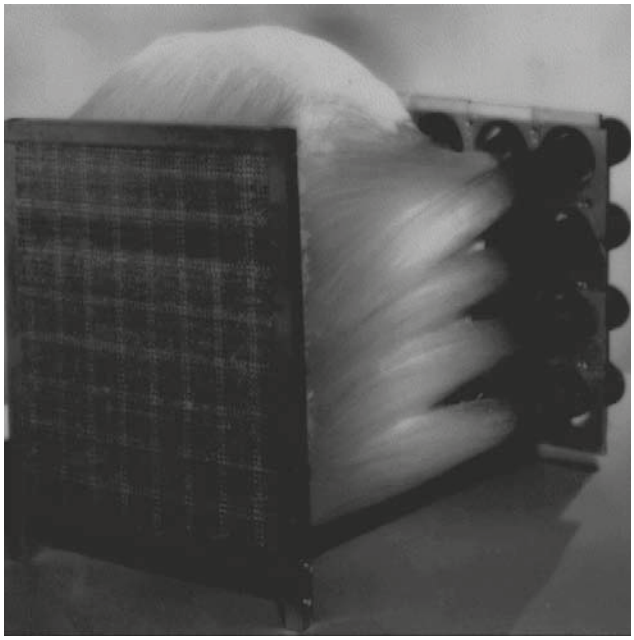
Previous page: Ron Smith and Steve Hull on POLARIS shortly after its installation on beamline N7 in 1996. Ron is resting his hand on the sample vacuum tank while Steve stands between the right low-angle detector bank and the transmitted-beam collimator.

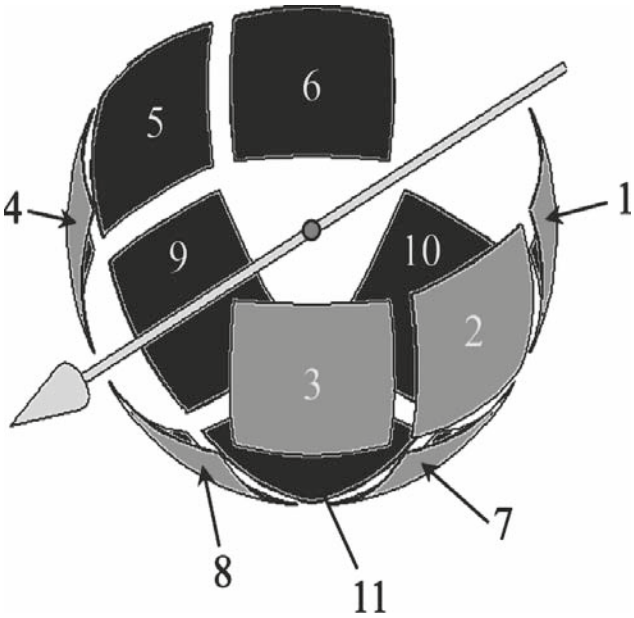
The POLARIS block-house in late 2011 awaiting the installation of the new instrument.



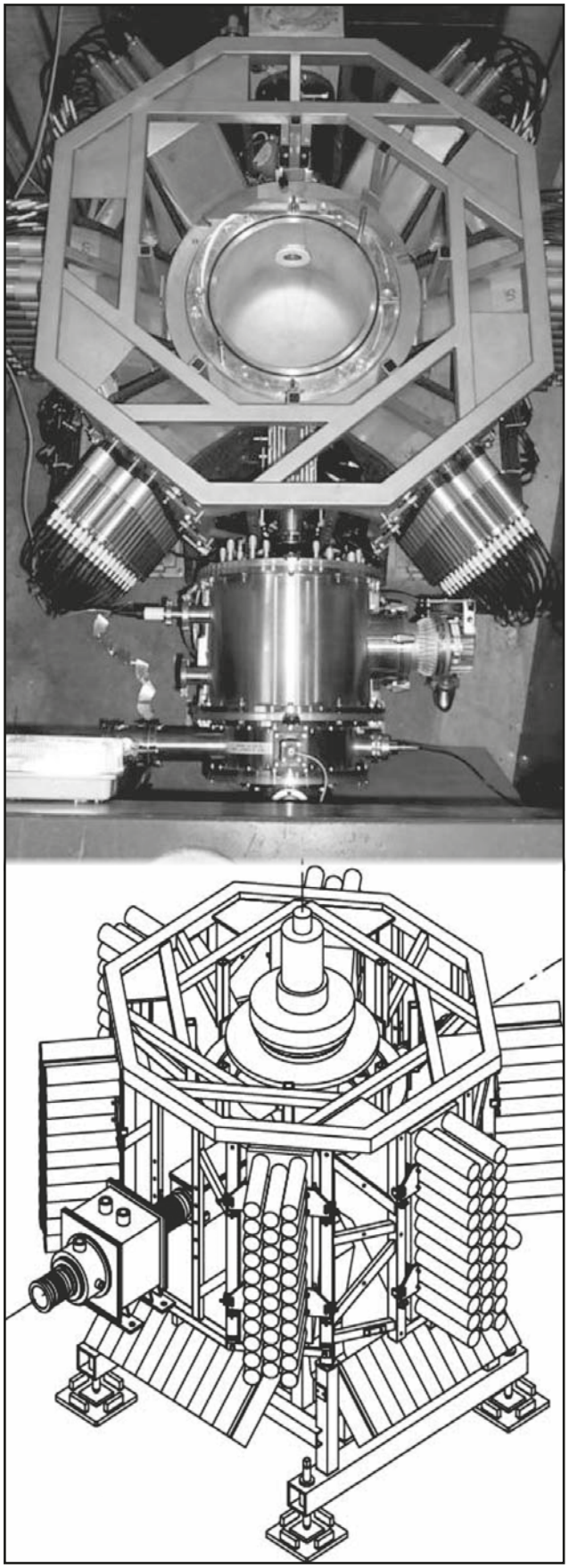


The new POLARIS vacuum vessel undergoing tests on the experimental hall floor of the TS1 building (centre left). The back of the detector modules, with their clusters of photomultiplier tubes, are clearly visible. In the new instrument there are 38 of these detector modules arranged in 6 detector banks. A schematic cut-away representation of the new instrument with the sample vacuum tank shown at the top (lower left). At the time of writing, the internal B_4C (crispy mix) collimators are being installed. The radial collimator, which will surround the sample tank, is not shown.





An individual SXD ZnS scintillator 64 × 64 pixel position sensitive detector from SXD (above). Each panel contains 16384 fibre optic cables which are connected to 32 photomultiplier tubes. SXD contains 11 of these PSD units and they are arranged to provide an approximately hemispherical region of angular coverage around the sample position (below).



A view looking down onto the SXD diffractometer with the roof of the block-house removed (above). A schematic representation of the SXD diffractometer indicating how the banks of detectors are supported (below).

Former IUCr President's Win

THOSE of us who attended recent meetings of the American Crystallographic Association as well as the latest Congress of the IUCr have been amazed by the maturity, enthusiasm and scientific competence of the presentations given by a series of high school students led by "Pied Piper" Bill Duax. Previously he had been President of the International Union of Crystallography between 2002 and 2005. The ACA is proud to announce that his high school science program has been selected as the regional winner in Time Warner Cable's Super Connector Search. Duax's program for high school students has now advanced to the national level among 20 regional winners.

The summer school program in Buffalo, New York at Hauptman Woodward Institute **www.hwi.buffalo.edu/outreach/high_school_program.html**, combines bioinformatics with macromolecular structural data to improve gene bank annotation, trace the origin and evolution of the genetic code and of ribosomal proteins, and develop bioinformatics techniques to design substrate and species specific enzyme inhibitors. Students in the program have made oral and poster presentations at ACA meetings in Toronto and Chicago and at the IUCr Congress in Madrid. Crystallographers of the future may well be among them.

IUCr General Assembly Madrid

THE IUCr General Assembly meets 3-4 times in the evening during the IUCr Congress. The Congress itself is 9 days long. Countries have varying numbers of voting representatives from their National Associations (1-5). The number of votes is related to the subscription paid by the National Association. Small countries can form a regional association. This time the newly formed Irish Crystallographic Association submitted an application for membership of the IUCr and the current membership of their National Committee is **P. McArdle** (Chair), **S. Lawrence** (Secretary), **T. Soulimane** (Treasurer), **A. Khan, J.F. Gallagher** and **N. Hamill**.

The IUCr are keen that there is a good geographical spread of the IUCr Officers, so the statutes were changed such that the election of Officers of the Union shall be arranged in such a way that there will not be more than two Officers from any one Country and that amongst the six ordinary members there will be at least one Officer from a Country from each of the three geographical regions (i) Europe and Africa, (ii) the Americas and (iii) Asia/Oceania. Since many scientists work and are resident in a country which is not the land of their birth, a person is regarded as belonging to the Country in which he or she is normally resident and where the main part of his or her work is conducted.

Issues come up from time to time that require ballots of Adhering Bodies or of the Executive Committee members. At present these are described as requiring postal ballots so the Statutes and By-Laws were revised to allow a postal or electronic ballot to be arranged.

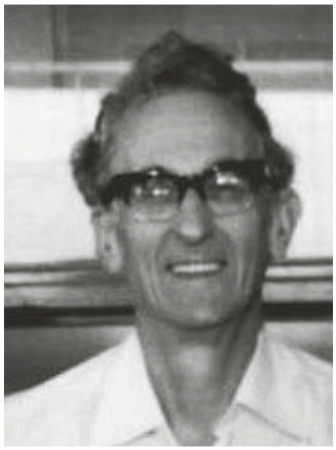
After the IUCr Congress in Osaka in 2008, the UK representatives made some suggestions for changes to voting at the IUCr assembly. We suggested that a Single Transferable Voting system should be implemented in order to substantially speed up the voting procedure. However, voting procedure changes had been raised back in 2002, and all the National Committees apart from the BCA and one other preferred the present system. This is because a candidate must receive at least 50% of the votes to be elected and delegates can change their votes after each round in order to adjust the balance of the Executive Committees as the voting progresses. The procedure was changed slightly so that a candidate was dropped off the list each time someone was elected which did speed up voting. Although no electronic/mechanical counting device was used in Madrid, provision of this facility was strongly recommended at the next IUCr Congress in 2014 which will be held in Montreal.

One of the main features of the IUCr General Assemblies is the vote on the venue for subsequent IUCr Congresses. This time we were voting on the venue for 2017 and the choice was Hyderabad (India) or Prague (Czech Republic). Both parties made impressive presentations of what their country and city could offer the IUCr Congress and delegates. A secret ballot was held and the Indian Crystallographic Association's bid for Hyderabad won. There are direct flights from London to Hyderabad and the congress will be held in the Hyderabad International Convention Centre which has a swimming pool as well as the expected lecture rooms, restaurants and bars.

All the discussions and voting make us hungry so, since there was little time to get something to eat, I went to the local supermarket to get emergency extra rations for the UK team including pastries, olives, crisps and surprisingly drinkable 250ml cartons of wine at 1 euro each. There were only tortilla (potato omelette) rolls or ham rolls on offer for everyone else and the beer ran out fast!

Georgina Rosair

George Kakabadse



COX'S Pippin from a Rare Graft: George Kakabadse (1917-2002)

Staff and research students in the Leeds University Structural Chemistry crystallography laboratories of **E G** (later Sir Gordon, FRS) **Cox** in the late 1940s and 1950s were associated in what was unsurprisingly called the Pippin Club. During 1947-1952, one junior member of staff was the quietly humorous, tall and athletic **George Kakabadse**. He played basketball for the University and taught **Keith Cox**, me and others to climb rocks at Almscliff and Ilkley; in his case this was often in bare feet, though he told us about these new vibram soles. In the laboratory, his experience aided our crystal growing, helped us keep our tempers with the Raymax continuously-pumped X-ray sets, and, in my case, guided autoclave preparations. As a demonstrator in the teaching labs, his oblique sense of humour enabled him to extract from students an awareness of the point of their experiments.

Cox we knew, as a TA Lieutenant-Colonel, had visited Germany at the end of the War, investigating scientific intelligence and also acquiring in the UK equipment such as parabolic mirrors and gun components potentially useful in projecting structures and analogue calculation of structure factors. He had left behind at Birmingham and Welwyn **G A Jeffrey** (later leaving Leeds to take up the first Crystallography Chair at Pittsburgh) and the crystallographic computing pioneer **A D Booth** (author of the textbook on Fourier Techniques in X-ray Structure Analysis). Cox had also worked at the former ICI research institute at Welwyn, helping to realize improbable concepts for Special Operations Executive devices. These contacts helped his recruiting of staff. Of George Kakabadse's remarkable early life and family, however, we knew little. His German and Russian were evidently good enough for him to give language courses to postgraduates. He was known to be of Georgian (USSR) extraction, to have been in Berlin before and during the War, and somehow contrived to be an army translator for the British in Austria in 1945. Much later I tried unsuccessfully to persuade him to write his memoirs.

Recently, with the collaboration of his exceedingly talented offspring (all four are graduates, two have PhDs, one a distinguished Professor, embracing fields from music to management but not science), some of the story of his pre-Leeds life has been assembled [*RSC History of Chem. Gp. Newsletter* No. 60, pp. 28-31, Aug. 2011]. It appears that George's father **Kyrill Kakabadse** had been a boyhood acquaintance of Stalin, commanded the Bolshevik garrison in Petrograd (St. Petersburg) in 1918-1919, and was Deputy Prime Minister of Soviet Georgia from 1921 to 1931. Kyrill was then sent, accompanied by his family, to Berlin to head a Russian minerals sales company. But when Kyrill denounced Stalin in 1933, a death sentence was passed on the family, should they be apprehended in the Soviet Union. In Berlin, George participated in the gymnastics display at the Opening of the 1936 Olympics, gained admission to the Technische Hochschule, graduated in Chemistry, and was awarded a Dr Ing in 1943. In 1945-47, despite a background in the USSR and Germany, George was kitted out as a Lancashire Fusilier when he acted as an army interpreter. He met his Greek wife in Vienna. After their marriage, their first child Andrew (now a Cranfield Professor) was born in Athens in 1948; by then George had been for some months at Leeds University and was not able to return to Athens until 1951.

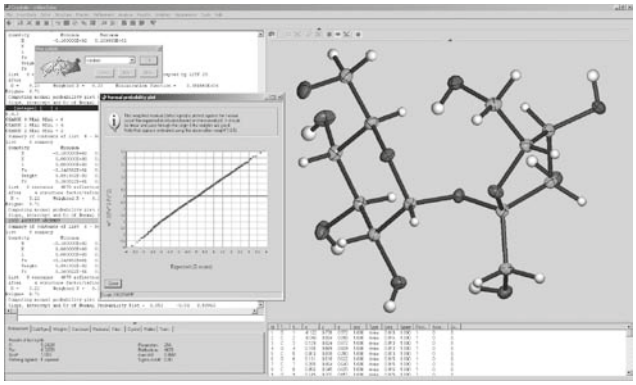
From 1952, the family was re-united in Manchester where George was, until retirement in 1982, on the Chemistry staff of the institution that for most of his time was called UMIST. He escaped from crystallography (apart from translations) in Manchester where his skills in analytical chemistry were much appreciated.

I am especially grateful for the recollections of Professor **Andrew Kakabadse**, Mrs. **Lydia Dyer** (nee Kakabadse) and Dr. **Joe Lee** (who along with Dr. **Roger Perry** also supplied the photograph).

Derry W. Jones
University of Bradford

The Future of CRYSTALS

THE CRYSTALS program is widely used by Chemical Crystallographers involved with running analytical services, research and teaching. It has been under continuous development since the first FORTRAN versions were created by **John Rollett** and **Bob Carruthers** during the 1970's. A large number of people have contributed code or concepts for dealing with specific crystallographic problems, leading to a richness of procedures. A small number of people, in particular **Paul Betteridge**, **Lisa Pearce** and **Richard Cooper** have made substantial changes to the infra-structure to ensure that the program remains suitable for modern users. As well as the monolithic code in CRYSTALS, the program also acts as a convenient interface to programs dealing with cifs and several diffractometer data files. It also links smoothly with checkCIF, PLATON, SIR92, SIR2011, Superflip, SHELXS, Mercury, Mogul, and MCE (an electron density visualiser). My own role has been to generally look after the code, to respond to users' requests and comments and run an e-mail help desk. Following my retirement in September 2011, I hope to continue to be involved with CRYSTALS.



After a period working with Oxford Diffraction, oXray and carrying out research into small-molecule docking with macromolecules at InhibOx, **Richard Cooper** (richard.cooper@chem.ox.ac.uk) has returned to Oxford to be my successor as head of The Chemical Crystallography Laboratory. In addition to all his other responsibilities, he plans to continue to look after CRYSTALS, and when time permits re-develop and extend it. Existing CRYSTALS users can be confident that it will be maintained into the foreseeable future, and non-users looking for a single integrated work environment might like to try the program. Oxford University has made the installation kit available to commercial and
non-commercial uses without cost from our website: www.xtl.ox.ac.uk. Contact Richard for more details.

David Watkin (david.watkin@chem.ox.ac.uk)

...Answer to Previous Puzzle Corner

THE winning response was submitted by Bob Gould. Along with supplying an analysis of the more-or-less exact symmetry of the ceramics from Stoke he reminds us of the symmetry of the BCA logo.

"Starting on the upper left and going clockwise:
1. The centre of the plate approximates to 4m symmetry, but the slightly lecherous figure seems to be significantly peering to his left, so that reduces the symmetry to 4. In any case, the symmetry is only very approximate. I'm afraid I don't have the patience to count the rim, but it approximates to something like 120m.Overall 4, near to 4m.
2. Centre: approximates to ∞m; second ring, good approximation to 5 - clearly mirror symmetry not envisaged! Outer ring: there seems to be a flaw in the printing; but ignoring this, the symmetry is 20. Overall: 5.
3. Also overall 5, and quite close to 5m.
4. The BCA logo (ignoring the letters) is a projection of m3m, giving 3m. Each face (with the letters) is a projection with an approximate m for A and C, a good m for B.
5. No overall symmetry. Inner ring (ignoring colours) is 8m. Outer ring is 14.
6. No overall symmetry. Innermost figure approximates to m. Next ring is part is nearly 3 and less nearly 3m. Next ring is nearly 11m, and final ring is nearly 8 and not quite so nearly 8m."

Bob Gould

SAXS Course Leeds 2012

UNIVERSITY of Leeds Astbury Centre for Structural Molecular Biology & Rigaku BioSAXS Workshop August 19th 2011

Small Angle X-ray Scattering (SAXS) is able to provide low resolution molecular envelopes as well as information about dynamic motion from a wide range of solution and sample conditions. It is a technique that has recently been attracting renewed interest within the crystallographic community with the development of new X-ray sources and detectors as well as improved data processing algorithms. With this in mind, **Arwen Pearson** (University of Leeds) and **Olivia Sleator** (Rigaku) organized a workshop at the University of Leeds to cover the basics of SAXS, provide practical instruction on the information SAXS data can provide and introduce some of the software associated with data processing and analysis. The workshop proved so popular that a pre-workshop had to be held for local Leeds attendees! This allowed space for graduate students, post docs and more seasoned scientists from laboratories in the UK and further afield.

In the morning, presentations were given by **Angela Criswell** and **Joseph Ferrara** from Rigaku USA, Houston, Texas and **Edward Snell** from the Hauptman-Woodward Medical Research Institute in Buffalo, New York. The talks focused on the practicalities of sample preparation, data collection and data processing. In the afternoon, a hands-on data processing practical session used real world examples provided by **Eddie Snell** and **Angela Criswell**. The workshop was wrapped up with a plenary presentation by Prof. **Samar Hasnain** (University of Liverpool) who gave an overview of the power of SAXS in combination with crystallography and other techniques. He succinctly explained how a comprehensive complementary approach provides biological information that no single approach alone could achieve.

The workshop was supported by a BBSRC International Partnering Award for the development and application of complementary biophysical methods for the study of macromolecular dynamics.

3rd Workshop on Simultaneous Combination of Spectroscopies with X-ray Absorption, Scattering and Diffraction

4-6th July 2012, ETH Zurich, Switzerland

THIS workshop is the 3rd in a series of workshops previously held at the ESRF in 2008 and at SOLEIL in 2010.

The objective of the workshop is to provide an international platform for an in-depth discussion of both the application and instrumentation aspects of the combination of in-situ optical spectroscopy and X-ray methods.

In recent years, many synchrotron-based research fields have seen an increase in applications taking advantage of the complementary information provided by UV/Vis and IR absorption, fluorescence and Raman spectroscopy. The main advantages of such a combination are the:

- Gain of complementary information under identical experimental conditions
- Minimization of systematic errors that result from sequential measurements
- Easier understanding of fast rate processes, detection and manipulation of kinetic intermediates via complementary but independent observations.
- Observation and avoidance of radiation damage effects

The presentations are organized in sessions focused on the different scientific fields where a combination of optical spectroscopies and X-ray methods are currently employed at synchrotron beamlines, namely:

- Biological / Pharmaceutical Research
- Catalysis
- Materials / Nanomaterials

The organizers encourage suggestions for sessions dedicated to additional fields such as time-resolved measurements or environmental sciences. Based on the response from the scientific community, additional sessions may be announced in the next circular.

The sessions will be focused both on instrumentation and scientific applications. By holding single sessions the participants will be able to attend all sessions and hence inter-disciplinary discussions will be promoted. As the field is still new, the focus on instrumentation and interdisciplinarity is expected to aid the quick adoption of instrumentation advances by the diverse scientific communities.

A poster presentation will be organized, with two poster sessions dedicated to discussions.

The meeting will be accompanied by a vendor exhibition pertinent to the conference topic. Based on previous events, we plan on hosting approximately 100 participants. The participation of students is strongly encouraged.

Website: **http://www.psi.ch/csx2012**
Contact: **Martin Fuchs**, Paul Scherrer Institute,
csx2012@psi.ch

Scientific organizing committee:
Olga Safonova
Antonio Cervellino
Luca Quaroni
Martin Fuchs

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Swiss Federal Institute of Technology Zurich

ECA Individual Membership

Individual Membership of the ECA – an invitation

THE European Crystallographic Association (ECA) is one of three large transnational organisations for crystallographers, the others being the American Crystallographic Association ACA (covering both American continents) and the Asian Crystallographic Association AsCA (which includes also Australia, New Zealand and the Pacific islands). The ECA encompasses Europe, Africa and some parts of the Middle East.

Individual national crystallographic societies within its geographical area are members of the ECA and have representatives on its Council. The ECA Council generally meets annually during ECM or IUCr conferences, and shares its policy-setting and decision-making role with a smaller Executive Committee that meets twice each year.

The ECA supports and encourages crystallographic activities and helps to bring national societies together in cooperation. It sponsors some educational, training and outreach events, but one of its main purposes is to plan and oversee the organisation of European Crystallographic Meetings (ECMs), which occur in the 2 out of 3 years when there is no IUCr International Congress. The most recent ECMs (of which there have now been 26) were in Darmstadt, Germany (2010) and Istanbul, Turkey (2009).

Since the BCA is a member society of the ECA, it has one representative on the ECA Council, currently **Georgina Rosair** as the BCA Secretary. As a BCA member you thus have a small stake in the ECA. However, the ECA also invites and encourages Individual Membership (IM). As one of the three currently elected representatives for Individual Members of the ECA (the others being **Helen Stoeckli-Evans** in Switzerland and **Giuanluca Cascarano** in Italy), I have written this article to explain something about the ECA and to urge you as a BCA member to take up this opportunity to be an IM yourself.

You will undoubtedly ask what is in it for you. I will answer that question, but it should go alongside the parallel question what you can do for the ECA. Like the BCA, this organisation is only as strong and effective as its members make it, and both the BCA and the ECA really value the input and contributions of their members to their work of promoting crystallography at national and international levels, through membership fees of course, but also by expressing your views through elected representatives and in other ways, and by getting involved in events and activities. As we approach 2013, which we hope will be officially designated International Year of Crystallography by UNESCO, we have an unprecedented opportunity to showcase our subject and catch the imagination of the public at large.

Being an IM of the ECA will entitle you to vote to elect representatives on the ECA Council; the number of these representatives depends on the number of IMs (1 per 100), and it would certainly be useful to have more IM representatives who can bring a wider perspective than the large number of national society representatives. More tangibly, IMs enjoy a discount on ECM registration fees, just as BCA members pay less for our own Spring Meetings. You may well find this attractive, given that the 2012 ECM will be held in Bergen, Norway; 2013 is at Warwick University, UK and is expected to be a major celebration of the International Year of Crystallography with some special contributions to the programme (and we have no BCA Spring Meeting in that year); and 2015 will be in Rovinj, a holiday resort on the Croatian coast.

The IM annual fee is only 10€, and this can be paid conveniently by credit card, either year by year or for 5 years in advance for even greater convenience, at the website http://www.xray.cz/eca/regist.asp, to which you will also find a link on the ECA website at http://www.ecanews.org/, along with lots of other information.

The ECA will warmly welcome you as an Individual Member. About 40 of the 360 or so current IMs are in the UK. Well, what are you waiting for...?

Bill Clegg, ECA IM Representative (bill.clegg@ncl.ac.uk)

Meetings of interest

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

4-6 January 2012
CCP4 Study Weekend, University of Warwick.
http://www.cse.scitech.ac.uk/events/CCP4_2012/

8-10 January 2012
Workshop on New Experimental Capabilities, Los Alamos, NV, USA.
http://lansce.lanl.gov/users/lug.shtml

8-13 January 2012
10th NCCR Practical Course and 3rd Winter School, Kandersteg, Switzerland.
http://www.structuralbiology.uzh.ch/index.php?q=node /162

9-10 January 2012
Workshop on Off-Specular Neutron Scattering, Université Libre de Bruxelles, Brussels, Belgium.
http://www.ulb.ac.be//sciences/physsol/conference/Workshop/Welcome.html

18-19 January 2012
7th SOLEIL Users' Meeting, Polytechnique and SOLEIL, Gif-surYvette, France.
http://www.synchrotron-soleil.fr/Soleil/ToutesActualites/Workshops/2012/SUM12/Accueil

23-27 January 2012
5th ILL Annual School on Advanced Neutron Diffraction Data Treatment using the FullProf Suite, ILL, Grenoble, France.
http://www.ill.eu/instruments-support/instruments-groups/groups/dif/FPSchool/

29 January - 1 February 2012
Neutrons and Food 2012, Delft University of Technology, Delft, The Netherlands.
http://www.iucr.org/news/notices/meetings/meeting_2011_256

12-15 February 2012
4th International Conference on Drug Discovery, Dubai, UAE.
http://www.icddt.com/index.htm

4-7 March 2012
14th EMPG Meeting, Christian Albrechts Universität zu Kiel, Kiel, Germany.
http://www.empg2012.uni-kiel.de/

5-16 March 2012
43rd IFF Spring School, Juelich, Germany.
http://www.fz-juelich.de/pgi/EN/Leistungen/SchoolsAndCourses/SpringSchool/_node.html

8-16 March 2012
32nd Berlin School on Neutron Scattering, Berlin, Germany.
http://www.helmholtz-berlin.de/events/neutronschool/index_de.html

12-15 March 2012
Annual Meeting, German Crystallographic Society, Munich, Germany.
http://www.iucr.org/news/notices/meetings/meeting_dgk_2012

25-29 March 2012
Powder Diffraction and Rietveld Refinement School 2012, Durham.
http://www.dur.ac.uk/john.evans/webpages/pcg_rietveld_school_2012.htm

26-27 March 2012
"Small Molecules in Interactions" International Symposium, Ruhr-Universität Bochum, Bochum, Germany.
http://www.ruhr-uni-bochum.de/smi/

3 April 2012
CPOSS Open Day, UCL, London.
http://www.cposs.org.uk

9-13 April 2012
2012 MRS Spring Meeting and Exhibit Moscone West Convention Center, San Francisco, CA, USA.
http://www.mrs.org/spring2012/

16-19 April 2012
British Crystallographic Association Spring Meeting, University of Warwick.
http://www.crystallography.org.uk/

19-20 April 2012
Science & Scientists @ ESS 2012, Berlin, Germany.
http://esss.se/ess_conferences/

14-18 May 2012
E-MRS 2012 Spring Meeting, Congress Center, Strasbourg, France.
http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=428&Itemid=1

31 May - 10 June 2012
Present and Future Methods for Biomolecular Crystallography, Erice, Italy.
http://www.crystalerice.org/Erice2012/2012.htm

17-20 June 2012
European Conference of Crystal Growth 2012, University of Strathclyde, Glasgow.
http://eccg4.org/

25-28 June 2012
IWPCPS-14 (International Workshop on Physical Characterization of Pharmaceutical Solids), Barcelona, Spain.
http://www.iucr.org/news/notices/meetings/meeting_2011_252

4-6 July 2012
3rd Workshop on Simultaneous Combination of Spectroscopies with X-ray Absorption, Scattering and Diffraction, ETH Zurich, Switzerland.
http://www.psi.ch/csx2012

22-27 July 2012
15th International Conference on Experimental Mechanics, Faculty of Engineering, University of Porto, Porto, Portugal.
http://paginas.fe.up.pt/clme/icem15/

28 July - 1 August 2012
ACA Meeting 2012, Westin Waterfront Hotel, Boston, MA, USA.
http://www.amercrystalassn.org/2012-meeting-homepage

7-11 August 2012
27th Meeting of the European Crystallographic Association, Bergen, Norway.
http://ecm27.ecanews.org/

2-6 September 2012
First European Mineralogical Conference (EMC2012), Frankfurt, Germany.
http://emc2012.uni-frankfurt.de/

2-6 September 2012
XXII Conference on Applied Crystallography (XXII CAC), Targanice/Andrychów, Poland.
http://www.cac.us.edu.pl/

2-7 September 2012
Aperiodic 2012, Cairns, Queensland Australia.
http://www.iucr.org/news/notices/meetings/meeting_aperiodic_2012

4-9 September 2012
22nd IUBMB and 37th FEBS Conference, Seville Conference and Exhibition Centre, Seville, Spain.
http://www.iubmb-febs-2012.org/IUBMBFEBS2012/

15-20 September 2012
6th European Charge Density Meeting, Štrbské Pleso, Slovakia.
http://ecdm6.stuba.sk/?page=home

17-20 September 2012
7th International Sample Environment Workshop, Amora Hotel Jamison, Sydney, Australia.
http://www.ansto.gov.au/research/bragg_institute/current_research/conferences_and_workshops/sample_environment_at_neutron_scattering_facilities

23-28 September 2012
ICCBM 14. 14th International Conference on the Crystallization of Biological Macromolecules, Huntsville, AL, USA.
http://iccbm14.org/

18-23 November 2012
International Small-Angle Scattering Conference (SAS2012), Sydney, Australia.
http://www.sas2012.com/

26-30 November 2012
2012 MRS Fall Meeting and Exhibit, Boston, MA, USA.
http://www.mrs.org/fall2012/

25-29 August 2013
28th European Crystallographic Meeting, University of Warwick.
http://www.crystallography.org.uk/

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