Crystallography News

British Crystallographic Association

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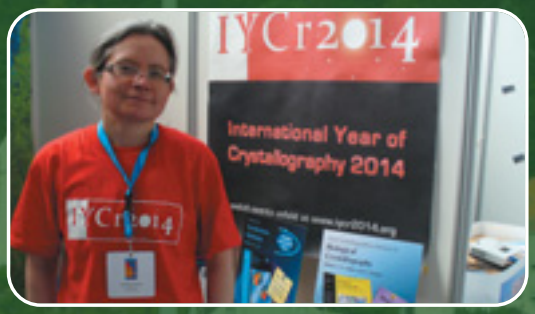

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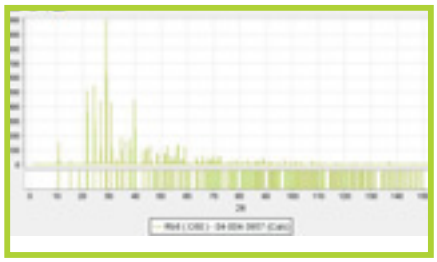

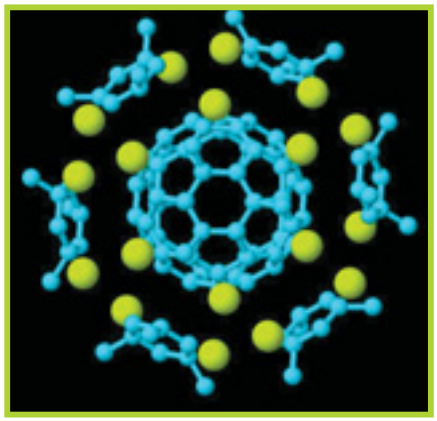

- All entries have digital patterns for use in total pattern analysis
- 171,856 entries with atomic coordinates
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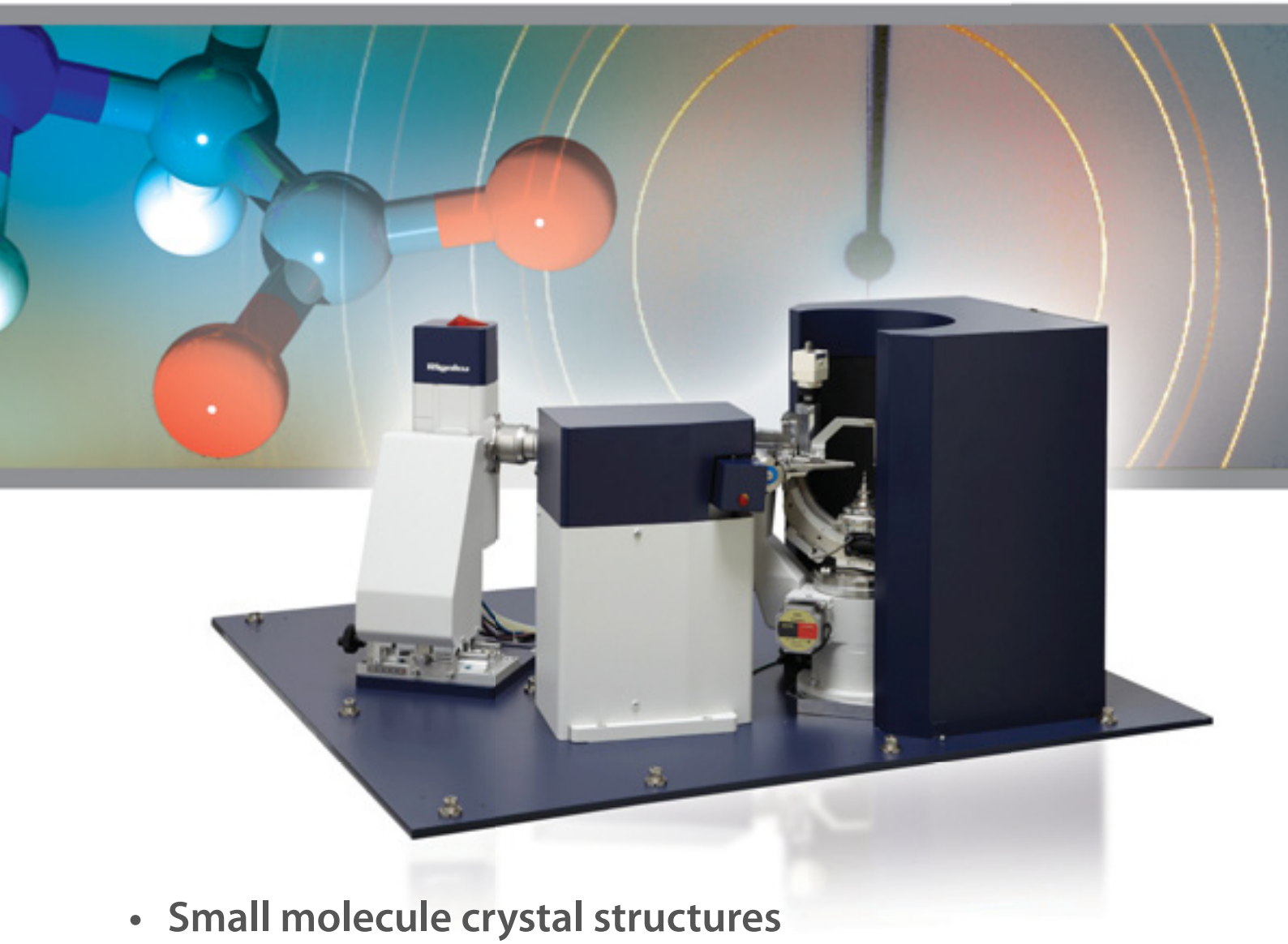

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- Twinned and disordered crystals

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This month's cover:

Scenes from Bergen, Norway, and ECM27

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by Bowmans, Leeds. Text should preferably be sent electronically as MSword documents (any version - .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (e.g. awards, honours, retirements etc.), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews. Please ensure that items for inclusion in the March 2013 issue are sent to the Editor to arrive before 25 January 2013.

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From the Editor

IT has been a wonderful summer for crystallographic meetings. Running the gamut from B to B, the two big ones were held in cities that offered fine culture as well as great seafood, set in areas of beautiful scenery. Both Boston, the venue for the American Crystallographic Association, and Bergen, the site of the European Crystallographic Meeting, were not cheap; but then we crystallographers are worth it, aren't we? Reports on both meetings appear in this issue. We can also anticipate with great pleasure the sophistication and natural beauty of the venues for next year's meetings: Honolulu for the ACA and Warwick University for the ECM. Neither should we lose sight of the smaller, more tightly focused meetings. In this issue we have reports on the May meeting of our Industrial Group and the conference of the South West Structural Biology Consortium. While it goes to press, the meeting of the Physical Crystallography Group and the joint meeting of the Chemical and Industrial Groups will take place. Readers should still be in time to attend the BSG Winter Meeting: 'From Genome to Proteome', MRC Cambridge, Tuesday 11 December 2012.

Notices in this issue demonstrate that next year will be an excellent one for crystallographic education, beginning with the very popular and highly effective Durham School from 6 to 14 April 2013. Our Durham colleagues are also organising the programme for "The Future of Dynamic Structural Science", which will take place in Erice from 30 May to 8 June. Finally I mention the long and comprehensive Zurich School to be run by our Swiss friends from the 9 to 22 of June.

I am grateful to **Derry Jones** for bringing to my attention a report written by **W H Brock** in the Newsletter of the RSC Historical Group about the life of **Alfred Tutton** (1864-1938). It can be found at **http://www.chem.qmul.ac.uk/rschg/Newsletter/NL2012summer.pdf** . Tutton already left school at 14 but carried on attending evening classes to improve himself. Winning a scholarship to the Royal College of Science in South Kensington, he compiled such an outstanding record that he was made a demonstrator. In 1895 he obtained a permanent job as Her Majesty's Inspector for Technical Schools, which kept him very busy. Notwithstanding this occupation, he was "obsessively determined to gain an FRS even if it meant working in his spare time day and night", in the words of his friend **Frederick William Westaway**. (Parenthetically, if the FRS's I know were obsessive about anything, it was their research; and Fellowship of the Royal Society "just happened".) Tutton built a private laboratory in each house where he lived, in which he undertook very precise measurements of dimensions and interfacial angles in crystals made from closely related series of elements. He initially studied sulphates and selenates of K, Rb, Cs, NH_4 and Th, and then their double salts with Mn, Cu and Cd (usually known as Tutton's salts). He concluded that crystal properties varied regularly with atomic number. His assiduous pursuit of the FRS was crowned with success already in 1899. By 1929 he had published data on over 90 salts in over 50 papers. While this year we rightly celebrate the momentous discovery of X-ray diffraction, Tutton showed that well into the 20th century it was still possible to obtain valuable information about crystals from goniometric and optical measurements.

I also thank Derry for helping the gifted instrument designer **Dennis S Beard** with the preparation of an autobiographical article. As well as designing instrumentation for high-end research applications, Dennis has been active in the production of apparatus that is simple, safe and cheap enough to be useful in schools for demonstrating topics such as X-rays.

This article and the sequence of the Laue and Bragg anniversaries and the International Year of Crystallography naturally prompt thinking about our public outreach activities. I am pleased that we have an article by **Gwenda Kyd** describing a joint initiative undertaken by CCDC and the Cambridge University Botanic Garden. Medicinal plants in the garden are associated with the crystal structures of the medicinally useful compounds that they contain. We also show the result of a bright idea by **Graeme Jones** of Keele University. To celebrate the Queen's Diamond Jubilee he organised teams of willing helpers, many from local schools, to construct and display in the centre of Uttoxeter a model of a diamond crystal of record-breaking size.

I continue with another request from **Kevin Lotery**, who is an art historian seeking crystallographic images from the 1950s produced by scientists such as **J W Jeffery**, **Kathleen Lonsdale**, **C H Carlisle**, **L Heller**, **I M Dawson** and **V Vand**. He is looking for high-resolution images or original negatives/prints of images from around this period by these or other researchers. He is based in London and can be reached *via* the following information: Kevin Lotery, Ph.D. Candidate, History of Art and Architecture, Harvard University, tel. +44(0) 75 2823 8040 (UK). While we contemplate the beauty of many crystallographic images and think about outreach activities, we should recall the work of **Helen Megaw**. With a distinguished record in science and a post of Assistant Director of Research at the Cavendish Laboratory in Cambridge, she turned her attention to the possibility of incorporating crystallographic patterns into commercial designs. As chief scientific consultant to the Festival Pattern Group, she inspired the exhibition at the 1951 Festival of Britain of a wide variety of manufactured products featuring crystal structure designs. In 2008 the Wellcome Trust put on a retrospective exhibition, "From Atoms to Patterns", with an associated book. In 2008 articles and reviews appeared in Crystallography News in the March (p 26), June (p 26) and December (p 27) issues, and the website for this exhibition is still accessible at **http://www.wellcomecollection.org/whats-on/exhibitions/from-atoms-to-patterns.aspx** .

It just remains for me to wish all our readers a happy holiday season. On an exam one of my students once wrote about "Brag's Law". As we enter the Year of the Braggs I hope it will bring all of us solid accomplishments that we can brag about.

Carl Schwalbe

BCA Council 2012

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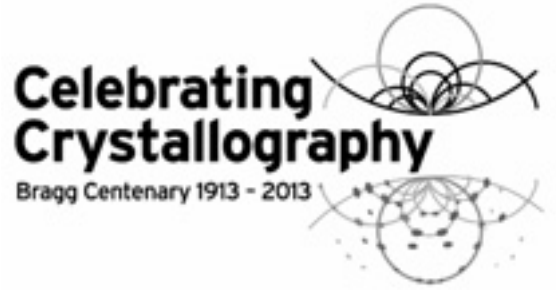
From the President



ELSPETH Garman, our past President, and I met for coffee in Oxford earlier this Autumn and discussed amongst other things how easy it is for the weather to creep into the Crystallography News "From the President" column. Perhaps we shouldn't be surprised since we are the British Crystallographic Association after all, but in my mind its topicality has risen above the UK norm this time because I have just returned from the European Powder Diffraction Conference in Grenoble where the weather played an unseasonable part in the meeting. The organisers had warned us to anticipate traffic disruption on the first day due to a marathon starting and ending near the conference venue, but instead we were greeted by snow falling in the city throughout the day and local transport at a virtual standstill. Indeed Lynne McCusker told me that the fabled Grenoble tramlines were the clearest and safest way to walk from the city centre hotels to the conference. Needless to say, the marathon had been cancelled, the sun came out and Grenoble looked stunning and the conference was very enjoyable. But I still don't know if Simon Billinge, who travelled with me on the bus back to Lyon Airport, has managed to get home to New York successfully (for other even more severe weather reasons)…

Work on the Bragg Centenary Celebrations is gathering pace. We now have a dedicated section of the BCA website (see www.crystallography.org.uk/bragg-centenary/) where we are listing events that are happening to coincide with this important milestone – some of which have already occurred. Please email me, or **Richard Cooper**, our Website Editor if you know of events that you think should be included. We even have a logo – thanks to **Laura Holland** at Diamond and others and shown at the top of this column. The logo incorporates a representation of Lawrence Bragg's interpretation of Max von Laue's diffraction pattern of zinc blende and will be made available for Bragg Centenary publicity via the BCA website. (As an aside, and for those punctuation gurus among us, I had a pre-conference dinner coach conversation at EPDIC as to whether we should be celebrating "Bragg's Law" or "Braggs' Law" next year. This was on the basis that Lawrence Bragg's first discussion of the equation in the 1913 Proceedings of the Cambridge Philosophical Society defined it as $\lambda=2d \cos \theta$ whereas we emphasise the more familiar $n\lambda=2d \sin \theta$, first published by William and Lawrence Bragg later in the same year. Perhaps we would've resolved our discussion better after dinner!)

More importantly, we are working with STFC and Diamond to produce a stand at the Big Bang Fair (www.thebigbangfair.co.uk), a national event held at London, ExCeL between 14 and 17 March 2013 for up to 60,000 school pupils, teachers and family groups. **Ross Harrington**, our Education and Outreach Coordinator, is coordinating this for us and I am certain that he will be looking for enthusiastic helpers to join him in this exciting outreach event.

I finish this column by announcing the sad news of the recent deaths of **Louise Johnson** and **Phil Lowe**. Please read their obituaries in this issue of Crystallography News and remember them.

David Keen

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Puzzle Corner

THIS codeword contains seasonal and crystallographic words, a few others, a smidgen of Latin, and lots of symbols for elements (only one of which you may want to give your special friends for Christmas). Find them by assigning the appropriate letter to each number in the squares.

14	3	●● ●●	11	26	11	9	23	●● ●●	3	23	22	19
●● ●●	11	2	●● ●●	●● ●●	8	24	●● ●●	11	9	●● ●●	●● ●●	24
●● ●●	8	22	23	1	23	10	14	1	●● ●●	8	11	18
●● ●●	8	12	10	●● ●●	●● ●●	13	●● ●●	●● ●●	17	13	22	●● ●●
1	16	10	2	3	22	24	14	22	24	10	●● ●●	●● ●●
23	●● ●●	2	24	●● ●●	●● ●●	1	●● ●●	24	10	23	●● ●●	8
●● ●●	2	3	22	13	1	14	21	11	1	●● ●●	19	11
●● ●●	22	16	23	●● ●●	●● ●●	11	●● ●●	1	●● ●●	14	13	2
26	16	●● ●●	●● ●●	22	24	14	11	14	24	22	●● ●●	6
●● ●●	1	2	11	10	1	●● ●●	●● ●●	●● ●●	●● ●●	23	22	11
●● ●●	14	●● ●●	20	●● ●●	●● ●●	●● ●●	5	24	10	23	●● ●●	9
25	11	10	12	11	22	16	●● ●●	18	23	●● ●●	14	23
●● ●●	15	●● ●●	11	15	23	●● ●●	4	24	7	23	15	1

To get you started, two numbers are matched to their letters.

1 S	2	3 H	4	5	6	7	8	9	10	11	12	13
14	15	16	17	18	19	20	21	22	23	24	25	26

Answer to September Puzzle

The winning entry was submitted by **Jim Trotter**. In the attached pictures he is comparing halite crystals (from the Natural History Museum in Vienna) and "cube" houses in Rotterdam.

American Crystallographic Association Annual Meeting

THIS year's ACA meeting began with four workshops running in parallel on the Saturday. BCA members provided major input into the two workshops that enhanced participants' understanding of important software. Paul Emsley, Garib Murshudov and Roberto Steiner gave instruction and led tutorials on Refmac and Coot. Oleg Dolomanov, Horst Puschmann and Ilia Guzei introduced advanced features for structure refinement and disorder modelling in OLEX2, after which they worked through in-depth examples and set problem structures. Another workshop, led by scientists from national laboratories at Los Alamos and Oak Ridge, dealt with modelling and refinement applied to the hot topic of nanoparticle structures. The final workshop has the catchy title "Crystallography – World of Wonders" and introduced imaginative ways to stimulate interest in our subject, primarily among student-age and younger people. Contributions ranged from "Making Structures with Lego, Ping-Pong Balls and Yarn" by Claudia Rawn – to British eyes reminiscent of Blue Peter, to "Remotely Enabled Instruments" by Katheriner Kantardjeff, to "Tackling Some Difficult Concepts in High School and College Chemistry, using the Cambridge Structural Database" by Colin Groom.

In the interest of conserving participants' time and money the main meeting ran from Sunday to Wednesday, ie one day shorter than past precedent with a corresponding increase in the number of parallel sessions. The meeting attracted 785 participants, including 23% from 30 different countries outside the USA. Other impressive statistics included: 258 posters, 294 lectures and 39 exhibitors. Inevitably this means that I can only describe a few of the high points in this summary.

This year's prestigious Transactions Symposium had the title "Transformations and Structural Oddities in Molecular Crystals: In Honor of **Bruce M Foxman**". Reflecting members' appreciation and admiration of Bruce and his work, this session ran for an entire day and continued through a second morning. **David Watkin** began the proceedings with a talk entitled "Z'>1 Structures. Just a Nuisance or Something More Interesting?" About 10% of the structures in the Cambridge Structural Database (CSD) have Z'>1. A proportion of these structures may be metastable with respect to a hypothetical structure with Z=1. In other cases all the strong interactions between molecules may be used to join them into an aggregate with only weak forces remaining between aggregates. The CRYSTALS team have embarked on the difficult task of providing automated analysis of Z'>1 structures. When participants returned after a break where they could imbibe good strong coffee, **Roger Bishop** enunciated a Clathrate Uncertainty Principle. Our understanding of hydrogen bonding is sufficiently advanced that we can often predict hydrogen bonded structures, particularly those involving OH groups. However, much weaker forces can be used to assemble clathrate hosts, although structure prediction then becomes unreliable. Factors that make a molecule likely to act as a clathrate host include C_2 or trigonal symmetry and an awkward shape that hinders packing. V-shaped butterfly hosts illustrate such features. A central alicyclic group offers (pseudo) symmetry and a limited degree of conformational flexibility. Aromatic "wings" provide edge-to-face or offset face-face interactions, and halogen "spikes" make packing awkward. A synthetic intermediate produced a surprise. It is insoluble and melts at 354°C even though the only intermolecular interactions are C-H…N, C-H…π and π… π. This observation raises the question: are weak forces really weak? Obviously, if enough of them are operating, the effect can be powerful ("the Gulliver effect"). If the coffee hadn't jolted us into wakefulness, **Richard Adams**'s opening statement did. He asserted that there are similarities between $(Ph_3P)Au\cdot$ and $H\cdot$ and justified this statement with the ability of both $Au(PPh_3)NO_3$ and HNO_3 to attack iridium and osmium carbonyl clusters, leading to novel subsequent reactions. **Carolyn Brock** began her talk "Learning from Outliers" with the maxim "Know what is normal; investigate the exceptions". Energy calculations show that unhindered biphenyls have minimum energy when the rings are twisted out of coplanarity by 42-45°. However, among the structures in the CSD the values for this twist angle found most frequently are near 0° and near 36°. A closer approach to planarity improves the packing. Mono-alcohols do not form dimeric hydrogen bonded interactions between OH groups. Instead, >51% of them in the CSD have Z'>1 so that better hydrogen bonding can occur. If possible, molecules crystallize with inversion symmetry. Enantiomerically pure materials often have Z'>1 so that two molecules can be related by a fake inversion centre.

While the Transactions Symposium continued after lunch, the General Interest I session with its hints of skulduggery drew a good crowd in a different room. **Edwin Pozharski** initiated the topic of Forensic Crystallography with "The Ligand That Was Not There". Protein-ligand structures provide more understanding than protein structures alone, but such structures present difficulties. (1) Validation is difficult since the standard evaluation measures are almost unaffected by the presence or absence of ligand. A useful exception is comparison of displacement parameters: B values of ligand should be similar to B values of protein. However, (2) occupancy by ligand at the desired site is seldom 100%, and this can affect the B values. In an illustrative example a complex with a fully and correctly fitted ligand led to good statistics. A correctly fitted partial ligand structure still led to good statistics. Even a full ligand fitted backwards gave good statistics. The only hint of this error was that the average B factor for ligand was 45, compared to 29 for the protein. However, reducing the occupancy of the incorrectly fitted ligand to 0.5 washed out the difference in B. It is necessary to check the correlation with the electron density, which the program TWILIGHT can do. About 5% of structures in the PDB are found to have an incorrect ligand! In the

absence of fraud, reasons are likely to be wishful thinking or over-reliance on "magic" methodology. Next, **Ethan Merritt** spoke on "Consider a Spherical Cow...Ruminations on Modelling Atoms in Crystals". With the highest resolution data on macromolecular crystals it is now possible to go beyond isotropic refinement to anisotropic or TLS. From the anisotropic displacement parameters B_{eq} values can be calculated and compared with B_{iso} values from isotropic re-refinement. In general the B_{eq} values are too high, and B_{est} fits the refined B_{iso} much better. Returning to the theme of Forensic Crystallography, **Bernhard Rupp** recounted "The F-Calc Files" in the manner of a spy thriller. It is a fact that X-ray structural models and structure factor amplitudes exist in the Protein Data Bank that are not based on measured data. Fraud may be detected by HUMINT: anonymous hints and emails, querying people who might know. Or it may be found by SIGINT. Faked data have atypical features. The data and the error model (random and systematic) may not match. The data and the model may fit too well. The electron density may be improbably clean. Errors in the imaginary model may propagate into the density. Based on counting statistics alone $I/\sigma(I)$ is calculated at around 100 for strong reflections, but even with synchrotron data the real $I/\sigma(I)$ levels out at around 30. Developing an ability to detect such anomalies also guards against innocent sloppiness such as interchanging the F_{obs} and F_{calc} columns.

Back at the Transactions Symposium, **Miguel Garcia-Garibay** introduced a topic more akin to Bruce Foxman's own research area. He began with a Topochemical Postulate: Molecular structure determines crystal and physical properties, which in turn determine reactivity. One must consider energetic and mechanistic feasibility. There is little kinetic energy in a crystal, so a lot of potential energy must be supplied if a reaction is to proceed. In other words, a high-energy reactant is required, eg a photochemically excited species. Examples of photodenitrogenation and photodecarbonylation were provided. After reaction a single crystal of reactant may turn into a single crystal of product, a crystal of product dissolved in reactant, or a completely amorphous product; but there always are the advantages that the reactions are selective and solvent-free. Next, **Victor Young** reminded his audience of crystallographers that they should not ignore other techniques, in particular differential scanning calorimetry (DSC). When ionic liquids are cooled, they usually crystallize first in a structure with nominal Z'=1, though often with disorder. Further cooling leads to an enantiotropic phase transition to a structure in a lower-symmetry space group with Z'>1, more twinning and less disorder. By revealing the occurrence of such transitions DSC provides the information necessary for planning the appropriate conditions for crystallographic data acquisition. The last talk was a fascinating personal account of disappearing polymorphs given by **Joel Bernstein**. Azobenzene and stilbene have similar spectra, but the spectrum of *N*-benzylideneaniline is different and suggests possible nonplanarity. A crystal structure was earnestly sought. Although crystals could be prepared from the p-methyl derivative, the first crystallographic experiment yielded only the unit cell dimensions and space group. Subsequent attempts to grow suitable crystals for a full structure determination failed. Instead, two new polymorphs called II and III appeared. It only became possible to grow Form I again when the group moved into a brand-new laboratory! The rings in Form I and Form III are coplanar while Form II shows a twist. Of immense financial importance is the issue of polymorphism in ranitidine hydrochloride (Zantac) with sales of $3.5 billion in 1991. A patent dispute hinged on whether a product that supposedly consisted of a new polymorph might contain any of the original patented polymorph. Factors that had to be considered were the relative stability of polymorphic forms, precise definition in the crystallization protocol of solvent, heating and stirring, and the development and use of analytical methods that can ascertain phase purity as well as identity.

The "Past Reflections and Future Directions" session neatly combined these two topics with strong implications for crystallographic teaching. **Brian Toby** chose the thought-provoking title "But Who Will Know What a Glide Plane Is?" He warned us about the irreversible tendency for parts of crystallography to become routine techniques, a process now far advanced with small molecule single-crystal structure determination but likely to spread to macromolecular and powder samples as well. It is futile to try to restrict the use of crystallography by non-experts, but we should be striving to incorporate the techniques and "language" of crystallography into university education. CheckCIF has done a lot to weed out bad structures, but more guidance is needed to tell non-experts when to consult a professional crystallographer. Those professional crystallographers will still have plenty of original research to do using more widely available neutron sources and microbeam synchrotron X-ray sources, phases that occur under non-ambient conditions, and the whole realm of structural science that uses structural information to design useful materials. **Hilary Jenkins** introduced us to MAX3D, which helps students to help themselves by providing a clear visualisation of data. Such visualisation makes clear when a wrong unit cell based only on strong reflections has been chosen, 2-component twins exist, or there is diffuse scattering. MAX3D is also useful for following phase changes and carrying out texture analysis. Under the title of "Enabling all Scientists to Utilize Crystallography" **Paul Swepston** reminded us of the importance of crystallographic entrepreneurs through an entertaining account of the history of the Molecular Structure Corporation. As colleagues of **F Albert Cotton**, **Jan Troup** and **Bert Frenz** set up the company with an agreement that they could use Cotton's diffractometer while Cotton's group could use their computer. They needed to be practical but also were visionary. To make the process of structure determination run as efficiently as possible, they devised the SDP package; but they also made the first attempt to determine charge density. This early effort was given a memorably devastating review by **Jack Dunitz**: "Troup's attempt at interpreting electron density maps was like people finding funny animals in clouds". **Christine Beavers** gave a very lively presentation entitled "A Fistful of Photons" focusing both on the synchrotron and on the beamline scientist. The first generation synchrotrons, eg the Bevatron, were built by physicists for exclusive use by physicists. The second generation were still devised by physicists, but chemists and biologists could use them. Starting with the SRS in Daresbury, third generation synchrotrons were purpose-built for chemistry and biology. In fact, we use X-rays from the storage ring, not the synchrotron. The users can be put on a 2-dimensional matrix ranging from knowledgeable to not knowledgeable and from kind to unkind. The beamline scientist has to provide support and encouragement ("make it look easy") but rein back unrealistic expectations ("keep it real"). Users should be made as self-sufficient as possible, but contact should be followed up to ensure that value is

obtained from the data and publications ensue where appropriate. **David Rae** provided his usual combination of thought-provoking comments and impressive mathematics in "Using Partial Observations, Partial Models and Partial Residuals in Least Squares Refinement." He stated that "An obsession with not biasing results obtained from diffraction intensities has led to the use of maximum ignorance statistics." We should make use of the information about variances provided by refinement.

The session on "Important Science from Small Molecule Structures" complemented the Transactions Symposium. **Bruce Foxman** described "Temperature and Pressure-Induced Phase Transitions in Metallocenes". First he defined the phenomenon of conservative twinning in a topotactic phase transformation. When the mother crystal has higher symmetry than the daughters, they twin to preserve the lost symmetry. He described the transformations in a series of ferrocenium salts, for which the rearrangements can be visualised as movies. Finally he presented the results of "Bruce's low-cost high-pressure crystallography". Touching a crystal with a needle caused the appearance under a polarising microscope to degrade and the diffraction pattern to disappear. **Alan Pinkerton** addressed the question "Why is Ferroelectric Croconic Acid so Dense". Its density of 1.912 g cm^{-3} seems astonishingly high for a small organic molecule. Its two enolic OH donors and three C=O acceptors can and do form very strong hydrogen bonds [d(H...O is about 1.68 Å], but other interactions must make a contribution. Calculations show that bond critical points also exist along O...O and O...π interactions.

I had an obvious interest in attending the session on "Crystallographic Information in Pharmaceutical Research and Development". **Patrick Connelly** started us off with "Getting Physical to Fix Pharma". The current challenge to the pharmaceutical industry is to make full use of structure-based drug design and structure-based pharmaceutical development. While airframers use modelling and simulation right from the start in designing aircraft, the pharmaceutical industry generally starts with a lot of empiricism. The combination of crystallography with other physical methods, particularly calorimetry, can reduce the failure rate in drug discovery. Even when a potent drug is found, poor solubility may make it difficult to administer. Making it amorphous may help; but, now that we are getting better at predicting crystal structures, we should now try our hand at predicting solubility. Next, our own **Peter Wood** discussed "Isostructurality in Pharmaceutical Salts: How Much and How Similar?" Pharmaceutical companies often reformulate a drug, eg to switch counter-ions in salts. This may be done to improve an important property such as solubility, but another reason may be to obtain new patent protection. Granting of a patent is not automatic; a new crystal form has to be both novel and unobvious. The analysis of structural similarity is difficult. Peter reported a comparison of Na^+ and K^+ salts by a variety of methods including 3D packing analysis, unit cell comparison, and X-ray powder diffraction patterns. If these salts are isostructural, a switch from one to the other would seem "obvious" and unlikely to be patentable. Full isostructurality shows up as clearly in the cell dimensions as in more sophisticated measures. Less than full isostructurality leads to poor correlation between cell dimension changes, and even changes in powder diffraction patterns, and the underlying alterations in packing. Even small deviations from isostructurality may lead to significant changes in physical properties. **Eugene Cheung** presented "Structural Insights from Variable Temperature X-Ray Diffraction Data". Typically PXRD is combined with thermal methods in the characterization of a drug. For instance, sodium tartrate monohydrate first shows the expected increase of unit cell volume with temperature; but then a decrease in volume occurs, attributable to dehydration. Thermal analysis suggests that ampicillin trihydrate undergoes 1-step dehydration and melting, but PXRD gives the additional information that crystallinity is retained for a while after dehydration.

Full of new ideas, I was on an eastbound flight the same evening on a journey that would ultimately lead to Bergen. I am grateful to **Peter Mueller** of MIT for the photographs that accompany this article.

Carl Schwalbe

David Watkin

Richard Cooper

Roberto Steiner

Images from American Crystallographic Association Annual Meeting
Boston, USA, 28 July – 1 August 2012

OLEX2 workshop

Crystal Towns draws the winner

Sunday PM Transactions speakers

CCDC in Boston

Public Domain Software speakers

Sunday AM Transactions speakers

Future Directions speakers

A lively poster session

Margaret Etter Student Lecture Awards

THE success achieved by British students at this year's ACA meeting should engender great pride among the student winners, their supervisors and the BCA in general. Of the nine winners of Margaret Etter Student Lecture Awards in 2012, six were from universities or research institutes within the United States, three came from the UK, and zero were from anywhere else. The ACA website describes these awards as follows: *"Each Scientific Interest Group (SIG) within the ACA has the opportunity to invite one student to receive an award and to present a lecture in one of the sessions organized by that SIG. Selections are based upon submitted abstracts and are independent of whether the student presenter originally requested an oral or poster presentation. Award winners are determined by the elected officers of the SIGs. Students who accept the invitation will receive a monetary award of $250, which is independent of any requests for support via the ACA Travel Awards."*

The photograph below shows: (L) **Karim Sutton** (University of Oxford, chosen by the General Interest SIG), (R) **Allan Pang** (Queen Mary University of London, chosen by the Small Angle Scattering SIG).

Congratulations should also go to **Simon Goodson** (Cardiff University, chosen by the Fiber SIG). It should be noted that the run of British success started already in 2011, when two of the eight awards were won by **Phoebe Allan** (University of St Andrews, Materials Science SIG) and **Lauren Hatcher** (University of Bath, Synchrotron Radiation SIG).

ECM Bergen 2012

THE 27th ECM held in Bergen, Norway promised to be an interesting and informative meeting, and I have to say I wasn't disappointed; the standard of speakers was excellent. As my work is currently focussed on low temperature / high pressure polymorphism, my conference kicked off with the high pressure workshop held in the two days before the main meeting. Not only was this the most useful part of the conference for myself, it was also the most enjoyable. Given the small meeting size the event is considerably more personal and the audience, shall we say, more "interactive" when they disagree with the speaker. In particular the correct use of SADABS promoted a lively debate.

Clivia Hejney's discussion of the ideal data collection methods through the medium of interpretive dance was a highlight as was the Bruker software session. **Ross Angel**'s discussion of the program ABSORB, (although the program is maybe not well suited to my work), was really informative and useful should I work in other areas of high pressure crystallography.

I was to give my talk on low temperature – high pressure polymorphism in the middle of the main conference. Naturally, I was mildly terrified at giving my very first presentation to an international audience. I felt it went quite well however, and that following a nervous start I grew into the talk. **Francesca Fabbiani** and **Simon Parsons** gave some very useful pointers and questions for which I am very grateful. There were many fascinating talks in the main conference, certainly too many to mention in an article of reasonable length; but a couple of highlights were **Paul Midgely**'s hugely interesting lecture, attempting to redefine how we view refinement in electron crystallography, and **Simon Parsons**, who was as ever excellent in both of his talks.

Norway was an extremely welcoming and friendly host location; the organisers **Karl Törnroos** and **Carl Hendrik Görbitz** were both really generous with their time and organised a wonderful programme. Sadly, the extreme generosity of the Norwegian people is matched by the extreme price of just about everything in Norway, an especially large impediment for this impoverished PhD student; but that didn't stop me having a whale of a time. Many thanks go to the BCA for supporting my trip.

Joe Ridout
University of Durham

Bryggen district in Bergen, a World Heritage site

JOE'S report gives a good summary of the highlights and the spirit of ECM-27. I just want to add a couple of additional highlights, and I thank Georgina Rosair and Joan Schwalbe for providing pictures to supplement my own. Before MS31, the "How to" session, took place, it seemed likely to merit a description of "worthy, useful but not particularly exciting". However, the actual experience proved to be very entertaining. If Harry Powell ever decides to give up crystallography, his thespian talent should land him a top job at RADA. Not only did he describe good and bad lecturing techniques, he acted them out, sometimes to cringe-making effect as we recognised our own shortcomings. John Helliwell did much to change the widely held image of journal editors as the modern equivalent of hanging judges. In fact, the mission of editors and peer reviewers is to help authors. It is rare for a manuscript to be either accepted with 'publish as is' or rejected out of hand. Usually some degree of revision is required, and the result is a better paper. Reasons for complete rejection include inadequate data, poor science, a total lack of conclusions, or incomprehensible English. A particular bête noire is a style of referencing that does not match the journal's style; it suggests that the manuscript had been submitted and rejected somewhere else, and this journal is regarded as the second- or third-best option. Under the title "How to survive in Academia" Alessia Bacchi recounted some horror stories from surprisingly recent times, particularly for women trying to build a career in science. Fortunately, equal rights legislation and increased emphasis on appointing the best candidate irrespective of gender or race have opened up a lot of previously "no-go areas" for women. Cultivating a network of colleagues can be very rewarding. Finally, Elena Boldyreva gave a typically thought-provoking lecture on "How to ensure the future of crystallography – a teaching perspective". In far-away Siberia she is stimulating interest in crystallography already among children by using appropriate exercises. Other objectives

that she put forward were to build links between consumers and producers of structural data, and to continue to train professional crystallographers with the ability to produce high-quality data from difficult samples.

For a long time at BCA meetings, and more recently at ECA meetings, I have envied the Young Crystallographers. They seemed to be having all the fun. I wondered why the Old Crystallographers couldn't have a similar group. Well, now we do! At the European Crystallographic Meeting the new General Interest Group 2 – Senior Crystallographers held two lunchtime meetings. The first one dealt with organisational matters, and the second one provided two enjoyable excursions into the history of crystallography.

MS31 "How to" session speakers

As soon as the first meeting had been called to order (not that we were particularly disorderly!), an election was held in which **Hans-Beat Bürgi** was unanimously elected chairman. The discussion then turned to our remit. We have a unique role in the history of crystallography. Many of us knew some great crystallographers who are no longer with us. While we still can, we should document our memories of them and curate memorabilia if we have any. It was also suggested that we could provide the inverse of a function fulfilled by the Young Crystallographers. While they provide advice and networking to members seeking a permanent job, we could provide similar help to members making the transition from a job to retirement but wishing to retain an interest in crystallography. This prompted members of the audience to say what they were doing in retirement. Several recurrent themes emerged. All of us welcomed the chance to shed

Mountain-top view of Bergen

Speakers at the award ceremony

administrative responsibilities. We had to downsize our laboratories and offices or relinquish them entirely, which could be a painful process. Two of us worked on databases without the need for laboratory facilities. We valued continuation of contacts with students and younger colleagues, and those of us who could supervise a few selected research students felt particularly fortunate. Finally we were reminded that the joys of retirement should be cherished, such as playing with grandchildren or hiking with a beloved partner.

In the middle of the final day of the conference we tucked into a generous packed lunch and enjoyed MS-48, "Historical Aspects of Crystallography". **Santiago Garcia-Granda** gave a beautifully illustrated presentation on "X-rays and Crystallography. A Story through the Stamps". As well as providing a feast for our eyes, it made us aware that even countries that we might regard as out-of-the-way celebrated our science in their stamps. This bodes well for the International Year of Crystallography. Then we had a wonderful show-and-tell presentation by **Theo Hahn**. Knowledge of the space group is essential to us as we solve a crystal structure. Who could explain the development of the concepts better than the long-time editor of this section of the International Tables? Theo reproduced some of the 19th-century correspondence between **Evgraf Stepanovich Fedorov** and **Arthur Schönflies** as they developed the mathematics of space groups. Their letters contain a fascinating mix of flowery compliments, important mathematics and the occasional barbed criticism. By 1919 **Paul Niggli** had published a system that successfully related the mathematics of space groups to the world of crystals. Unfortunately, his notation was cumbersome and his "explanations" were in German that was impenetrable even to a native German-speaker. During the early 1920s **Ralph Wyckoff** developed an analysis of special positions that is still used today, and our own **Kathleen Lonsdale** developed a far more understandable pictorial notation. Finally, in the early 1930s **Carl Hermann** and **Charles-Victor Mauguin** produced fairly similar schemes which they reconciled into the system we use today. (Biographical details about these two admirable men appeared in the December 2010 issue of *Crystallography News*.) Theo passed around several priceless old books by the authors he mentioned. Despite their age, they were in remarkably good condition – a description which could also be applied to the members of GIG-2!

Carl Schwalbe

BCA IG May Meeting

XRD: Phase Identification & Crystallography in Industry

Morning Session

OPTIMISING YOUR DIFFRACTOMETER

Judith Shackleton, Senior Technologist, Pilkington Group Limited, European Technical Centre, Lathom, Hall Lane, Ormskirk, Lancashire, L40 5UF

THE first talk, by **Judith Shackleton** from NSG Pilkington Group, focused on the importance of sample preparation and instrument optimisation. The presentation gave an overview of the various configurations that are currently available for analysis, highlighting some of the common pitfalls of XRD and methods to avoid them along the way. Judith described the need to tailor the analysis to the sample to ensure good data is obtained. The presentation was finished with by stressing the importance of regular calibration checks and the use of suitable standards.

PHASE ID WITH THE POWDER DIFFRACTION FILE

David Taylor, Treasurer, International Centre for Diffraction Data

THE presentation by **Dave Taylor** started by highlighting some of the Powder Diffraction File's (PDF) 75 year heritage. Dave provided a live demonstration of the current PDF software walking though examples of phase ID with an insight into some of the ways that the data can be manipulated along with the data mining tools to determine a match from the 700,000+ phases in the database. A brief insight into some new features in the upcoming September release was given at the end of the live demonstration.

PHASE ID OF GEOLOGICAL MATERIALS

Cheryl Haidon, University of Leicester

CHERYL **Haidon**'s talk and presentation covered the qualitative phase identification of geological materials by powder diffraction. The challenges of mineral identification were discussed, such as issues with peak assignments, overlaps and amorphous or fluorescing materials increasing the background. This highlighted the need for supporting information from other sources, such as sample provenance and chemical (XRF) analysis. Also a significant proportion of the geological materials of interest contain solid solutions (eg framework and sheet silicates). Cheryl showed how it is possible to discriminate many of these forms in pure phases or with extensive chemical treatment, but that in a flat-plate "whole-rock" sample, it is more difficult.

Alex Abbott
NSG/Pilkington Group Limited

Afternoon Session

POLYMORPHISM AND THE FORMULATION PROCESS

Sandie Dann, University of Loughborough

DRUG formulation must be predictable and involve 3 components: a coating, a filler and the active pharmaceutical ingredient. The particle size of the materials is very important. This is especially so when used in inhalation devices where solvents are used as carriers. An example given was where sugar (alpha lactose) is used as the filler and ethanol used as a solvent. Any water involved in the process can increase the particle size of the lactose after hydration. This is obviously a bad thing in an inhaler where consistency of drug delivery, and removal of side effects, is important.

XRD can be used to look at the form of lactose used in the material stored in the inhaler canister and also after it has been used. This allows judgements to be made as to how the lactose may behave if water is present in the process.

USES OF X-RAY AND OTHER DIFFRACTION METHODS IN UNFOLDING AND DISCOVERING NEW MATERIALS

Paul O'Brien, University of Manchester

CRYSTALS can be grown in unusual and exotic forms. Examples were given of crystals of potentially complex materials. XRD can be used to track any changes in crystal growth. Nanoparticles and mesocrystals were described which could be grown with core materials and outer layers of compounds such as lead selenides.

USING PXRD IN SUPPORT OF THE INVESTIGATION OF LITHOFACIES IN CARBONIFEROUS MUDSTONES

J J Graham, University of Leicester

SHALE gas is a potential new source of energy and, although only just being looked at in the UK, the industry is growing rapidly in the United States. There are many different types of mudstones and shale and a better understanding of them may lead to better identification of where the gas deposits may be. Mudstone types include carbonate rich, lenticular, homogenous and those that are fossil rich.

XRD can be used to differentiate between the carbonate and silicate minerals present although other techniques are also used such as XRF and TOC. The Polysnap software package is used to group XRD plots from different samples together thus greatly increasing the speed of interpretation.

DETECTING COUNTERFEITS USING OPTICAL SPECTROSCOPY

Prof George Fraser, University of Leicester

PRCI is a spin off company from the University of Leicester. It is developing products to differentiate between real and counterfeit goods. This is important for the Whiskey industry where the revenue loses half a billion dollars of tax each year due to counterfeiting.

Any solution to the problem of testing goods needs to be quick, portable and able to give a YES/NO answer. The development of a simple optical spectroscopy method is able to differentiate between malts and blends and between ethanol, water and air. By plotting the ratios of peaks against wavelength, very reproducible 'fingerprints' of product type and origin are possible.

X-RAY DIFFRACTION WITHOUT SAMPLE PREPARATION

G M Hansford, University of Leicester

AN XRD system will land on Mars this year. This is part of the Mars Science Lab that was sent on the Mars Carrier mission. This is a back-reflection XRD unit that uses an ED-XRD detector at an angle of 100 degrees. Due to the unique instrument geometry it is insensitive to sample morphology and no sample preparation is required. The system that went to Mars weighed less than 1 kilogram.

Healthy count rates were recorded when testing the system on a single mineral sample and a basalt. More testing is required as fluorescence interference can be a problem. Monochromators can be used in order to improve peak resolution.

Andrew Scothern
Saint-Gobain

THIS year's conference of the **South West Structural Biology Consortium** was hosted by the recently founded **Institute for Life Sciences (IfLS)** at the University of Southampton on 16 and 17 July. The conference is a great opportunity for young and early career scientists to present their work and exchange ideas and get to know each other. With a hundred participants, over 40 posters and about 20 talks the conference offers ample opportunity to catch up with the latest research. The conference has a long tradition to involve manufacturers and industrial partners adding a valuable dimension to the meeting in a field that has a strong technology component. Together with CCP4 and the BCA BSG the industrial partners also make a substantial contribution to the meeting that has enabled us over the years to make the meeting accessible to everyone.

This year the scientific programme broadly fell into five areas: mechanistic enzymology, molecular microbiology, extracellular matrix and fibres, molecular immunology and novel technologies. The presentations as well as the posters were of very high quality and the discussions open and engaging. For a fair few, the conference extended well beyond the conference dinner accompanied with live music from an up-coming Southampton band into the early hours of the morning in some of Southampton's live music pubs.

The meeting is a vital element of creating and maintaining a vibrant structural biology community and the many connections, the sharing of ideas and resources as well as collaborations that are initiated at these meetings are testament to their importance. We are all looking forward to a great SWSBC meeting in Bristol next year.

Applications for the June 2013 School are now open. Applications close January 15, 2013.

Intended audience and purpose of the course

The course is intended primarily for Master's and Ph.D. students in the molecular and solid state sciences, particularly from across Europe, but applicants from other regions will be considered. The goal is that the participants gain hands-on experience plus a theoretical background in the art and science of routine crystal and molecular structure determination of small molecules by single-crystal X-ray crystallography, as well as in the interpretation and presentation of results. The course will consist of lectures, computer exercises and practical work.

Elementary knowledge of general-purpose, first-year university-level chemistry and mathematical concepts is helpful. No specialized knowledge of crystallography is required, but some prior experience is useful. The course language is English and participants must be sufficiently proficient in English to be able to understand the lectures and participate in discussions without difficulty.

The course is **not** suitable for students interested specifically in powder diffraction techniques or macromolecular crystallography.

Bring Your Own Crystals

The unique aspect of the School is that participants get to collect data and determine the structure of one of their own compounds that they are currently interested in and that they have not worked on before. Participants prepare and send their own crystals of one compound several weeks before the School, so that the crystal quality and suitability of the problem may be assessed. At the end of the School, participants give a ten minute presentation of the results of their analysis.

ECTS credit for course

The University of Zürich offers 3 ECTS points, equivalent to 90 contact hours, for the course to successful students. Receiving credit requires:

- attendance during the full duration of the School.
- passing a two-hour written examination on the final morning of the School and a positive assessment of the practical course work by the directors of the School.

Acceptance of the credit points by the student's home university must be negotiated by the students themselves on the basis of the detailed School programme, the result of their examination and the course assessment by the School directors.

On the Trail of Crystallography in the Garden!

SINCE the beginning of human history we have exploited plants as a source of medicines, foods, dyes and many other things. Scientists have, therefore, tried to extract and study the active chemical compounds, to help them to understand their actions and maximise the benefits. This has led to many compounds of natural origin being studied by X-ray crystallography and so included in the Cambridge Structural Database (CSD).

A new "Chemicals from Plants" Trail aims to highlight some of these chemical compounds in their natural environment. The Trail is the result of a collaboration between Cambridge Crystallographic Data Centre (CCDC) and Cambridge University Botanic Garden.

The 26 compounds and 22 plants on the Trail were selected to show the wide range of uses and properties of plant-derived compounds but also to try to engage with people of all ages and levels of interest and knowledge of science.

One of the plants on the Trail is wild carrot (Daucus carota), a source of the orange pigment beta-carotene. This conjugated polyene acts as an antioxidant. It is related to Vitamin A (retinol), which promotes good eye health, so eating carrots really is good for you! However, excessive consumption can lead to carotenodermia, which makes your skin turn orange.

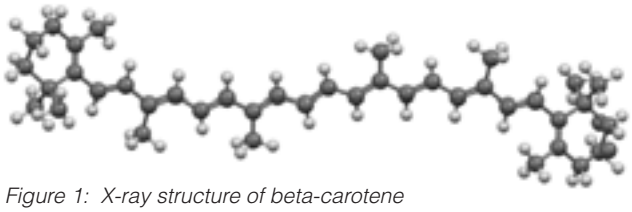
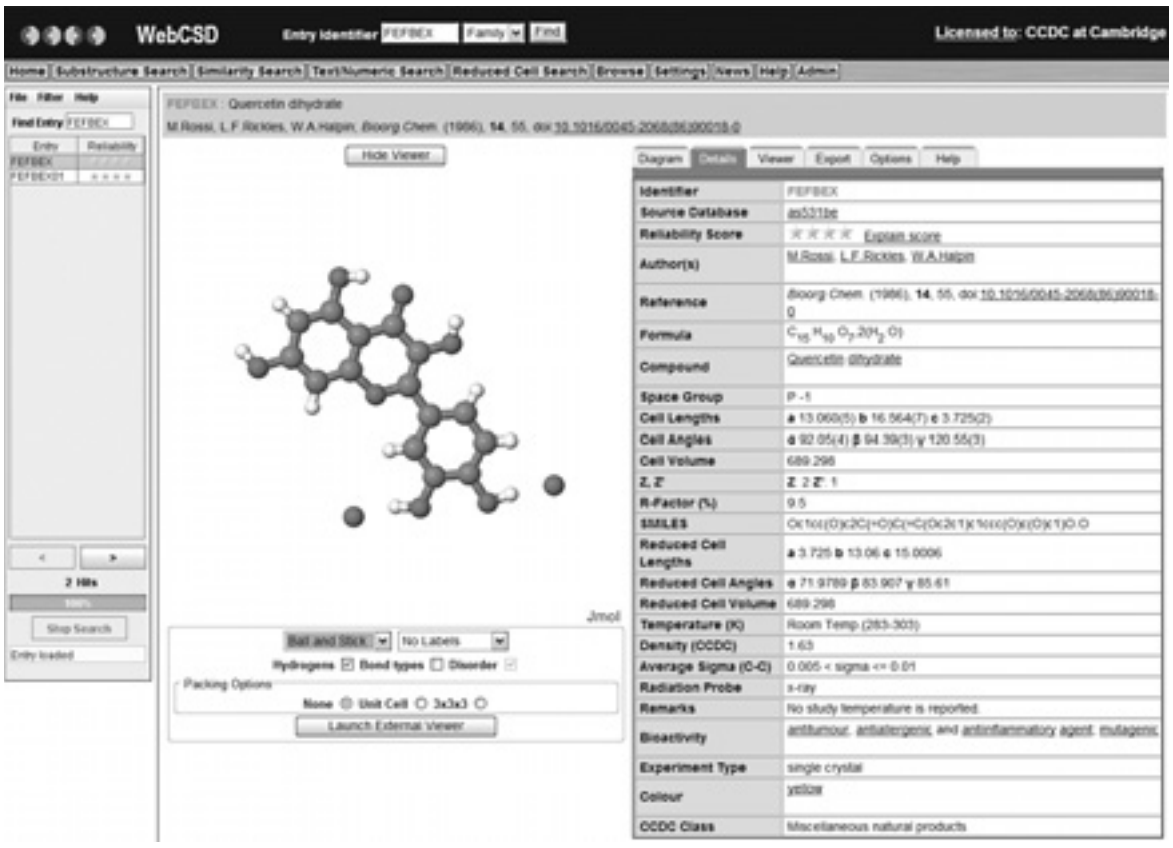


Figure 1: X-ray structure of beta-carotene

This effect is also seen in other species- the characteristic colour of flamingos and salmon is due to carotenes in their diets. Flamingos living in captivity must be fed food enriched with carotenes, otherwise they appear white. Recent studies also indicate that Greater Flamingos use the carotenoid pigments as "cosmetics" spreading them to their cheek, neck, breast and back feathers. This behaviour is more prevalent in females than males and there is some evidence to suggest that more highly coloured birds attract mates more easily. As carotenes are photo-sensitive, the pigments need to be applied frequently to maintain the effect! Wild carrot roots are less highly coloured than cultivated varieties and both wild and cultivated carrots can be purple, white, yellow or orange depending on their species. Although beta-carotene is an orange pigment, purple carrots actually contain more beta-carotene than orange ones.

Figure 2: WebCSD entry for quercetin dihydrate



Like carrots, many other plants contain health-promoting chemicals. One of these is quercetin, a flavonoid widely found in plants including prickly pear (Opuntia). This has anti-cancer, anti-allergy and anti-inflammatory properties. It is an anti-oxidant, scavenging free radicals in the body and protecting LDL cholesterol from oxidation. Quercetin is commonly taken as a food supplement. The plant itself features in Disney's "The Jungle Book". As highlighted in the song "The Bare Necessities", the spines are extremely prickly. These were used, before the introduction of stainless steel needles, to play 78 rpm vinyl records. If you can avoid the spines, the prickly pear fruits are edible.

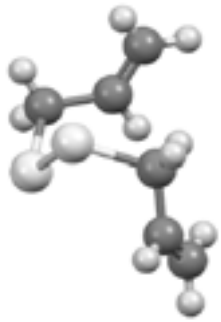


Figure 3: X-ray structure of diallyl disulfide

Plants need to protect themselves from being eaten so often contain foul-smelling or poisonous compounds. For example, garlic (Allium sativum) contains allicin, which forms diallyl disulfide (DADS) when the cells are broken down eg by cutting or chewing. DADS has the well-known sulfurous odour which many consider unpleasant. This smell is perceived through the transient receptor potential cation channel, member A1 (TRPA1). This ion channel has long been present not only in humans and animals, but also in fungi. Thus, Alliaceae plants probably developed the DADS-TRPA1 protection mechanism against predators in the early stages of their evolution. DADS is the principal cause of skin reaction to garlic but has a number of beneficial effects such as anti-bacterial, anti-cancer and cardio-protective properties. Garlic is used to add flavour to food and as a supplement, particularly for its effects on the heart and blood pressure.

One of the poisonous plants on the Trail is henbane (Hyoscyamus niger), the source of scopolamine. This hallucinogenic alkaloid has allegedly been used as a truth drug and was suggested as the cause of death of Dr Crippen's wife, Cora, after traces were found in her body. In small quantities, however, it can be used medicinally, to treat nausea and motion sickness. The whole plant is toxic, but, in 2008, celebrity chef Antony Worrall Thompson mistakenly recommended using the leaves in salads, confusing it with the plant fat hen.

Many plants contain compounds which are either used medicinally or have been developed to produce drug molecules. One example is willow (Salix) which contains salicin in its bark. This is oxidised to give salicylic acid, an anti-inflammatory agent. Extracts of willow bark have been used to treat pain since the time of Hippocrates (around 400 BC). The acetyl derivative of salicylic acid is commonly known as Aspirin. This non-steroidal anti-inflammatory drug is widely used for pain relief and in the prevention of heart attacks and strokes. Estimates suggest a global usage of above 120 billion aspirin tablets per year. Cricket bats are made of willow and willow is also the Bach Flower Remedy for self-pity and resentment.

Each plant on the Trail has an information board and QR code which links to the online version of the Trail. This contains more information on the plant and the compound(s) of interest and their uses, a 2D chemical diagram and a representation of the 3D crystal structure. From here you can also link to the full X-ray structural data in WebCSD. Even if you can't visit Cambridge in person, or in inclement weather, the virtual Trail can be followed at **www.bit.ly/CCDCTrail** .

Gwenda Kyd CCDC

Figure 4: WebCSD entry for scopolamine (as hydrobromide)

(Figure 5 is on next page)

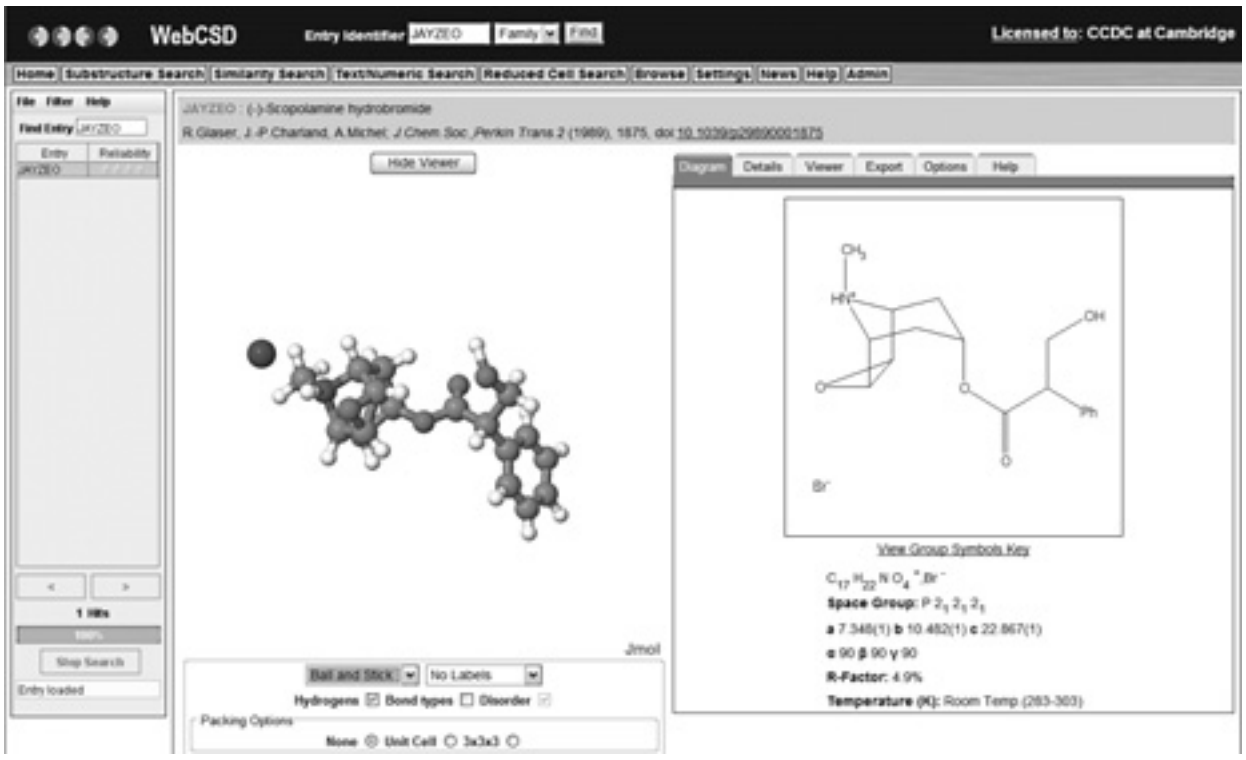


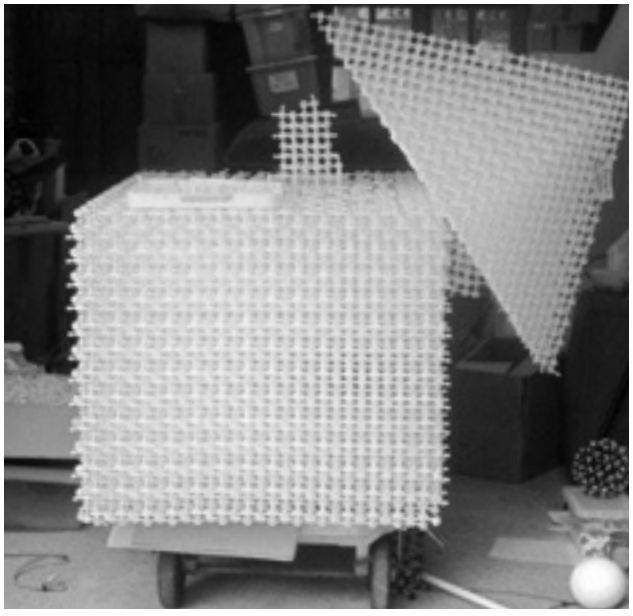
Figure 5: "Chemicals from Plants" entry for Salix (willow)

Uttoxeter Jubilee Diamond

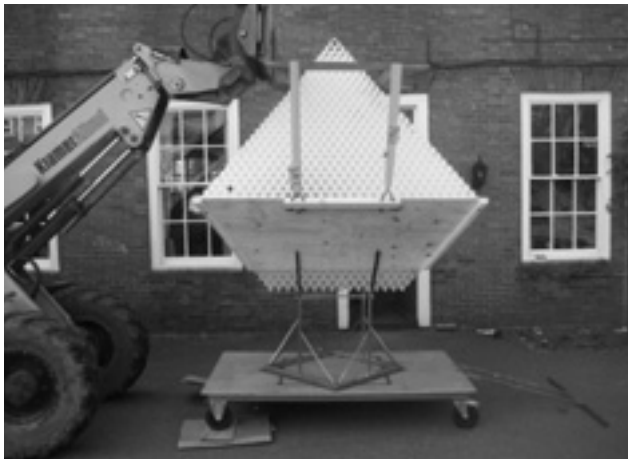
THE guiding spirit was Graeme Jones, Senior Lecturer in Organic Chemistry at Keele University. His objective was to create in Uttoxeter a Scientific Celebration of the Queen's Diamond Jubilee. He and his large team of helpers assembled an array of 35990 transparent balls representing atoms of carbon into the largest molecular model of diamond in the world. It has been submitted for recognition as a Guinness World Record.

An excellent example of scientific outreach, this enterprise provided people of all ages in Uttoxeter with an appreciation of the beautiful regularity of crystal structures along with an opportunity to build civic pride. A total of eight schools, Uttoxeter Cubs and Brownies plus two more groups, a museum, a service club and a church took part. Being more efficient than the designers of the Egyptian pyramids, Graeme assigned different parts of the crystal to the various teams of builders. After they were finished, he assembled the resulting modules into the finished crystal. One problem remained: how to move the finished model to the display site in the middle of town without knocking off any bits. As Graeme put it: "It is amazing who you bump into at 5.30 in the morning in Uttoxeter. There I was with my tape measure sizing up the doors of the local garages and what should I find but the Maltings Garage is open!! And I now have Ed who has a telescopic handler and can help me put it on the stand." The big but delicate operation was a success.

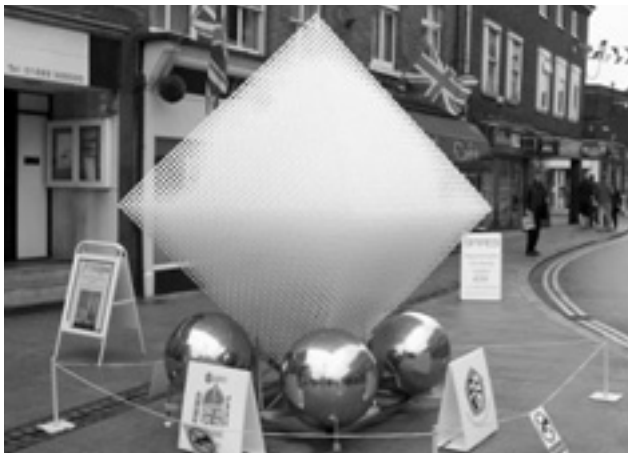
On the great day **Sarah Elsom**, the High Sheriff of Staffordshire, came to unveil the model at 11.00 am and did a splendid job despite the rain. The Rev **Ted Whittaker** read the Jubilee Prayer, the townsfolk sang the national anthem and everybody did three cheers for the Queen and three cheers for the children and adults who made the model.



Diamond in pieces



Diamond in transit



Diamond in situ

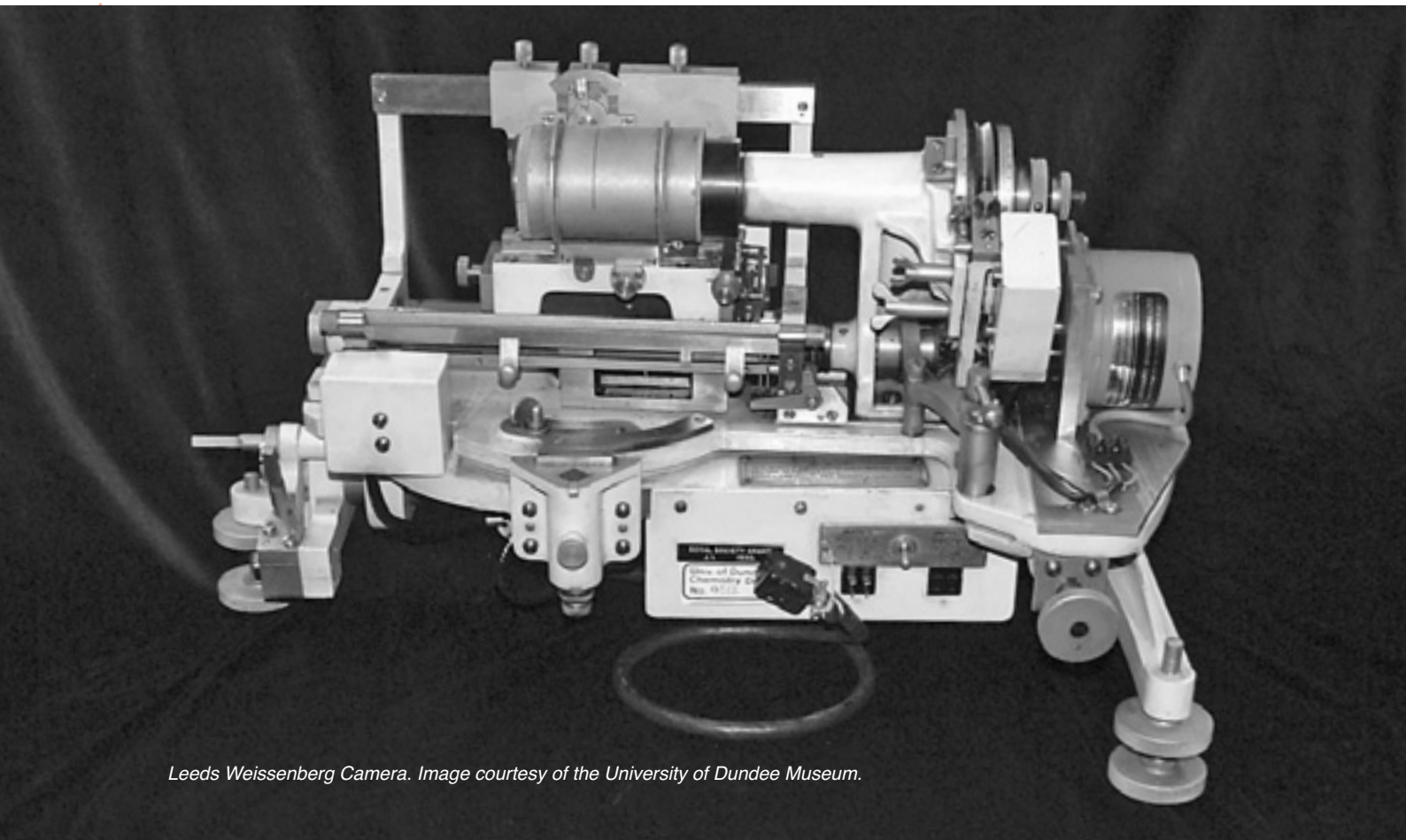
Crystal Clear Reflections: a Londoner Physicist in Yorkshire, 1947-51

The personal account below has been assembled and redrafted from many long and detailed letters from **D S Beard** (born 1922 and now less active) to **Derry W Jones**, following enquiries; I apologise for any remaining inaccuracies.

Wartime spectroscopy and naval X-radiography were the prelude to a London physicist aiding the development of X-ray crystal-structure analysis in a Yorkshire Chemistry Department around 1950.

AS a fresh physics graduate from Imperial College, I was engaged in 1942 in spectroscopic analysis of transition metals and then X-radiography of pressure hulls of submarines and aircraft carriers before a spell on emission spectroscopy of precious metals in Yorkshire. Since C P Snow opposed my continuation in the Scientific Civil Service, I wrote in 1947 to Prof E Gordon Cox (met when working for the Admiralty) about developing Geiger-Muller tubes for X-ray diffraction. Cox (later to run the Agricultural Research Council and be knighted), a physicist heading the Dept of Inorganic and Physical Chemistry at Leeds University, offered me an ICI Fellowship. The post was to devise and develop instruments to speed up X-ray analysis in determining accurate bond dimensions, then taking a year or more for one small structure. I familiarized myself with the procedure: collection of relative intensities on multiple-film X-ray photographs from small crystals, visual intensity estimations to yield relative structure amplitudes, trial-and-error solution attempts, and many laborious cycles of structure factor/Fourier syntheses calculations on mechanical hand machines.

Inspired by Cox, I co-ordinated a project for the design and manufacture of a versatile new Weissenberg moving-film X-ray goniometer (reflection indices were much more readily identified with a moving rather than fixed camera). Supported by ICI and the Royal Society's Paul Instrument Fund, and through the detailed work of a consultant engineer, **G J Sutton**, the Leeds equi-inclination Weissenberg camera was designed and a prototype built by Research Engineers Ltd in London. In operation, a crystal principal axis was aligned (by double-oscillation stationary photographs) along the instrument's rotation axis. The new instrument (1) could align its camera horizontally or vertically, the latter using a tripod to cope with the troublesome continuously evacuated Raymax X-ray unit. For recording intensity data, the camera carriage traversed synchronously with crystal rotation, eg 0.1 cm per 2 deg rotation, loaded with a pack of four half-plate X-ray films, often interleaved with metal foil (to extend the intensity range). Since exposure times of many hours



Leeds Weissenberg Camera. Image courtesy of the University of Dundee Museum.

were needed to record the weakest reflections, thousands of rotations and translations had to coincide so that mechanical requirements were demanding. The last batch of Leeds Weissenbergs was made in 1964 but instruments were in use in several UK laboratories into the 1970s, when commercial diffractometers were becoming available.

Further funding enabled us to design a Wiebenga (2) integrator accessory for the Weissenberg. The camera body underwent small additional lateral and rotational movements in 12 by 12 steps; a given X-ray reflection thus registered 144 spots close enough for overlap to yield a 1 mm by 1 mm square of uniform blackening. This intensity could then be measured by a microdensitometer more objectively than by eye estimation. The required movement was effected by ratchets and pawls driving cams and a lever. Bases were also devised so that a crystal on goniometer arcs (for mutually perpendicular angular orientations of the crystal) could be interchanged between fixed-film S25 and moving-film cameras (which did not apply to the 1930s Unicam instruments). Incidentally, few precautions were taken at this time over stray X-radiation.

A separate instrumental project aimed to reduce the labour of repeated structure factor/ electron-density-projection calculation sequences (with the Beevers-Lipson strips); digital hand calculation would be partly replaced by analogue devices (3). Post-war shortages encouraged the acquisition of ex-Service (including German) equipment. We experimented with summing voltages on a series of capacitors connected via electro-mechanical switches or uniselectors as used in telephone exchanges; the resulting voltages were read by quartz-fibre electrometers as in Stephens dosimeters. Success was limited by problems with stray capacitances and leakage and of acquiring a high-resistance voltmeter and capacitors of reproducible value; but bigger summations were soon to be tackled with punched-card Hollerith tabulators (initially at the Electricity Board). [Incidentally, a Hollerith Sorter is on display at the Science Museum Turing Exhibition.] Another instrumental project in 1950 was to construct, with Dr **G E Pringle**, a diffractometer based on a German (war reparations) Bertholt unit. One GM tube monitored the incident beam and another could be positioned at almost any inclination in the hemisphere above the centrally mounted crystal to measure the diffracted beam. We devised a 2:1 (crystal/detector) rhombus rotation device based on a divided circle from Cooke, Troughton and Sims at York. Twelve years later, I incorporated much of the design in a small portable diffractometer for teaching in schools X-ray properties, including detection by film and GM tube, radiography and diffraction.

The Yorkshire crystallography experience proved a valuable preparation, three jobs later, to setting up a company for small-scale commercial production of cloud chambers and other apparatus for demonstrating X-rays, radiation, etc to schools. I thank Prof **Derry W Jones** for his persistent encouragement to tell this story.

Dennis S Beard

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(1) D S Beard, E G Cox, and G J Sutton, J *Sci Instrum* **28**, 246-0251 (1951)

(2) E H Wiebenga and D W Smits, *Acta Cryst* **3**, 265 (1950)

(3) Instruments of this kind are shown in A D Booth, *Fourier Technique in X-ray Organic Structure Analysis* (Cambridge University Press, 1948)

Editor's note: the Beevers Lipson strips have been described in a recent Crystallography News.

A Crystallographic Might-Have-Been: June Broomhead

READERS of my previous articles about June Sutor will recall that she provided the first crystallographic description of C-H...O hydrogen bonding exactly 50 years ago but received precious little recognition. Just over a decade earlier, another June was making an important contribution to the crystallography of organic molecules, including their hydrogen bonding interactions.

The "From Atoms to Patterns" exhibition put on by the Wellcome Trust in 2008 documented the many manufactured products such as textiles, ceramics and furniture with designs based on crystallographic images that were on show at the Festival of Britain in 1951. **Helen Megaw**, described in *Frieze* magazine as "a leading crystallographer with a passion for pattern", made the original proposal and provided the crucial links between crystallographers and industrial designers. Alongside the famous names who supplied images there was...**June Broomhead**.

At this time June M Broomhead [not to be confused with J A Broomhead when searching the Cambridge Structural Database (CSD)] was a very promising research student at Cambridge who began her PhD research in 1948. The structures that she solved included adenine hydrochloride hemihydrate and guanine hydrochloride monohydrate. In the CSD their values for R factor and (C-C) look unimpressive. However, in 1946 the Edinburgh-educated Scot **William Cochran** had joined the Cambridge group as Research Assistant to Lawrence Bragg. His idea to use ($F_o - F_c$) Fourier syntheses improved the clarity of the maps sufficiently to give some clues about the location of hydrogen atoms. In turn these data provided an important structural foundation for the model of DNA proposed by **James D Watson** and **Francis Crick**. Indeed, Watson was so impressed by the hydrogen-bonded base pair dimers of adenine found in Broomhead's structure that he initially and erroneously postulated their existence in DNA as well. By studying hexa-aqua-magnesium bis(benzenesulfonate) and hexa-aqua-zinc bis(benzenesulfonate) June Broomhead also obtained information about the interaction of water with metal ions and anions. On 20 August, 1951, she married the Canadian nuclear physicist **George Lindsey**. For a while the new Mrs June Broomhead Lindsey carried out research with **Dorothy Hodgkin** on the structure of vitamin B12. Working on "air-dried" B12, she did not achieve as much success as colleagues working on "wet" B12; but comparison of the unit cell dimensions was instructive, and J Lindsey appears as a co-author on a 1954 *Nature* paper. Late in 1951 she moved to Canada to be with her husband. As well as achieving a distinguished career with the Canadian Department of National Defence, he became known as the Darwin of the Diamond for his compilation of baseball statistics and showed enough skill as a sculptor to create a statue of the dragon slaying St George! Meanwhile, June curtailed her career to be a full-time mother of two children, both of whom became distinguished academics. One wonders what great further achievements she might have accomplished if she had lived at a more favourable time for career women.

Carl Schwalbe

Invitation to ECM28

Dear Colleagues

THE 28th European Crystallographic Meeting will be held in Warwick during August 2013, organized by our British crystallographer colleagues.

We would like to welcome and invite to Warwick all crystallographers and scientists with interests in crystallography and crystal growth to share with us their scientific views and new achievements. It will also provide an excellent opportunity to strengthen the links with the IUCr and the regional associates AsCA and ACA.

The Program Committee is organizing a diverse scientific program of microsymposia and keynote lectures in five focus areas to illustrate the growth in science of the ECA Special Interest Groups and the additional networking activity of the General Interest Groups. At ECM28 we will celebrate the centenary of the first crystal structure determinations, and have the opportunity to view at first hand some of the original equipment used by the Bragg father and son, William Henry and William Lawrence. The award ceremony of the 7th Max Perutz Prize of the European Crystallographic Association will also take place during ECM28.

Another important component of the meeting is the ECA Council, where the councillors from 33 national members get together with the three individual members' representatives and the corporate associate members' representative to review the work of the Association.

Everything is in place for a successful 28th European Crystallographic Meeting, and I hope that you will accept this invitation from the ECA and our British crystallographer colleagues. I also look forward to welcoming you in person at Warwick.

Andreas Roodt
President
European Crystallographic Association

IT is a pleasure to invite you to join us for the 28th Meeting of the European Crystallographic Association at Warwick University 25-29 August 2013. Warwick is a great location for the meeting, with good quality on-site accommodation, easy transport links from Europe and, in the Warwick Arts Centre, an excellent conference venue. We are in the process of finalising a wide-ranging scientific programme and hope to also have exhibits and activities to celebrate our crystallographic heritage, 2013 being one hundred years since the pioneering work of William and Lawrence Bragg.

We encourage you to come to what we are confident will be an exciting meeting and all of us in the British Crystallographic Association look forward to welcoming you to Warwick next August.

Prof **Sandy Blake** (Chair) and
Prof **Elspeth Garman** (co-Chair)
ECM28 Organising Committee

Prof **David Keen**
President of the British Crystallographic Association

OLEX2 Satellite Meeting

OLEX2 has become established in the community of small-molecule crystallographers as an easy-to-use unified package that provides tools needed for day-to-day analyses of small molecule structures.

This workshop will introduce a number of advanced structure refinement features available in OLEX2 to a wide audience.

We will introduce a typical OLEX2 workflow followed by several in-depth examples of how non-routine structures may be refined. Particular attention will be paid to refinement of disordered structures and what advantages OLEX2 offers in handling them.

The day will consist of structured 'instruction' sessions, interspersed by plenty of 'hands-on' sessions, where you can apply these procedures and new skills to your own structures.

The number of places is limited to 50 participants, and the provisional cost will be 80 euros for this full-day workshop.

European Young Crystallographers Satellite Meeting

THE European Young Crystallographers Satellite Meeting will take place at ECM28, Warwick, UK on Sunday 25 August 2013. This satellite meeting will be the first of its kind at a European level and will run from 9.00 am to 5.00 pm, with three sessions dedicated to young crystallographers (anyone under the age of 35) presenting their work.

This meeting is organised by the European Young Crystallographers' General Interest Group and the Young Crystallographers' Group of the British Crystallographic Association, in order to promote interaction between up-and-coming and more established crystallographers. We feel that this satellite meeting is an extremely valuable event for young researchers and believe that it will help create a network for young crystallographers, enabling them to communicate their research in an informal environment and to establish connections with other young crystallographers. Given the significance of 2013 to many crystallographers around the world with the Bragg centenary, we want to ensure that we celebrate the contributions of younger members and to continue promoting the fantastic work of these up-and-coming scientists.

Further details will be published on this website. Everyone is very welcome to attend this meeting, and we look forward to welcoming you to Warwick!

Introduction to Software Development for Crystallographers Satellite Meeting

ECACOMSIG, the European Crystallographic Association's Computing Special Interest Group, is organising a two day Computing School on 23 – 24 August 2013, immediately before the European Crystallographic Meeting (ECM28) at Warwick University.

The School will provide an introduction to software development for crystallography students and post-docs – especially those who are not currently involved with software development (or at an early stage of this). We will not be teaching the basics of programming, so students will need to be familiar with at least one programming or scripting language in current use. These include both modern languages (e.g. Python, C++, Java) or older languages, such as Fortran, C, Perl or Tcl.

The School will be held over two full days, starting in the morning of 23 August 2013, so students and teachers should plan to arrive on the evening of Thursday 22 August.

The School will be open to a maximum of 30 applicants. A limited number of bursaries will be available to assist with the cost of attendance. For more information on bursaries, please contact **Harry Powell**.

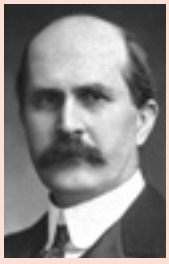
The registration fee (including dinner on 22 and 23 August, and lunch and refreshments on 23 and 24 August) is currently planned to be €125.

Registration (including accommodation bookings) will be via the ECM28 website.

Further details will be posted on the ECACOMSIG website as they become available.

We look forward to seeing you in Warwick!

"The Two Braggs" Exhibition



William Henry Bragg

William Lawrence Bragg

APPROXIMATELY 100 years ago in Germany Max Theodor Felix von Laue (1879-1960), Paul Karl Moritz Knipping (1883-1935) and Walter Friedrich (1883–1968) showed that X-rays could be diffracted by crystals. Laue was subsequently awarded the Nobel Prize in Physics in 1914. Following this discovery, the unique partnership, father and son, William Henry Bragg (1862-1942) and William Lawrence Bragg (1890-1971) in England, successfully showed how x-ray diffraction could lend itself to the solution of crystal structures, for which they shared the Nobel Prize in Physics in 1915. A major exhibition is planned to coincide with the ECM28 at the University of Warwick to celebrate their lives: for the first time it will be possible to view historic equipment, notebooks, honours, letters, films and artwork. The exhibition will be open to all participants and to the public at large.

The registration form for ECM28 will be released at the end of November. As more information about the main meeting and other satellite meetings becomes available, it will be posted at http://ecm28.ecanews.org/ .

Professor Dame Louise Napier Johnson FRS, DBE

26/9/40 – 25/9/12

LOUISE Johnson, biophysicist and structural biologist, died on 25/9/12 after a 13-month illness which she bore with quiet fortitude and grace. Her life and work impacted very many people worldwide, due both to her scientific activities in protein crystallography and enzymology, and her tireless interest and effort in supporting and encouraging scientists in developing countries to establish effective research laboratories as far apart as South America, the Middle East and Pakistan.

I am one of those whose life course was changed by a chance conversation with Louise, who I first met in 1987 when I was tutoring physics at Somerville College where Louise was then a Fellow. Over lunch she asked me what I was going to do when my fixed term contract at Somerville expired and since there was still a whole year to go, I threw away the comment 'Oh, I don't know, I will probably have to change fields since nuclear physics (my then research area) is no longer being funded in Oxford.' She visibly brightened and said 'We are looking for someone with just your skills at the moment to look after our new cutting edge X-ray equipment for protein crystallography which is about to arrive.' As a result of my rash statement and Louise's quiet persuasiveness, I visited her the very next day at the Laboratory of Molecular Biophysics (LMB) where she and her research group were then working on the mechanism of action of glycogen phosphorylase, a large protein (842 amino acids) present in muscle which turns inert glycogen into the sugar needed to power physical activity. They had succeeded in obtaining a structure (1,2) and showed how the enzyme was regulated by reversible phosphorylation and allosteric effects. Her group were in the vanguard of those using synchrotron radiation at Daresbury Laboratory near Runcorn for macromolecular crystallography in the early 1980s (3). Louise's lifelong interest in applying new techniques to structural biology questions came to the fore much later when she became Life Sciences Director of Diamond Light Source in 2003. There she oversaw the building and development of this highly effective national facility which is now bearing great fruit for the UK physical and biological sciences research community.

As a result of my visit to LMB that day I went to work there a few months later, and when Louise was appointed to the **David Phillips** Chair in Molecular Biophysics in 1990, worked under her until her retirement in 2007. Her management style was 'hands off' but 'attention on' in that she was always there if advice or guidance was needed, but did not offer it unless it was requested. She encouraged a highly cooperative working environment among the different groups and PIs in LMB which was extremely productive. Since synchrotron data collection time was allocated in aliquots of 24 or 48 hours and was much more efficient as a team effort, we regularly had the opportunity to work together closely with colleagues, thus developing a highly effective research effort. Although Louise did not normally accompany us on these trips to the synchrotron, during one of her sabbatical terms, she asked to be brought up to speed in using the current X-ray equipment and software for crystallography. She determinedly and methodically worked her way through our usual training programme for new researchers, asking penetrating and pertinent questions at every stage. This was a great example to us of how a senior scientist should keep in touch with what the daily research really involved, so that challenges faced by students and postdocs could then be better appreciated and overcome.

Her book written with **Tom Blundell** and published in 1976 (4), although now a collector's item judging by the price of a second hand one on Amazon, is a classic text in the field worthy of attention today: I still regularly consult my well thumbed copy. Louise, with **Wolfgang Baumeister**, **Alasdair C Steven** and **Richard Perham**, had just completed work on a book entitled 'Molecular Biology of Machines and Assemblies' before she became ill, and it will be published in 2013.

Louise was very modest and unassuming about her many achievements and honours, and this quality was brought home to me forcefully on one occasion in June 2010 when she very kindly offered to substitute in giving a conference lecture for me. At the time my husband was critically ill and I was unable to go and deliver it. We were trying to work out over the phone if she could give it on a Tuesday afternoon, and she mentioned she had to go to Cambridge on Sunday evening and for the whole of Monday and then to London on Tuesday morning, but that she might be free later in the afternoon. I assumed that the Cambridge trip was to visit her twin granddaughters, and asked after them, upon which she hesitantly told me that actually she was going to collect an honorary ScD degree from Cambridge. After some more convoluted discussion, it gradually transpired that the

London engagement was at Buckingham Palace at a garden party given by the Queen, and that getting to Cardiff in time to give the conference lecture was unfortunately just not going to be possible. I was left wondering what her Wednesday commitments might be! Her schedules were punishing, and her energy amazing.

When Louise's death was announced, I received many e-mails from ex-LMB members expressing their appreciation for Louise's role in their lives, and retrospective realisation of the positive atmosphere she nurtured: eg 'After working in other places, only now do I realise what a special place it was under her leadership.', ' A great lady', and 'Such a big presence within the field'.

Thus because of Louise I am a protein crystallographer and no longer a nuclear physicist. She had an enormous and lasting influence on my life, as she also had on the lives of many others. Along with her numerous colleagues throughout the world, I will miss her inspiration both scientifically and personally. I feel privileged indeed to have known her and worked with her.

Elspeth Garman

Louise with Robin Owen after his DPhil viva

Career:

1962: University College, London. Graduated with BSc (Hons) Physics.

1965: The Royal Institution, London. PhD supervised by David Phillips, University of London.

1966: Department of Biophysics, Yale University. Post-doctoral research assistant in Prof F M Richards Laboratory.

Departmental Demonstrator in the Zoology Department, University of Oxford.

University Lecturer in Molecular Biophysics, University of Oxford.

1973-1990: Fellow and Janet Vaughan Lecturer, Somerville College, Oxford.

1990-2007: David Phillips Professor in Molecular Biophysics, University of Oxford.

1990-2007: Professorial Fellow, Corpus Christi College, Oxford.

2008-2012: Emeritus Fellow Corpus Christi College, Oxford.

1991-2012: Honorary Fellow, Somerville College Oxford.

2003-2008: Director Life Sciences, Diamond Light Source.

2008-2011: Diamond Fellow.

Major Honours:

1990 Elected a Fellow of the Royal Society

1992 Honorary DSc University of St Andrews

2004 Hon DSc University of Bath

2000 Associate Fellow Third World Academy of Science

2002 Dame of the British Empire

2004 Hon DSc University of Bath

2009 Hon DSc Imperial College London

2010 Hon ScD University of Cambridge

2011 Foreign Associate of the US National Academy of Sciences.

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(3) J Hajdu, K R Acharya, D I Stuart, P J McLaughlin, D Barford, N G Oikonomakos, H Klein, and L N Johnson. EMBO J. 1987 February; 6(2): 539–546. PMCID: PMC553427Catalysis in the crystal: synchrotron radiation studies with glycogen phosphorylase b.

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Dr Philip R Lowe

1948-2012

WHEN I joined the Department of Pharmacy at Aston University in 1972 as a brand-new Lecturer, I was offered assistance from a technician who, though junior in status, had already established a reputation for skill and the fearlessness necessary to tackle an arcane subject like X-ray crystallography. That man was Phil Lowe. During the years that followed, Phil became indispensable to my research. Our first X-ray generator was scrounged from another department, and Phil quickly developed an understanding of what the temperamental beast required in order to keep it running happily. This was also the period when the culture was changing from "Wild West" to "'Elf and Safety". Phil devised the modifications to equipment and operating procedures that brought us into compliance with regulations that seemed burdensome then and seem sensible now.

Though busy with a full-time job and family life, Phil had the determination to gain an impressive set of academic credentials. Phil began by earning his first degree through the Open University, an experience which left him with a keen appreciation of the Open University. He became a tutor there for many years. Phil's next step was to obtain the MSc in Physics at Aston. With his understanding of the underlying physics allied to his skill with apparatus, I was delighted that he then chose to do PhD research under my supervision. When the Big One came up, requiring a high-quality structure determination, of course I asked Phil to work on it. This was temozolomide, Aston's own blockbuster drug. Discovered in the research group of **Malcolm Stevens**, it became the drug of choice for the treatment of glioma and achieved annual sales in excess of $1 billion. Phil duly delivered the goods, obtaining an R factor of 4.2% with data from our CAD4 diffractometer. Comparison of this structure with those of related molecules, also studied by Phil, demonstrated the existence of rotamers which had to be taken into account in any attempt to relate structure to activity.

Of course, many BCA members will remember Phil through the Intensive Courses in X-ray Structure Analysis, which ran at Aston for a decade before transferring to Durham. When **David Watkin** came up with the original idea, he found that Oxford colleges would charge so much that the course would become prohibitively expensive. Seeking a location that would be both central and cheap, David discussed the matter with Phil and me. Because of Phil's cheerful and outgoing nature, he had a circle of friends at Aston that extended well beyond the scientific departments. In particular, he was able to call in favours from friends in Residences and Catering, who offered the course very attractive prices that came within David's available budget. Even if the financial rewards to Aston were meagre, the intangible rewards were great, putting Aston on the map in the subject of crystallography which was to gain so many Nobel Prizes. Phil and I assisted David as Local Organisers. While we both helped out with academic matters, it was Phil who worked tirelessly on everything else. He would be there first thing in the morning to solve any problems with photocopying or projectors, and he often would be found in the evening cheerfully pulling pints for participants.

Phil is survived by his widow Jean and his sons Adrian and Scott. He will be much missed by his many friends and colleagues.

Carl Schwalbe

Meetings of interest

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

2-5 December 2012
AsCA 12/CRYSTAL 28, Adelaide, Australia.
http://www.sapmea.asn.au/conventions/crystal2012/index.html

6 December 2012
Bragg Symposium: Celebrating 100 years of Crystallography, Adelaide, Australia.
http://www.sapmea.asn.au/conventions/crystal2012/bragg.html

10-12 December 2012
Seeding and Self-Seeding at New FEL Sources (SSSFEL12), Trieste, Italy.
http://www.elettra.trieste.it/SSSFEL12/

11 December 2012
Biological Structures Group Winter Meeting, MRC Cambridge.
http://bsg.crystallography.org.uk/

11-12 December 2012
International Workshop – Advances in Neutron Triple-Axis Spectroscopy, Berlin, Germany.
http://www.helmholtz-berlin.de/events/tas/index_de.html

6-11 January 2013
Carotenoids – Gordon Research Conference, Ventura, CA, USA.
http://www.grc.org/programs.aspx?year=2013&program=carot

8-11 January 2013
International Conference on Biomolecular Forms and Functions: A Celebration of 50 Years of the Ramachandran Map, Bangalore, India.
http://icbff2013.com/

13-18 January 2013
5th MaNEP Winter School – Understanding Electronic and Magnetic Correlations, Saas-Fee, Switzerland.
http://www.manep.ch/en/events/saasfee13/

14-17 January 2013
International Symposium on Neutron Scattering, Mumbai, India.
http://www.barc.gov.in/symposium/isns2013/

20-25 January 2013
Metals in Biology – Gordon Research Conference, Ventura, CA, USA.
http://www.grc.org/programs.aspx?year=2013&program=metalsbio

21-22 January 2013
Synchrotron Radiation for Electrochemical Energy Storage (SYREES-2013), Gif-sur-Yvette, France.
http://www.synchrotron-soleil.fr/Soleil/ToutesActualites/Workshops/2013/SYREES-2013/Welcome

21-25 January 2013
7th International Symposium on Hydrogen and Energy, Stoos, Switzerland.
http://www.empa.ch/plugin/template/empa/22/123773/---/l=2

22-24 January 2013
Nagoya Symposium: Frontiers in Structural Physiology, Nagoya, Japan.
http://symposium.cespi.nagoya-u.ac.jp/

23-24 January 2013
8th SOLEIL Users' Meeting, Gif-sur-Yvette, France.
http://www.synchrotron-soleil.fr/Workshops/2013/SUM2013

23-25 January 2013
Flipper 2013: International Workshop on Single-Crystal Diffraction with Polarised Neutrons, Grenoble, France.
http://www.ill.eu/news-events/events/flipper-2013

24-27 January 2013
Bioinorganic Chemistry – Gordon Research Seminar, Ventura, CA, USA.
http://www.grc.org/programs.aspx?year=2013&program=grs_bioin

25 January 2013
DESY Photon Science Users' Meeting – Research With Synchrotron Radiation and FELs Hamburg Germany.
http://hasylab.desy.de/news__events/users%27_meeting/index_eng.html

3-8 February 2013
Nanomaterials for Applications in Energy Technology, Ventura, CA, USA.
http://www.grc.org/programs.aspx?year=2013&program=nanomat

10-15 February 2013
Fibronectin, Integrins & Related Molecules – Gordon Research Conference, Ventura, CA, USA.
http://www.grc.org/programs.aspx?year=2013&program=fibronec

14-18 February 2013
AAAS Annual Meeting – The Beauty and Benefits of Science, Boston, MA, USA.
http://www.aaas.org/meetings/2013/

25-26 February 2013
Annual International Conference on Chemistry, Chemical Engineering and Chemical Process (CCECP 2013), Hotel Fort Canning, Singapore.
http://chemistry-conf.org/

3-8 March 2013
Glycobiology – Gordon Research Conference, Ventura, CA, USA.
http://www.grc.org/programs.aspx?year=2013&program=glycobio

5-14 March 2013
ISIS Practical Neutron Training Course, March 2013, ISIS, Abingdon.
http://www.isis.stfc.ac.uk/learning/neutron-training-course/

19-22 March 2013
21st Annual Meeting of the German Crystallographic Society, Freiberg, Germany.
http://www.conventus.de/dgk2013/

1-5 April 2013
2013 MRS Spring Meeting and Exhibit, San Francisco, CA, USA.
http://mrs.org/spring2013/

6-14 April 2013
14th BCA/CCG Intensive Teaching School in X-Ray Structure Analysis, Durham.
http://www.dur.ac.uk/durham.x-ray-school/

7-12 April 2013
2nd International School on Aperiodic Crystals, Bayreuth, Germany.
http://old.crystal.uni-bayreuth.de/aperiodic_crys_school_2013/

14-19 April 2013
4th Annual Accelerator Reliability Workshop, Clayton, VIC, Australia.
http://www.synchrotron.org.au/index.php/news/events/australian-events/arw-2013

20-21 April 2013
TOPAS Users Meeting, Gaithersburg, MD, USA.
http://www.bruker.com/?&tx_ttnews[tt_news]=311&cHash=fd79a9509e33f955a414a209b333457c

22-25 April 2013
APD-IV: Accuracy in Powder Diffraction Meeting, Gaithersburg, MD, USA.
http://www.iucr.org/news/notices/meetings/www.nist.gov/mml/apdiv_conference_2013.cfm

4-5 May 2013
Chemistry of Supramolecules & Assemblies – Gordon Research Seminar, Les Diablerets, Switzerland.
http://www.grc.org/programs.aspx?year=2013&program=grs_supra

5-10 May 2013
Chemistry of Supramolecules & Assemblies – Gordon Research Conference, Les Diablerets, Switzerland.
http://www.grc.org/programs.aspx?year=2013&program=supramol

5-10 May 2013
5th International Conference on Recrystallization and Grain Growth, Sydney, Australia.
http://www.rex-gg2013.org/

17-22 May 2013
EMBO Conference – The Biology of Molecular Chaperones: From Molecules, Organelles and Cells to Misfolding Diseases, Santa Margherita di Pula, Italy.
http://events.embo.org/13-chaperone/index.html

27-31 May 2013
E-MRS 2013 Spring Meeting, Strasbourg, France.
http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=569&Itemid=1583

30 May - 8 June 2013
Crystallographic Course: The Future of Dynamic Structural Science, Erice, Italy.
http://www.crystalerice.org/Erice2013/2013.htm

2-7 June 2013
Electron Distribution and Chemical Bonding – Gordon Research Conference, Les Diablerets, Switzerland.
http://www.grc.org/programs.aspx?year=2013&program=elecdist

9-14 June 2013
Polymers – Gordon Research Conference, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2013&program=polymers

9-22 June 2013
The Zürich School of Crystallography 2013, Zürich, Switzerland.
http://www.oci.uzh.ch/group.pages/linden/zsc/Location.html

16-21 June 2013
Liquid Crystals – Gordon Research Conference, Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2013&program=liqucryst

30 June - 5 July 2013
Nucleosides, Nucleotides & Oligonucleotides – Gordon Research Conference, Newport, RI, USA.
http://www.grc.org/programs.aspx?year=2013&program=nucleo

2-5 July 2013
International Workshop on Neutron Optics and Detectors (NOP&D-2013), Munich, Germany.
http://www.iucr.org/news/notices/meetings/meeting_2012_299

6-7 July 2013
Thin Film & Crystal Growth Mechanisms – Gordon Research Seminar, Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2013&program=grs_thin

7-12 July 2013
Thin Film & Crystal Growth Mechanisms – Gordon Research Conference, Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2013&program=thinfilm

8-12 July 2013
International Conference on Neutron Scattering, Edinburgh.
http://www.icns2013.org/home

13-17 July 2013
9th European Biophysics Congress, Lisbon, Portugal.
http://www.ebsa2013.org/

14-19 July 2013
Enzymes, Coenzymes & Metabolic Pathways – Gordon Research Conference, Waterville Valley, NH, USA.
http://www.grc.org/programs.aspx?year=2013&program=enzymes

20-24 July 2013
2013 American Crystallographic Association Meeting, Honolulu, HI, USA.
http://www.amercrystalassn.org/2013-meeting-homepage

4-10 August 2013
ISSCG-15. 15th Summer School on Crystal Growth, Gdansk, Poland.
http://science24.com/event/isscg15/

11-16 August 2013
ICCGE-17. 17th International Conference on Crystal Growth and Epitaxy, Warsaw, Poland.
http://science24.com/event/iccge17/

25-29 August 2013
28th European Crystallographic Meeting, University of Warwick.
http://ecm28.org/

1-6 September 2013
12th International Conference on Quasicrystals, Kraków, Poland.
http://www.icq12.fis.agh.edu.pl/

8-11 September 2013
11th International Conference on Biology and Synchrotron Radiation (BSR), Hamburg, Germany.
http://www.nature.com/natureevents/science/events/17286-

8-13 September 2013
11th European Conference on Accelerators in Applied Research and Technology, Namur, Belgium.
http://www.ecaart-11.be/

30 September - 5 October 2013
8th International Workshop on Bulk Nitride Semiconductors, Seeon, Germany.
http://www.iwbns2013.iisb.fraunhofer.de/index.html

30 September - 5 October 2013
International School on Fundamental Crystallography: Introduction to International Tables for Crystallography, Vol.A: Space-Group Symmetry and Vol. A1: Symmetry Relations Between Space Groups, Guletchitza, Bulgaria.
http://www.bgcryst.com/index.php?option=com_content&id=62

1-6 December 2013
2013 MRS Fall Meeting and Exhibit, Boston,, MA, USA.
http://www.bgcryst.com/index.php?option=com_content&id=62

2-6 December 2013
Thermec 2013: Neutron Scattering & X-Ray Studies for the Advancement of Materials, Las Vegas, NV, USA.
http://www.thermec.org/template3s/

5-12 August 2014
IUCr2014. 23rd Congress and General Assembly, Montreal, Quebec, Canada.
http://www.iucr2014.org/

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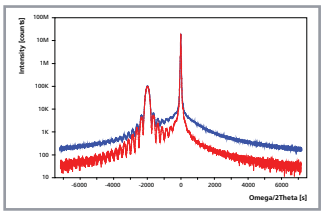

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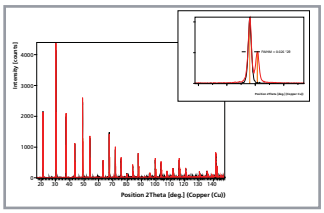

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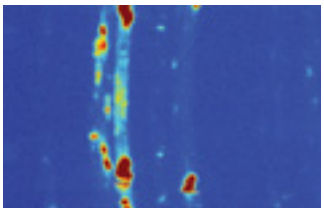
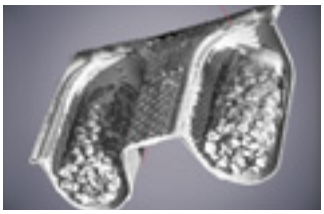


3D



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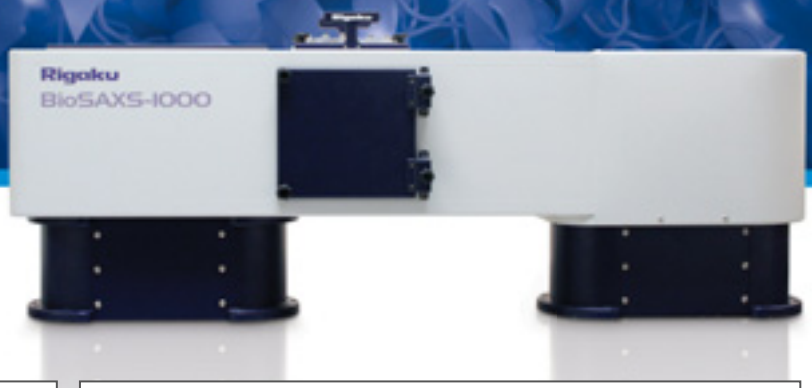
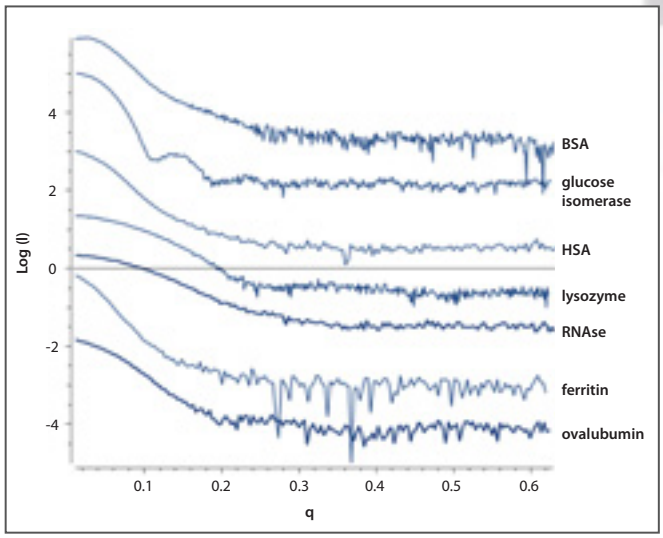
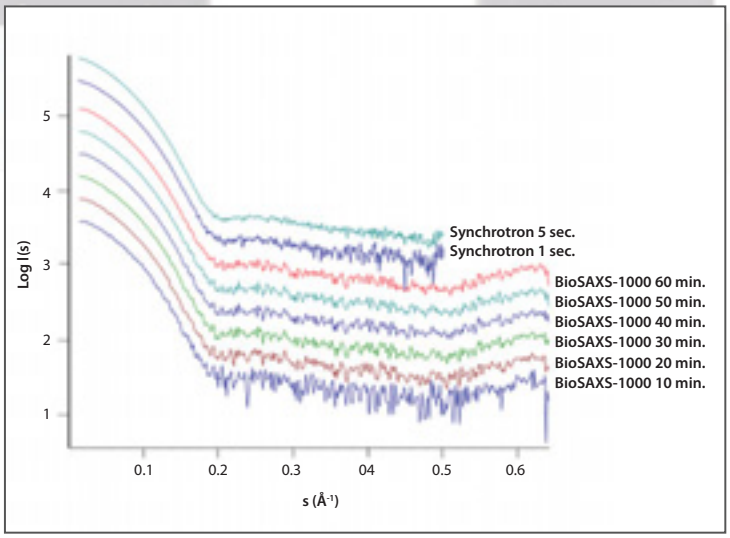




Actual scattering data for protein standards (data are scaled for display purposes)
Exposure time for each – 30 minutes



Comparison data: Synchrotron data (top 2 scans) and BioSAXS-1000 (bottom 6 scans)
Data are scaled for optimal display. Synchrotron data courtesy of T. Grant, J. Luft and E. Snell (HWI)

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