Crystallography News

British Crystallographic Association

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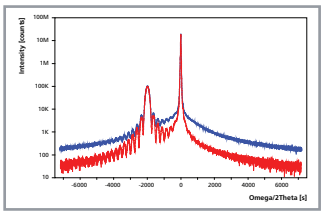

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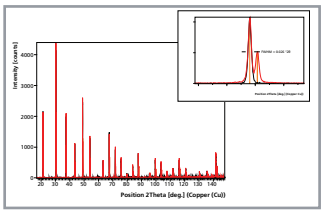

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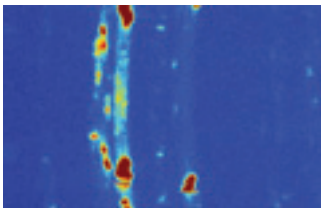

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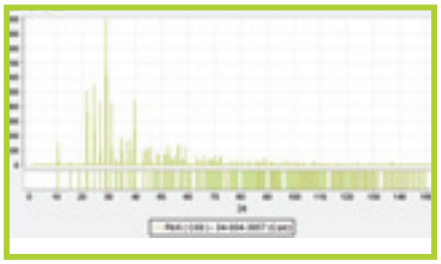

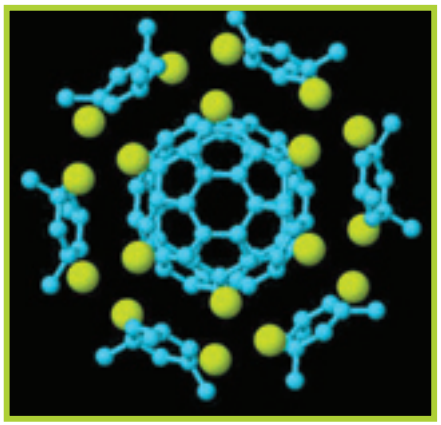

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Contents

BCA Administrative Office,
Helen Leese
First Floor
Hornbeam House
Hornbeam Business Park
Harrogate HG2 8QT
Tel: +44 (0)1423 855 990
Fax: +44 (0)1423 855 999
e-mail: bca@hg3.co.uk

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Carl Schwalbe
15 St. Augustine Dr.,
Droitwich,
Worcs WR9 8QR
Tel: 01905 775257
e-mail: carlschwalbe@hotmail.com

Printed by Bowmans
Westland Square, Westland Road, Leeds, LS11 5SS
Tel: 0113 272 0088
Web: www.bowmans77.co.uk

This month's cover:

Photos of the Shard (B J Mullan) and tourmaline (C Ralph)

From the Editor

I hope that most readers will have noticed no significant change in "look and feel" between the June issue and earlier issues of *Crystallography News*. However, those of you with the keenest eyes will have seen something new at the bottom of the left-hand column of page 1: "Printed by Bowmans". For many years we have had a happy and productive relationship with William Anderson Printers of Glasgow. Their designers (and for most issues that meant Ross Mushet) received individual articles and pictures from the editor and jigsaw-puzzled them into an efficient and artistic combination. I have received a number of compliments about the appearance and content of *CN* from the editors of other crystallographic societies' news magazines. However, the relationship between our agents and our printers is very important: our agents work directly with the printers on the encouragement, production and billing of advertising material and the implementation of mailing lists. When HG3 Conferences submitted the winning tender and became the BCA's new agents, their proposal included printing by their usual associates, Bowman Studio. The June issue was the first one produced by Bowmans. I am most grateful to Tony Hopps, their designer, for the very efficient way he handled the transition and his talent for absorbing the *"spirit of CN"*. Tony even spotted and corrected an occurrence of "densiy" where I missed it in an article that I wrote and I missed again when proofreading. The lesson that I draw from these very positive experiences with both printers is that we are living in a new Golden Age of British printing. The first Golden Age was started by William Caxton in 1476 when he set up a printing press in Westminster. Sometimes showing more zeal than accuracy, he defined early standards for English spelling and translated many foreign-language works into English for the benefit of British readers. His associate and successor, the wonderfully named Wynkyn de Worde, innovated the wide application of high-tech woodcut printing to illustrate his books. I hope that some of that zeal and that love of illustration, but not the dubious accuracy, show through in *CN* today.

The efforts by the crystallographic community to persuade the United Nations to declare an International Year of Crystallography have achieved success at last, with 2014 as the designated year. The UN General Assembly resolution is reproduced in this issue. The main reason is for us to revel in the compliments paid to crystallography and crystallographers. A second reason is to note that the language can be turgid at times. If you have been thinking of abandoning crystallography in order to join the diplomatic service, you may not want to hang up your radiation monitoring badge just yet.

The declaration of an International Year is particularly appropriate because of the high degree of international cooperation in crystallography. When the earthquake and tsunami of March 11, 2011 inflicted a terrible tragedy on Japan, crystallographers worldwide quickly offered practical help as well as sympathy. While displaced Japanese researchers were accommodated at a variety of international installations, the resourceful Japanese engineers repaired their facilities with remarkable speed. Even though the Photon Factory, located about 60 km north of Tokyo, was a good distance from the epicentre, it still was heavily shaken. A small diffractometer toppled from its pedestal, a larger one derailed from its positioning rail, vacuum bellows broke and some floor levels were displaced. Working long hours even through the Golden Week national holiday, crews were able to commence test operation on June 6 and provide user service on July 27. At J-PARC, whose location on the coast south of Sendai was much closer to the epicentre, it took until December to repair the very severe damage, particularly to ancillary structures which suffered distortion and flooding. On December 9 the Linac was switched on once again, and the Materials and Life Science Experimental Facility produced neutrons on the 22nd. Important results followed swiftly. This year a research team including collaborators at Cambridge collected neutron data at J-PARC and X-ray data at Spring-8 that enabled the structures of the mono-, di- and trihydrides of lanthanum to be determined, a series of interest for hydrogen storage.

The wet and gloomy summer in England has been enlivened by the completion of the Shard in London, which has become the tallest building in the European Union. The cover of this issue features a photograph of the Shard by **B. J. Mullan**. To my eye the tapered profile and multi-faceted sides bear a certain resemblance to a photograph of a tourmaline crystal by **C. Ralph**, which also is featured on the cover. Is this another example of crystallography preceding art?

Carl Schwalbe

BCA Council 2012

COUNCIL MEMBERS

President (2015)
Prof David Keen
ISIS Facility, Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Didcot Oxfordshire, OX11 0QX
Tel: 01235 446556
david.keen@stfc.ac.uk

Vice President (2013)
Dr David R. Allan
Diamond Light Source Diamond House, Chilton Oxfordshire, OX11 0DE
Tel: 01235 778644
david.allan@diamond.ac.uk

Secretary (2013)
Dr Georgina Rosair
School of EPS - Chemistry Perkin Building, Heriot-Watt University, Edinburgh, EH14 4AS
Tel: 0131 451 8036/4241
g.m.rosair@hw.ac.uk

Treasurer (2014)
Dr Andrea Mulholland
4 Rosling Road, Horfield, Bristol, BS7 8SX
Tel: 0117 951 4253

ORDINARY MEMBERS

Prof Simon Parsons (2015)
Room 90, King's Buildings, University of Edinburgh, West Mains Road, Edinburgh, EH9 3JJ
Tel: 0131 650 5804
s.parsons@ed.ac.uk

Dr Arwen Pearson (2013)
Astbury Centre for Structural Molecular Biology, Institute for Molecular and Cellular Biology, Astbury Building, Leeds, LS2 9JT
Tel: 0113 343 3032
a.r.pearson@leeds.ac.uk

Dr Amber L Thompson (2014)
Chemical Crystallography Service Manager, Department of Chemistry, University of Oxford, 12 Mansfield Road, Oxford, OX1 3TA
Tel: 01865 285018
amber.thompson@chem.ox.ac.uk

GROUP REPRESENTATIVES

Biological Structures
Dr John McGeehan
Biophysics Laboratories, School of Biological Sciences, University of Portsmouth, Portsmouth, PO1 2DY
Tel: 02392 842042
john.mcgeehan@port.ac.uk

Chemical Crystallography
Dr Peter Wood
Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ.
Tel: 01223 336408
wood@ccdc.cam.ac.uk

Industrial
Dr Elizabeth Shotton
Diamond Light Source Diamond House, Didcot Oxfordshire, OX11 0DE
Tel: 01235-778797
elizabeth.shotton@diamond.ac.uk

Physical Crystallography
Dr Kirsten Christensen
Inorganic Chemistry Laboratory, University of Oxford, Oxford, OX1 3TA
Tel: 01865 285023
kirsten.christensen@chem.ox.ac.uk

Young Crystallographers
Dr Anna Warren
Postdoctoral Research Associate, Diamond Light Source, Didcot, Oxfordshire, OX11 0DE
Tel: 01235 777455
anna.warren@diamond.ac.uk

CO-OPTED MEMBERS

Dr Alexandra Griffin (2015)
Oxford Diffraction Ltd., 10 Mead Road, Oxford Industrial Park, Yarnton, Oxfordshire, OX5 1QU
alex.griffin@oxford-diffraction.com

Prof Elspeth F. Garman (2013)
Department of Biochemistry, South Parks Road, Oxford, OX1 3QU
elspeth.garman@ bioch.ox.ac.uk

EX-OFFICIO MEMBERS

Education Coordinator
Dr Ross Harrington
School of Chemistry Newcastle University Newcastle upon Tyne, NE1 7RU
Tel: 0191 222 6641
ross.harrington@ncl.ac.uk

Editor "Crystallography News"
Prof Carl H. Schwalbe
15 St. Augustine Drive, Droitwich, Worcs, WR9 8QR
Tel: 01905 775257
carlschwalbe@hotmail.com

Webmaster
Dr Richard Cooper
Department of Chemistry, University of Oxford, 12 Mansfield Road, Oxford, OX1 3TA
Tel: 07525 687431
richard.cooper@chem.ox.ac.uk

GROUP CHAIRMEN

Biological Structures Group
Prof Vilmos Fulop
School of Life Sciences, University of Warwick, Coventry, CV4 7AL
Tel: 024 7657 2628
vilmos@globin.bio.warwick.ac.uk

Chemical Crystallography Group
Dr Hazel A. Sparkes
Department of Chemistry, University of Durham, University Science Laboratories, South Road, Durham, DH1 3LE
Tel: 0191 334 2004
h.a.sparkes@durham.ac.uk

Industrial Group
Judith Shackleton
Senior Technologist-Building Products R&D NSG Pilkington, European Technical Centre, Hall Lane, Lathom, Ormskirk, Lancashire, L40 5UF
Tel: 01695 54595

Physical Crystallography Group
Dr Ivana Radosavljevic Evans
Department of Chemistry, Durham University, Durham, DH1 3LE, UK
Tel: 0191 334 2594
ivana.radosavljevic@durham.ac.uk

Young Crystallographers
Dr Anna Warren
Postdoctoral Research Associate, Diamond Light Source, Didcot, Oxfordshire, OX11 0DE
Tel: 01235 777455
anna.warren@diamond.ac.uk

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

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

From the President

FIRST I must confess that I am sitting at the back of an underground lecture theatre in the Grieghallen conference venue in Bergen typing this, my second 'From the President' column, on my phone while waiting for a talk on high pressure crystallography by Wilson Crichton of the ESRF to start. Needless to say this furtive typing was prompted by bumping into Carl, our *Crystallography News* editor, who has gently reminded me about the September CN copy deadline that has just passed. So, greetings from the 27th European Crystallography Meeting where, despite the meeting only being half way through, we have already been treated to the usual vibrant mix of varied crystallography from high pressure mineralogy to free electron laser studies of micrometre protein crystals in water jets. We have also been very well fed and watered, although apparently Norwegian prices are such that some exhibitors and most participants are restricting themselves to only one beer a night!

Being at ECM27 of course inevitably leads our minds rapidly to ECM28 next year, which will be in Warwick at the end of August. **Sandy Blake** is chairing the organising committee for us and we are already working with the ECA Special Interest Groups on a programme outline that will hopefully have a distinct UK flavour, but maybe (for those of you who can still recall the Olympics) without disappearing oak trees, luminous hospital beds and growing chimneys. **Mike Glazer** is working on a display of Braggs' work for the meeting to coincide with the Bragg centenary (see below) and the programme will include the Bragg Symposium that would have been part of our BCA Spring Meeting next year. If you have any thoughts about content that can be brought to the programme committee then please let me or Sandy know.

Most of you I hope will by now have witnessed a smooth administrative transition from NNE to HG3, with perhaps the only clear evidence being an email with a username and password appearing in your inbox. These allow you to access and change your personal membership details and view member-specific areas of our website. I am also aware that this has not been the case for all of us and I hope that the teething troubles seen by some are just that. Please let me know if this is not the case for you and we will continue to work hard with HG3 to ensure that our membership database is kept up to date and accurate. With this in mind please do check on your membership status online – or indeed check that you have been sent a membership username and password – and contact HG3 to sort out any anomalies as soon as possible.

In early July a number of us met with various representatives of other organisations (including people from STFC, Diamond, a number of national museums, Leeds University, the Royal Institution and funding bodies) who are interested in commemorating the Bragg centenary next year. This in an exciting opportunity to celebrate all the contributions that crystallography has made, particularly in the UK, over the previous 100 years. The aim of the meeting was to ensure that the various endeavours of the various organisations – including those of the BCA – are coordinated without clashes or duplication. We will be hosting a calendar of centenary events on the BCA web site and hope to establish a common branding. If you have ideas about specific events that we might do next year, or are aware of events that should be included in the calendar, then please contact **Ross Harrington**, our Education and Outreach Coordinator.

These events will naturally feed into ideas for the following year because I am delighted to be able to relay the news that the United Nations have officially agreed that 2014 will be the International Year of Crystallography. As many of you know through emails from the IUCr President, **Gautam Desiraju**, this initiative was proposed by the International Union of Crystallography and spearheaded by the Moroccan Crystallographic Association working closely with the Permanent Representative of the Kingdom of Morocco in the UN along with support from a number of delegations to the United Nations from other countries. This means that we have two fantastic opportunities to champion our subject to the widest possible audiences in the UK and internationally over the next two years and I hope that, like me, you are looking forward to being a part of these celebrations.

Wilson's excellent talk on the developments of a large volume press for very high-pressure x-ray diffraction and spectroscopy at the ESRF has just finished and I hope that he will forgive my partial attention from the back. Now all I have to do is to detangle my poor phone-based typing and rapidly email this to Carl…

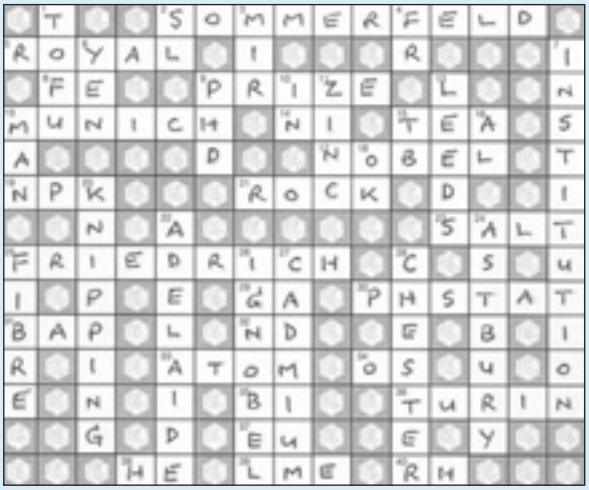
I hope that you have all enjoyed your summer-based vacations and conferences and I commend this issue of *Crystallography News* to you!

David Keen

Puzzle Corner

OUR cover shows a building and a crystal which have some similarity, at least to my possibly astigmatic eyes. Can readers come up with other examples of buildings and crystals that resemble each other?

December 2011 & March 2012 Puzzle Corner:
The answers to both the December 2011 and the March 2012 puzzles contributed by Jim Trotter were spot-on. Jim's answers are reproduced below.



The only one about which I am uncertain is 31 across: Bragg's food. "Bap" is a good old Scottish breakfast bun, which I often had as a child, but I do not know whether it was also popular in England or in Australia. Bragg's drink I am more confident about, as an old student of mine, Norman Camerman, who went to work with W.L. Bragg, once told me about going to "tea" with Lady Bragg.

As for the Cambridge Data Base names, all seem random, except CARPET = CARdioPETaline. SURFER and WASHER don't contain any water, at least in the Data Base. I don't have access to the Data Base at home, so I have to thank Brian Patrick at UBC Chemistry for looking the names up for me.

Jim Trotter

BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
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BCA Spring Meeting Reports

Meeting Reports

WE have now had time for reflection after the very successful BCA Spring Meeting, so that a representative selection of reports could be prepared. This issue starts with summaries of the four excellent Plenary Lectures. It continues with reports on various sessions prepared by the Session Chairs, and it concludes with quotes about the BCA Meeting from bursary recipients. I have not individually reproduced their praise for the meeting and their gratitude for financial support from the BCA and sponsors since every recipient expressed similar sentiments. Neither have I put in much about the Young Crystallographers' sessions since these have already been ably summarised by the YCs themselves.

The BCA meeting was not the only one for which bursaries were awarded. I am pleased to include reports on the Erice school and two Gordon Conferences that give good descriptions of these internationally renowned events.

Carl Schwalbe

BSG Plenary Lecture:

STRUCTURAL BIOLOGY OF THE DNA DAMAGE RESPONSE

Laurence Pearl

THIS lecture, which could hardly have dealt with a more important topic, provided the main meeting with an inspiring start. When a cell suffers damage to its DNA, it must detect the damage and mount a response. The cell cycle must be arrested until repairs have been made or programmed cell death (apoptosis) is initiated. Failure of this response may result in the replication of cells with damaged DNA, which can lead to cancer. Structural biology now gives us key insights into the relevant mechanisms.

Laurence's group has investigated the DNA damage checkpoint at G2/M in the cell cycle, particularly the significance of phosphorylation. Along the way we learned a number of the cell biologists' acronyms. Upon detection of damage ATR phosphorylates itself, becoming an active kinase which can intervene in a delicately balanced competition between Cdc25 (which evokes fond memories in old-time computer enthusiasts like me) and Wee1. While

Laurence Pearl

Wee1 phosphorylates Cdc2, rendering it inactive, Cdc25 restores phosphorylated Cdc2 to the active form. If ATR has been activated, it phosphorylates Cdc25, marking it for degradation by the proteasome. Then Wee1 wins the competition, Cdc2 is inactivated and the cell cycle stops.

Laurence presented further beautiful illustrations, including important dimer formation and a checkpoint clamp with a hole in the middle where the DNA fits.

Carl Schwalbe

CCG Plenary Lecture:

PREDICTING LOW-ENERGY CONFORMATIONS OF SMALL ORGANIC MOLECULES: IS CRYSTAL STRUCTURE DATA REDUNDANT?

Robin Taylor

THE CCG Plenary Lecture also constituted the BCA Prize Lecture in honour of Frank Allen. Fittingly, it was given by Robin Taylor, drawing on his wide experiences at Oxford, Cambridge, Pittsburgh and the CCDC, and now as a consultant. Thanks to the compilation of crystallographic databases, in which Frank played a major role, and to the structure prediction methods which they inspired, we are achieving increasing success in predicting small-molecule structures.

Robin began by enumerating 3 good reasons and 1 less good one for determining such structures: (1) to find out


Robin Taylor

what the chemist made, (2) to understand the molecular shape, (3) to improve our understanding of intermolecular interactions, and (4) just because we can, e.g. to pad out the PhD thesis. According to Chen & Foloppe (2010) in *Drug Dev. Res.,* 72, 85-94, "it is reasonable to ask whether conformational sampling of small organic molecules is an essentially solved problem". In decreasing order of accuracy and increasing order of speed, computational approaches include *ab initio*, density functional, semi-empirical and molecular mechanics. If we are to carry out high-throughput virtual screening on a company database of up to a million compounds, speed is essential. However, rapid methods encounter problems with transferability of force fields, electrostatics and charge representation, the dielectric model (a big term), rigid bond angles and the *in vacuo* approximation. The latter can be particularly troublesome with a long-chain molecule bearing polar groups at intervals: an extended conformation found in the Cambridge Structural Database (CSD) may fold up to make hydrogen bonds when optimised *in vacuo*.

Crystallographic experience embodied in MOGUL can filter out bad conformations and identify suspicious protein ligand geometries. To prevent the "folding up" optimisation error one can delete the van der Waals term, but then one must use atom clash criteria [Taylor (2011) *J. Chem. Inf. Model.,* 51, 897-908] based carefully on crystal structures. On a final topic, which has seen major advances through Frank Allen's work, we aim to predict which of the possible intramolecular hydrogen bonds will actually occur in condensed phases.

Carl Schwalbe

PCG Plenary Lecture:

SYMMETRY MODES: NATURE'S FAVOURED DESCRIPTION OF STRUCTURAL DISTORTIONS

Branton J. Campbell

THIS lecture also served as the Teaching Plenary Lecture. It was a tall order to teach us some group theory on the morning after an excellent conference dinner and a lively ceilidh; but thanks to the clarity of his presentation, Branton Campbell achieved this. While the atomic xyz coordinates are excellent for describing an individual structure, comparison of coordinates between a distorted structure and its undistorted parent can bewilder the observer. The symmetry modes of a distortion provide much more insight.

As an example Branton tabulated the symmetry operators in point group 222:

	I	C_{2x}	C_{2y}	C_{2z}
I	I	C_{2x}	C_{2y}	C_{2z}
C_{2x}	C_{2x}	I	C_{2z}	C_{2y}
C_{2y}	C_{2y}	C_{2z}	I	C_{2x}
C_{2z}	C_{2z}	C_{2y}	C_{2x}	I

Representations map group elements onto matrices that obey the same multiplication table as the group, e.g. $C_{2x}\ C_{2y} = C_{2z}$.


Branton J Campbell

An example of irreps in abstract space is R1: I becomes (1), C_{2x} (-1), C_{2y} (1), C_{2z} (-1). Distortions occur at specific k-points (hkl points), and irreps are recipes for breaking the parent symmetry. The residual symmetries form a subgroup, distortion-symmetry. The space group of the distorted structure includes not only 1-230 but also the location of operators, specifying the origin of the supercell relative to the origin of the parent cell. Branton demonstrated an impressive program, ISODISTORT, which enables even non-specialists to calculate symmetry modes straightforwardly.

Carl Schwalbe

IG Plenary Lecture:

QUASI-PERIODIC MATERIALS – CRYSTALS REDEFINED

Prof Dan Shechtman

IN a hugely entertaining Industrial Group plenary lecture, the 2011 Chemistry Nobel Laureate Prof Dan Shechtman described his discovery, in 1982, of a material exhibiting an electron diffraction pattern with apparent five and tenfold symmetry that had previously been considered forbidden by crystallographers for over 100 years.

Rapidly-cooled 2μm grains of the metallic solid Al_6Mn showed icosahedral symmetry, which was inconsistent with conventional crystallographic teaching. In the lecture, the audience learned how Dan came across tenfold symmetry in the alloy of aluminium and manganese that he was studying by transmission electron microscopy, an observation that he recorded in his lab notebook for perpetuity, complete with two exclamation marks!!


Prof Dan Shechtman

It was some two years before Dan was able to publish his seminal work in 1984, having had to endure ridicule and ostracism. His critics, including **Linus Pauling**, maintained that what Dan saw was as a result of twinning. The audience were then enthralled by the story of how Dan and his later co-workers had to fight to have the truth of their observation recognized: that 10-fold symmetry (and other forbidden symmetries) could exist in particular types of material known as aperiodic crystals, or "quasi-crystals".

Larger crystals were grown, and Laue photographs confirmed the presence of fivefold, threefold and twofold axes, consistent with icosahedral symmetry. A period of reluctant acceptance followed until in 1992 the definition of a crystal was modified by the International Union of Crystallography to accommodate aperiodicity. Since then, many other examples of quasi-crystals have been reported which are all metallic in nature. Amongst their physical properties they exhibit extreme hardness, poor heat and electrical conductivity, and like Teflon, low surface friction. Potential applications are in surgical instruments and other stainless steel appliances.

This very human story of argument and counter-argument against strong opposition from members of the scientific establishment was received with great interest by the audience and the recommendation to the many PhD students that they must pursue their research with "tenacity, professionalism and courage" was surely appreciated by the many young crystallographers attending the BCA Spring Meeting.

Dan concluded his talk by encouraging scientists of all disciplines to show professionalism, courage, tenacity and self-belief when advancing a new concept that goes against current scientific thinking.

The interest sparked by the lecture was revealed by the diversity of questions at the end, which spanned the range from whether quasi-crystals are always metallic materials to a comparison of Dan to another famous scientist, who was initially much opposed - **Charles Darwin**. Dan's humorous and well-informed replies brought the session to a lively and thought-provoking close.

David Rendle and **Judith Shackleton**

Sessions

Piecing Together the Puzzle – Multidimensional Approaches (CCG, YCG & PCG)

LYNNE Thomas (Bath) kicked off 'Piecing Together the Puzzle – Multidimensional Approaches,' which was a joint session between the CCG, YCG and PCG. She gave a presentation entitled 'Beyond the Structure: Investigating Properties in Molecular Materials.' She spoke about the approaches she'd taken to investigate the structural chemistry of target drug molecules for example, in order to improve their physical properties. One particular way of doing this is with co-crystallisation. Crystal engineering can be used to match hydrogen bond donors and acceptors with the addition of a second 'template' molecule. She then moved on to talk about experiments she had carried out with both X-ray and neutron sources, and also materials she had studied with diffuse scattering to help gain a better understanding of why materials behave in a certain way.

Andrew Goodwin (Oxford) then went on to talk about 'Frameworks, Flexibility and Frustration.' He spoke about how framework materials can be designed and constructed with a degree of flexibility within them; this can lead to interesting crystal dynamics. In particular he spoke about framework materials that behaved in a similar way to a foldable wine rack when temperature and pressure were applied to the sample. It was possible to reversibly convert between different phases of the materials, without any loss in crystal quality.

The session was concluded by two talks from Young Crystallographers, **Mark Eddleston** (Cambridge) and **Christopher Woodall** (Bath). Mark talked about using transmission electron microscopy combined with crystal structure prediction to help in structure determination. The combination of these two techniques allowed the solution of structures from very small samples, which would otherwise be impossible with conventional single crystal diffraction. The technique requires just a few experimental electron diffraction images, which are used to identify the corresponding crystal structure from a calculated set of low energy crystal structures.

Chris completed the session with a presentation entitled 'An Investigation in the Luminescent Behaviour of Gold(I) Trimers at Variable Temperature and Pressure.' He spoke about a number of Gold(I) complexes he had synthesised and studied at a number of different pressures and temperatures. The compounds underwent a number of phase transitions, and Chris has been studying them to understand the unusual phase transitions that he had been observing!

Anna Warren
(Diamond Light Source)

Hydrogen-bonding: From Water to Supermolecules (Part 1)

THIS session was part of a double session jointly organised by the PCG and CCG to highlight the importance of the phenomenon of hydrogen bonding for crystallography. The PCG session focussed mainly on hydrogen bonding between water molecules, and the topic was approached from the experimental as well as theoretical side.

Pictured L - R: Dr Ben Murray, Prof Angelos Michaelides, Dr Dominic Fortes and Dr Christoph Salzmann

The first talk by **Dr Ben Murray** (University of Leeds) was entitled "The Structure of Ice Crystallised from Supercooled Water" and showed that a metastable phase of ice, which has previously been called cubic ice, should in fact be named stacking-disordered ice in order to emphasise the fact that this phase contains considerable amounts of hexagonal stacking faults. The implications of the stacking disorder for ice under atmospherically relevant conditions were discussed.

Prof Angelos Michaelides (University College London) spoke about the "Quantum Nature of the Hydrogen Bond". His talk reported on new insights into the effect of the quantum nature of the hydrogen atoms on the strength and length of hydrogen bonds.

"More Ice than Salt – New Observations of $M^{2+}XO_4$ cryohydrates" was the title of the last talk in this session given by **Dr Dominic Fortes** (University College London). A variety of binary phase diagrams of salts and ice were explored, and several new water-rich hydrates were discovered. The importance of those phases in planetary geology was discussed.

The wide range and number of questions asked after the talks illustrated the vibrant character of this area of research, and lively discussions extended well into the coffee break.

Christoph Salzmann, Chair

Hydrogen-Bonding: From Water to Supermolecules (CCG) (Part 2)

THIS second half of a PCG/CCG double session on the topic of hydrogen bonding focussed on the crystal engineering aspects of the hydrogen bond. The first talk of the session, by Doris Braun (UCL), picked up where the PCG session left off – looking at water in the solid state, but extending the scope to organic hydrates. Doris presented the results of an impressive study looking at predicting the hydration behaviour and structural role of water in a range of phenol and hydroxybenzoic acid derivative hydrates. We heard about the difficulties associated with predicting hydrates including identifying the stoichiometry, assessing hydrogen bond energies accurately and achieving accurate conformation analysis of the organic molecule. Despite all these issues it would seem that the state-of-the-art methods can indeed predict the correct structures, get the stoichiometry right and even identify cases where no hydrate is likely to be observed!

Pictured L - R: Dr Laszlo Fabian, Dr Doris Braun, Dr Peter A. Wood and Prof Carl Schwalbe

Laszlo Fabian (University of East Anglia) then took our hydrogen-bonding journey into the area of co-crystals – in particular looking at the physical properties of these multi-component solid forms. One of the major aims of co-crystal research is to achieve rational design of solid-state materials with tuneable physicochemical properties. Laszlo presented a systematic analysis of work from the literature and his own lab towards rationalising the behaviour of solubility/dissolution rate and melting points across a range of co-crystals. There is clear scope for modifying the physicochemical properties of solid forms through judicious choice of co-former. Using a modular approach through consideration of the respective properties of the co-formers seems to have promise, though the trends observed are by no means clear. In this area there are more questions than answers at the moment, but the prize of being able to select the properties of the resulting co-crystal material remains a big one.

The final talk in the session wrapped up our tour of hydrogen-bonding by covering a third area of significant importance in crystal engineering – that of pharmaceutical salts. **Carl Schwalbe** (Aston University & CCDC), who was speaking in place of his collaborator at Aston **Miren Ramirez**, took us on a tour through the hydrogen-bonding and conformational behaviour of a range of salts of the drug compound diclofenac. In this system Carl explained that there are a number of competing hydrogen-bonding possibilities including some very strong charge-assisted interactions (H-bonding lions!), plus some weaker interactions (H-bonding pussy-cats). Interestingly one of the weaker interactions, which forms an S(7) intramolecular ring, occurs in almost all of the 24 diclofenac salts. It would seem that in this situation the pussy-cat can compete successfully with the lions due to conformational preference.

Peter A. Wood, Chair

BCA IG/BSG Session: SAXS

THE Joint IG/BSG SAXS session started with an introduction to SAXS from Nick Terrill (Diamond Light Source). Nick gave an introduction to scattering theory and explained what information can be obtained for biological systems using SAXS; size and shape of proteins and protein complexes are common outcomes from these experiments. The worldwide SAXS community is gradually bringing in standard protocols for experiments and automation is increasing; the new high throughput SAXS beamline at Diamond, B21, will have a sample changing robot as well as an HPLC (which will allow straightforward production of concentration series of proteins). A range of experiments already done at Diamond was also presented covering topics as diverse as liquid crystal structure, accelerated aging of prosthetic heart valves and mapping of diseased corneas.

Pictured L - R: Arwen Pearson, Allan Pang, Nick Terrill, Clair Baldock, Elizabeth Shotton and Ingrid Dreveny

Clair Baldock (University of Manchester) demonstrated the power of a combined structural biology approach using SAXS, TEM with single particle analysis, MALLS, AUC and a domain deletion approach to study the calcium dependent dimerisation of tolloid (TLD), a mammalian metalloproteinase that is involved in dorsal ventral patterning and extracellular matrix deposition. A comparison between truncation mutants, wild-type and the related proteinase bone morphogenetic protein BMP-1 suggests a substrate exclusion mechanism in the EGF2 domain mediated dimeric form of TLD. Furthermore, advances on the collagen VI structural characterisation using SAXS and TEM were described. Ab initio 3D reconstructions of the microfibrils showed that the N-terminal region is flexible.

The topic of the session then altered from SAXS to macromolecular crystallography. **Arwen Pearson** (University of Leeds) gave a presentation about time-resolved structural studies of macromolecules. Using the analogy of a horse crossing a field, Arwen explained why it is important to see proteins in motion to understand how they function. Both high spatial and temporal resolution are needed to study short lived intermediates. Synchrotrons such as Diamond and ESRF can help with these studies and there are exciting possibilities with the advent of free electron lasers where pulses are at the femtosecond timescales. Laue methods can used to ensure that there are enough photons per timeslice to get measureable diffraction and an example from **Phil Anfinrud**'s group showing photolysis of CO from myoglobin with 100ps time resolution was shown. Alternatively, single shots on multiple crystals can be used; advantages over Laue diffraction include the use of smaller crystals, being able to automate the experiments and the possibility of studying irreversible reactions. Development of this approach is underway in collaboration with Diamond and some preliminary experiments using aspartate decarboxylase were shown.

Allan Pang (Queen Mary University of London) reported on the challenges of the crystallisation and structure solution of propanediol-utilization (Pdu) bacterial microcompartment shell proteins. Mutational analysis provided insight into the pseudo-icosahedral assembly of the protein shell.

Elizabeth Shotton and **Ingrid Dreveny**

BCA IG: Process Analytical Technologies (PAT) – Online Processing

Held 3.30pm Wednesday 18th of April

THE first speaker of the PAT session was Dr Ali Saleemi from the Department of Chemical Engineering at the University of Loughborough. He spoke about PAT-based crystallisation control and monitoring and gave two interesting case studies of how PAT could be applied to crystallisation processes. In the first case study he described how PAT was applied to troubleshoot issues

observed for an AZ developmental drug where solvent inclusion had lead to an issue with poor particle size distribution. By using the automated direct nucleation control method (ADNC), which used focus beam reflectance measurement (FBRM) combined with attenuated total reflectance (ATR) and UV/visible spectroscopy, they were able to remove solvent inclusion and produce larger non-agglomerated crystals. In the second case study he described how the procedure could also be applied to monitor polymorphism during polymorphic phase transitions to provide better control polymorphism during crystallisations in the future.

Pictured L - R: Dr Paul Dallin, Dr Ali Saleemi, Dr Paolo Avalle and Dr V. Brett Cooper

The second speaker of the session was **Dr Paul Dallin** from Clairet Scientific Ltd. During his talk entitled "Converting Molecular Spectroscopies into useful PAT Tools" he highlighted how tools that have been around for decades, such as IR, NIR, UV/Vis and Raman, are now being applied to become the cornerstones of PAT. He provided examples of how these techniques could be applied to control and monitor the drying process of API's to ensure downstream quality, demonstrating how the process could vary from batch to batch. He described how crystal habit could be monitored and controlled using ATR/FT-IR. He also demonstrated how solubility could be monitored during the crystallisation process using ATR measurement.

Finally, during the last talk of the session, **Dr Paolo Avalle** from the MSD Development Laboratories talked about the development of PAT methods to help analyse the film coats of controlled release pellets used in pharmaceutical products. Paolo described how a controlled release system could be developed by adding a polymer coat to slow API release. He then described how he had developed NIR methods to determine how much API was being added to pellets and how thick a layer of polymer was being added to the pellets, by comparing the NIR data to HPLC assay and Morphologi Optical Microscopy data. Finally he described how the final drug release of the product could be estimated utilising a PAT NIR method correlated to the in vitro drug dissolution methods routinely used to monitor drug product behaviour by the Pharmaceutical Industry.

V. Brett Cooper – Session Chair and Secretary of the BCA-IG.

BCA IG Session Evaluation of Coatings

THE EVALUATION OF RESIDUAL STRESS IN COATINGS BY X-RAY DIFFRACTION

R.H.U. Khan, School of Metallurgy and Materials, University of Birmingham, Edgbaston, Birmingham, B15 2TT.

DR Raja Khan (School of Metallurgy and Materials, University of Birmingham) gave a fascinating talk about coatings produced by Plasma Electrolytic Oxidation (PEO). The properties of such coatings are critical to their service lifetime, particularly if any excessive residual stresses are present. Excessive in-plane tensile stresses may cause cracking and spalling while compressive stresses may cause buckling. The measurement and control of residual stresses in coatings is important in the development of a successful, 'industrial scale' coating process.

The properties of the coatings produced by various commonly employed Industrial coating processes were compared with PEO,

- Anodising tends to produce amorphous, hydrated coatings which have good adhesion to the substrate.
- Plasma spraying gives a more laminar structure with poorer adhesion.
- The PEO coating process has many advantages over conventional anodising in that it employs no toxic chemicals; it gives a dense, thick, highly crystalline coating with good adhesion and is relatively low-cost. The coating has a thin porous surface layer on a denser, crystalline base layer.

Raja described the PEO process and showed a video of the micro discharges which occur during the coating process enabling the formation of high temperature phases, such as α-aluminium oxide (corundum). However, the PEO process does subject the component to some rather harsh conditions and residual stresses are to be expected, although a coating has never been seen to delaminate.

Two X-ray diffraction methods were employed to measure the residual stress in the coating. Firstly, the $\sin^2\psi$ method was used to measure the macro stresses - both normal and shear. Glancing incidence geometry was also used to assess the stress in the coating which was found to be relatively low at about 350 mega pascals (MPa).

SYNCHROTRON GLANCING ANGLE STUDIES OF TURBINE BLADE COATINGS

Professor R J Cernik, School of Materials, Grosvenor St, University of Manchester, Manchester, M13 9PL.

UNFORTUNATELY Prof Bob Cernick was unable to give his talk due to transport difficulties. The text of his abstract is given overleaf.

Thermal Barrier Coatings (TBCs), produced by the Electron Beam-Physical Vapour Deposition technique, have been widely used in the airspace industry to increase the engine efficiency and to protect the engine components from oxidation.

There are four primary constituents in a TBCs system. They comprise (i) a yttria-stabilised zirconia (YSZ) coating, (ii) the superalloy substrate, (iii) an aluminium containing bond coat between the substrate and the YSZ top coat, and (iv) a Thermally Grown Oxide (TGO), predominantly alumina, which forms between the YSZ coating and the bond coat. The YSZ layer is the thermal insulator, the TGO on the bond coat provides the oxidation protection.

Typically, failure of TBCs occurs at the interface between the bond coat and the TGO, which is driven by the strain energy in the ceramic layers (e.g. YSZ and TGO), and resisted by the interfacial toughness. In particular, the interfacial toughness plays a dominant role on the durability of TBCS. These structural details have been evaluated by glancing angle synchrotron XRD.

X-RAY DIFFRACTION AND X-RAY REFLECTIVITY IN THE GLASS INDUSTRY

Mark Farnworth, Senior Technologist, Pilkington Group Limited, European Technical Centre, Lathom, Hall Lane, Ormskirk, Lancashire, L40 5UF.

THE final talk, by Mark Farnworth from NSG Pilkington Group focused on the evaluation of coatings on glass. He started with a history of the evolution from Pilkington (the inventors of the float glass process) and their acquisition by Nippon Sheet Glass (NSG). He described how the glass is floated on a bath of molten tin.

Many of the critical properties of the coatings applied to glass are evaluated by X-ray diffraction at NSG Pilkington. XRD is also used in conjunction with surface analysis techniques for example, X-ray Photoelectron spectrometry (XPS) and Time of Flight Secondary Ion Mass Spectrometry (ToF SIMS).

The laboratory at Lathom, in Lancashire, provides support to production sites and downstream operations around the world, support for internal R&D projects as well as the evaluation of glass making raw materials for impurity type and amount. Other work includes the evaluation of new glass compositions as well as the evaluation of current and new “Off Line” (PVD) and “On Line” (CVD) coatings on glass.

Mark started by describing the evaluation of an “On Line” coating of tin oxide, Cassiterite applied by CVD. This produces a very hard coating with columnar growth; the {200} plane is preferentially orientated parallel to the sample surface. There are large Cassiterite grains, each made up of smaller crystallites. The grain sizes are measured by SEM and crystallite size determined by XRD using the Scherrer equation. Lattice parameters are used to evaluate residual stress and chemical composition.

The next example was an “Off-Line” coating with highly textured Ag and Zn oxide with pole figures being used to evaluate the texture of the Ag {111} reflection. We then moved to a description of X-ray Reflectometry (XRR). Mark illustrated the method using a series of scans, starting with simple single layer coatings and building up to more complex, multilayer, finishing with a six layer stack of Glass/TiO_2/ZnO/Ag/ZrO_2/SnO_2/TiO_2.

It was very interesting to see the fitting process as the samples became more and more complex. Mark illustrated clearly, the sensitivity of the technique to the changes in the layers. Modelling software is used to extract layer thickness, density and interface roughness. XRR has a good repeatability (<5%, as determined by a round robin of Technical Committee 19 of the International Commission on Glass).

Finally, Mark showed how XRR is used to calibrate the sputter yields for ToF SIMS which enables depth profiling of the chemical species in a coating. Also, data from other analytical techniques (optical modelling, cross-sectional SEM, profilometry, XPS profiling) has been found to be in good agreement with XRR.

David Rendle and Judith Shackleton

30th Annual BCA Spring Meeting - Phase Transitions: Transformations in the Solid State

THE first speaker in this session was Prof Kenneth Harris from the University of Cardiff. Prof Harris set the scene by providing some background to the structural phase transition behaviour of urea and thiourea inclusion complexes and how they can provide a fundamental understanding for organic systems of this nature. Kenneth went on to contrast commensurate versus incommensurate behaviour (for thiourea and urea respectively) and detail how this is characterised by various complementary techniques. Aside from single crystal and powder diffraction and solid state NMR for static studies ^{2}HNMR was used to probe rotational motion whilst Incoherent Quasielastic Neutron Scattering provides information on translational movement. Finally Kenneth showed results from the exciting new application of X-ray birefringence using Diamond for characterising these phase transitions.

The second speaker of the session was **Dr Spoorthi Dharmayat** from Pfizer. She started by speaking about phase transitions observed for a tetra-hydrated drug candidate. This included discussion of the characterisation techniques used to understand the phase transformations this crystalline form undergoes and an exploration of the effect of varied temperature and humidity conditions. Spoorthi went on to discuss the impact these transformations have on the development of such a form as a drug candidate. Next the successful on-line monitoring of a polymorphic phase transformation was presented using real time capillary

PXRD data monitoring of a solution mediated slurry. Spoorthi demonstrated that the design space exploration of polymorphic systems in this manner enabled an optimised crystallisation process to be developed.

Pictured L - R: Dr Cheryl Doherty, Prof Kenneth Harris, Dr Mateusz Pitak, Dr Spoorthi Dharmayat and Dr Simon Coles

The final speaker of the session, and indeed the meeting, was **Dr Mateusz Pitak** from the University of Southampton. Mateusz presented a thorough study, mainly by single crystal diffraction, differential scanning calorimetry and hot stage microscopy of phase transition behaviour in the related family of aliphatic chain amino acids. Surprisingly, across the whole family of compounds there are some striking similarities in behaviour – particularly in that all transitions are reversible and they follow the same basic pattern. Mateusz then went on to demonstrate how the concerted mechanism for the transformation was derived and showed animations of how it actually takes place.

Simon Coles
University of Southampton

BCA session: Protein Crystallization: Magic versus Logic

THE session started with a very informative and entertaining talk by Terese Bergfors who related to us the story of how IspD from *Mycobacterium tuberculosis* as well as IspDs in complex with substrates were successfully crystallised following two years of effort. She discussed her crystallization strategy including the choice of construct, screening kits, buffer, protein concentration and seeding. It was encouraging to see that her logical approach of employing a minimalist approach to screening chemical space led to success.

Emmanuel Saridakis spoke about a new diagnostic tool using dual polarization interferometry (a surface analytical technique) for probing the different possible outcomes of protein crystallization experiments. The application of this technique provides a "signature" of crystallization events, thus predicting if there will be protein crystal formation, amorphous precipitate or clear solution. He showed examples of how DPI was used to discover crystallization conditions and to obtain information on the crystallization process for aiding crystal optimization.

Lesley Haire presented several case studies of experiments to optimize crystallisation conditions by introducing a new "combinatorial" experimental design where several precipitants can be combined with several additives or buffers. The Oryx crystallisation system was used to "reshuffle" the ingredients from several hits, to optimize the dilution of seed stock in microseeding experiments and to introduce and test up to twelve ligands. The same liquid handling procedure was employed for all three scenarios and yielded impressive results.

The last (but certainly not least) speaker was **James Hall** who showed an interesting study in which a DNA-ligand crystal, with data collected at room temperature, gave more structural insight than a cryo-cooled crystal which diffracted to 1.1 Å resolution. Collecting data at room temperature enabled the experimenters to change the humidity and thereby obtain a different crystal form with significant structural differences through dehydration of the crystal. Moreover, transition between the two crystal forms could be achieved by changing the relative humidity.

Naomi Chayen
Chair

BCA Spring Meeting: Quotes from our Bursary Recipients

OUR bursary recipients provided comprehensive reports. Because accounts of the Plenary Lectures and summaries of some sessions by their Chairs are presented separately in this issue, in the main only their comments on other sessions are reproduced. Their general opinion of the meeting was overwhelmingly positive.

Carl Schwalbe

"Twenty twelve is already grabbing headlines for many reasons: the Olympics, the Diamond Jubilee, the second and last solar transit of Venus this century, and the BCA Spring Meeting held at the University of Warwick. Indeed the ultimate social barometer, Twitter, briefly saw #BCAMeeting2012 trending. With a Nobel prize winner, disagreement on exactly when the International Year of Crystallography will happen, and fascinating sessions planned on all days it was the place to be... Highlights were **Mark Senn** and his work on the canonical magnetic material, magnetite; the PCG teaching plenary bringing a new technique to my own research; all the prize lectures; **Claire Murray**'s last-minute stand-in presentation and **Angelos Michaelides**' video!"

Andrew Cairns

"ONE particularly engaging talk which stood out for me was the Parkin Lecture given by **Lynne Thomas** taking crystallography beyond the normal boundaries to include the diffraction patterns of wood – definitely worth getting out of bed for on Tuesday morning! The following sessions investigating the physical properties of materials and the ability to tune these to requirements I found particularly interesting, and relevant to some of my work... As a third year University of Southampton MChem undergraduate student (on Industrial Placement in small molecule crystallography) this was a fantastic opportunity for me, being able to meet experienced people in the field as well as talking to and finding out about current PhD students' research. Hearing about the scope and wider applications of crystallography and other areas of research such as the more biological applications definitely expanded my knowledge and understanding of crystallography whilst introducing many new ideas and techniques. By attending I have definitely been enthused and further motivated to continue in this field and hope that this is the first of many crystallography events I am able to attend."

Lucy Mapp

"The main conference was opened by an interesting plenary by **Laurence Pearl** entitled: Structural Biology of the DNA Damage Response, where an overview was given of the work undertaken by his group to isolate and understand the structure and assembly of the proteins which recognise and repair damaged DNA strands... Of particular interest to myself was the double session on "Hydrogen Bonding: From water to supermolecules"... Overall the conference was very informative and will doubtlessly help with my work in many ways."

Alan R. G. Martin

"The theme of the 2012 BCA meeting held at Warwick University, was "Challenges in crystallography". Recently, the crystallographic analysis targets have been shifted from the "low hanging fruits" to more challenging targets such as protein complexes and membrane-associated proteins. Many talks were aimed to address difficulties encountered during such endeavours, and much insight was shared during the meeting this year, which will undoubtedly help in obtaining structural information of the proteins and extending their applications. Many successes derive from rational and/or systematic approaches, but also rare occasions of accidental and serendipitous findings were important. Such observations can easily be overlooked; to accept the observations and initiate further investigations requires open minds. Those elements were emphasised during a very memorable talk by a Nobel Laureate, Professor Dan Shechtman who discovered quasi-periodic crystals."

Soshichiro Nagano

"One of the main challenges a protein crystallographer faces, which was discussed in the final session, is to obtain a crystal fit for X-ray diffraction... When 'tips and tricks' fail, one can employ the surface entropy reduction technique. This has been reported successfully by **Soshichiro Nagano** (Queen Mary University of London). By introducing multiple mutational points on lysine, glutamate and glutamine into alanine, he was able to obtain crystals that behave and diffract considerably better than the wild type crystal. This technique, however, requires some sort of prior knowledge of the structure of your protein in order to find suitable surface mutational points. When crystals are beyond achievable, multiple techniques or approaches can still be used to get a three-dimensional structure of a protein. For instance, **Claire Baldock** (University of Manchester) uses small angle X-ray scattering (SAXS), cryo-transmission electron microscopy and analytical ultracentrifugation to show the structural detail of microfibrillar proteins.

A software workshop on two programs (Coot by **Paul Emsley** and CrysAlisPro by **Tadeusz Skaryzynski**) useful for protein crystallography was also tackled. Paul Emsley gave detailed developments on Coot, most specifically targeting the ligand fitting on the structure. CrysAlisPro, on the other hand, was first used mostly in small molecule crystallography but now has branched out to deal with

bigger molecules such as proteins. This program might be helpful in my case as he has shown how it manages to solve a crystal with lattice disorder."

Allan Pang

"The meeting continued with the Multidimensional Materials session of the PCG and CCG groups. **Mark T. Weller** give an interesting talk about Transition Metal Fluorophosphates with different applications in one, two and three dimensions such as: nanowires (1D), battery materials (2D), catalysts (1, 2 or 3 D). He also addressed the importance of the presence of the fluoride on a metal site acting as a bridge for transition metal centres. The following speaker **Paul J. Saines** described a series of inorganic-organic framework materials containing 2,2-dimethylsuccinate ligands with the role of weakly bonded hybrid layers in their bulk crystals. Despite their layers formed which prevent three dimensional magnetic order, these new family materials present antiferromagenetic coupling. **Elena Marelli** gave an interesting talk about the existence of Cu(II) with cyanide in a square-planar environment. $Cu(CN)_2$ had not been found till now. Our speaker showed that it can be stabilised in a cyanide environment containing copper-nickel mixture $[CuNi(CN)_4]$. The crystal structure solved from powder diffraction contains flat layers of square planar $[Ni(CN)_4]$ and $[Cu(CN)_4]$ linked by cyanide groups."

Ioana Sovago

"Highlights from the YC sessions included an insight by **Robin Owen** into the workings of MX beamline I24, which I found interesting despite being a small molecule crystallographer myself. Another highlight was an entertaining and confectionary filled overview (by **Claire Murray**) about some of the outreach work currently taking place entitled 'Chemistry for the People'... One highlight from the second day of the main meeting was the prize lecture session: **Gareth Lloyd** (winner of the CCDC/CCG prize) showed us the movement of CO_2 through porous MOF materials while **John Wright** (PCG prize winner) explained an impressive technique for untangling X-ray diffraction data from multiple, macromolecular crystallites allowing for simultaneous solution of their structures."

Karim Sutton

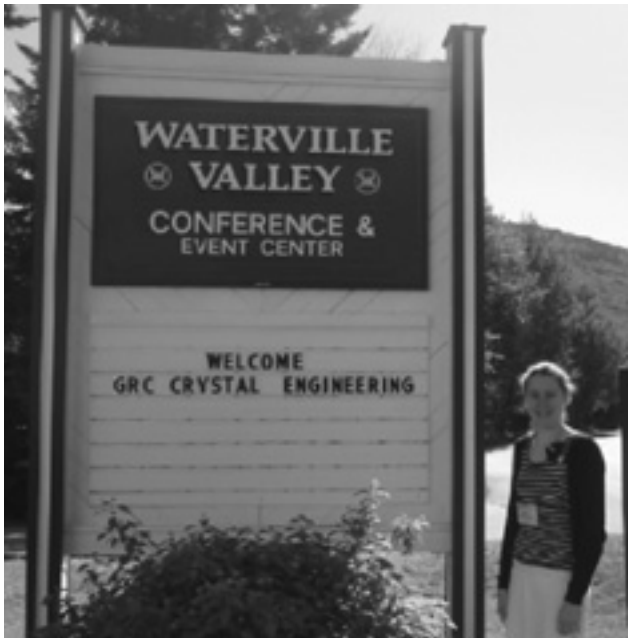
BCA Spring Meeting - *More images from Warwick 2012*

Colin Groom invites Gareth Lloyd to deliver the CCG CCDC Prize Lecture, chaired by Hazel Sparkes

Dynamic crystallographers at the ceilidh

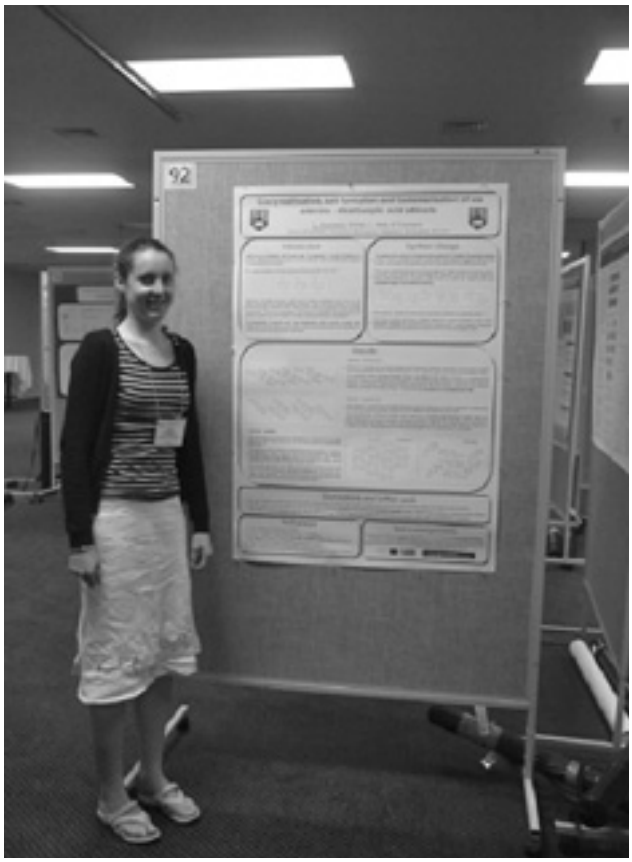
Gordon Research Conference Crystal Engineering 11-15 June 2012

GORDON Research Conference (GRC) is an organization managed by and for the benefit of the scientific community providing an international forum for the presentation and discussion of frontier research in the biological, chemical, and physical sciences, and their related technologies where leading investigators from around the globe discuss their latest work and future challenges in a uniquely informal, interactive format.



Having now attended a GRC, I wholly agree with the above statement. There were three sessions of talks per day in which the invited speakers presented their most recent (and unpublished) work followed by a 20 minute discussion session, enabling the attendees to further discuss and share experiences in the specific area and ask questions to aid further understanding. The different sessions were split into specific subject areas; since the conference was focussed solely on the crystal engineering field of crystallography, all sessions were relevant, though I personally found the Polymorphism and Crystal Structure Prediction and Design, Synthesis, and Properties of Co-crystals the most interesting with talks directly relating to my research and ideas presented that I can utilise to further my project. A presentation delivered by **Susan Bourne** from the University of Cape Town was a prime example of a talk in which I could gain knowledge and inspiration from her presentation of new results in systems very similar to the ones I study.

Along with the talks, there were daily poster sessions, in which I presented a poster entitled 'Cocrystallisation, salt formation and tautomerism of adenine : dicarboxylic acid adducts' (see picture below). All poster sessions were well attended, leading to numerous discussions of results and ideas to move projects further. One of the rules of a Gordon Research Conference is that all work presented is to be unpublished, and discussions regarding my poster and similar results found within another academic group have resulted in the commencement of a joint project and research paper.



The conference was held at Waterville Valley resort in New Hampshire, a resort offering a number of activities such as mountain biking, swimming, tennis and mountaineering, which were all utilised by delegates of the conference in the afternoon breaks, altogether making the conference very enjoyable.

Laura Thompson

Gordon Research Seminar and Conference on Biocatalysis 7-13 July 2012

THE Gordon Research Conference on Biocatalysis was held at Bryant University in Smithfield, Rhode Island from 8th – 13th July 2012. As is now the case with several of the Gordon Research Conferences, the conference was held in conjunction with a Gordon Research Seminar from 7th – 8th July, which is a two-day event aimed at PhD students and post-docs. The seminar provided a much more informal, non-intimidating environment than the main conference and gave the 45 attendees a chance to discuss our work and get to know each other before the more senior attendees arrived for the main conference. The seminar consisted of a key-note speech by Kristala Jones-Prather from MIT followed by three sessions of talks from PhD students and post-docs. Each session was chaired by a PhD student and I was lucky enough to be selected as chair for the first session. This was not an intimidating task at all as the group was relatively small and the chairs, Helge Jochens and Aram Panay, had already set a relatively relaxed atmosphere for the event in their introduction. There was also an evening discussion session on the variety of potential career paths available to the audience which gave us all some food for thought, and two poster sessions gave us plenty of opportunity to present our own work and find out exactly what everyone else was working on.

The seminar ended at 3pm on 8th July giving us a few hours of spare time before the main conference began at dinner. In total there were 172 attendees at the main conference and the group was very diverse in terms of career stage, nationality, gender and industry vs. academic backgrounds: nearly a third of the attendees came from an industrial employer rather than academic research. The topics covered in the conference were very broad, meaning everybody had a few sessions they were familiar with and some others that were relatively unknown areas of biocatalysis; for example, I work on changing the reaction catalysed by a single purified enzyme whereas many people there were interested in the use of whole cells to catalyse a cascade of reactions. The key-note speech was given by **Jay Keasling**, a giant figure in the biocatalysis field following his work in the biofuels domain, and needless to say there was an extensive discussion session following his talk. In fact following each of the talks over the five days of the conference the 15 minute discussion session was taken full advantage of and it was good to see that it wasn't only the established professors asking the questions but some of the younger researchers as well. The four poster sessions of the main conference gave everyone ample time to discuss all the research going on in the field. This was my first conference in the biocatalysis field and it was great to see how many people were interested in my work – I even had two industrial guys give me their business cards with the potential of future collaborations if my work progresses as I hope! Seeing some of the other posters on display also confirmed to me what an exciting area of research this is and gave me a few ideas of things I could try with my own project. As a result of discussions in the poster session I am planning to visit the lab of a group working on a similar project to my own to learn a specific technique they have developed.

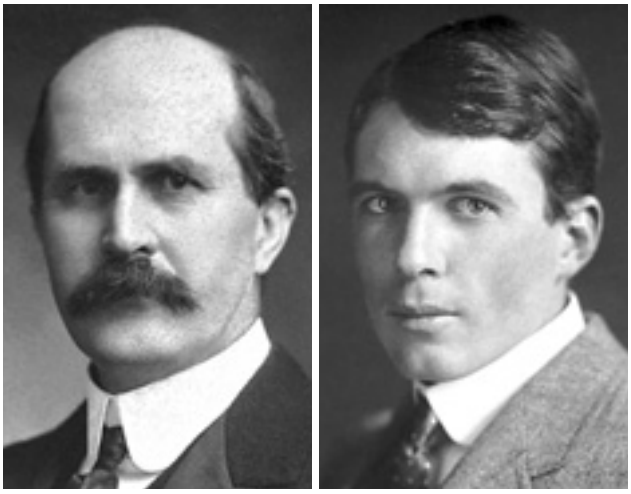
The Bryant University conference site itself was beautifully landscaped with plenty of green spaces and a couple of beautiful lakes and, along with the endless tasty food that we had for every meal and beer and wine available each evening, it was a very comfortable conference. I feel I have learnt a lot from the people I met there and the science that was presented and hope to keep in touch with several of the young researchers I met at the Gordon Research Seminar. Having this less formal introduction to the main Gordon Research Conference certainly enhanced the experience of all of us that attended and I look forward to attending again in two years' time if I can make it!

Lucy A. Chappell
University of Leeds

The Two Braggs: Who were they and what did they do?

X-RAY crystal structure analysis and its development were instigated 100 years ago. The nature of X-rays as waves or corpuscles was a controversy and the thinking on the nature of the electron distributions in an atom was before quantum mechanics. The structures of molecules were undetermined. **William Henry Bragg** (1862-1942) and **William Lawrence Bragg** (1890-1971), father and son, played the pivotal roles, at Leeds University and Cambridge University, in pioneering X-ray crystal structure analysis through 1912 to 1914, interrupted by the eruption of World War I in Europe in August 1914. The Braggs had promptly built upon the first 'X-ray diffraction from a crystal' set of experiments undertaken in Munich by **Max von Laue**, **Walter Friedrich** and **Paul Knipping**, with key roles by **Paul Ewald** and **Arnold Sommerfeld** in early1912. This proved conclusively that X-rays as waves were diffracted by the crystal as a 3D diffraction grating. Today we refer to the number of X-ray photons per second incident onto our crystal and our crystal diffracts the X-rays, now as waves. We live with 'wave particle duality' as a commonplace. Strong evidence of X-rays as waves came from **Charles Barkla's** research at Liverpool University on the polarisation of X-rays. There were direct clashes in the science literature of the time with William Henry Bragg, then at Adelaide University, Australia, as he, unlike Barkla, was convinced that X-rays were corpuscular by nature. Nobel Prizes in Physics were awarded to Laue (1914), both the Braggs (1915) and Barkla (1917). The X-ray spectroscopy of the elements by **Henry ('Harry') Moseley** in Manchester was tragically ended when Moseley, by then at the war front in Gallipoli, was killed in 1915. William Henry Bragg (WHB) and **Ernest Rutherford**, Head of Physics in Manchester, were regularly in touch, since Adelaide days for WHB and in Canada for Rutherford, which continued when they were both in the North of England. **C G Darwin**, also in Manchester Physics, grandson of Charles Darwin, derived a key equation for the diffraction of X-rays by a crystal (1914). In late 2012 the AsCA (Asian Crystallographic Association) will be held in Adelaide, because of the WHB work there over more than two decades, mainly physics teaching but building up research on radioactivity and the nature of X-rays. The research into the stopping distance of alpha particles in matter by WHB in Adelaide, and its medical potential, was arguably the most important. ECM 2013 will be hosted by the UK at Warwick University, and will have a special Centennial celebration session. Recently in March 2012, there was a special celebration conference held in Munich by the German Crystallographic Society.

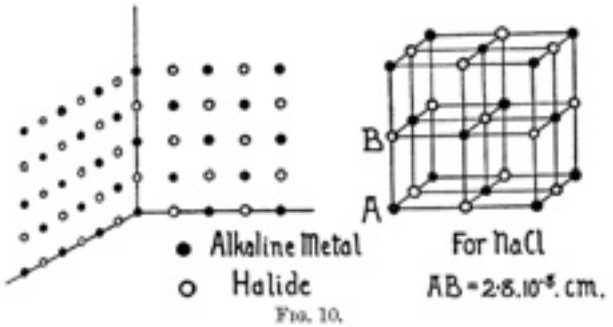
William Henry Bragg and William Lawrence Bragg (WLB) developed, over many decades, X-ray crystal structure analysis, including, by then, WHB based at University



William Henry Bragg *William Lawrence Bragg*

Photographs of W. H. Bragg and W. L. Bragg commissioned by the Nobel Foundation in 1915

College London and WLB firstly at Manchester University (1919 to 1937) then at the Cavendish Laboratory in Cambridge (1938 to 1953) and finally at the Royal Institution (up to 1965). Of those initial years 1912 to 1915, in the modern era we refer back to 'Laue diffraction', to Bragg's Law (WLB 1912 in Cambridge), the first crystal structures, which were of the alkali halides (WLB 1913 in Cambridge using Laue diffraction photos, and also in Leeds with his father's diffractometer; see ref 1 and figure below), the first X-ray diffractometer (WHB ref 2) and Fourier analysis (WHB at UCL in 1915).



From ref 1 - the caption shown is the original.

The sequence of events above is described in various biographical works, including by **Gwendolyn Caroe** on her father (3, 4, 5). There is an extensive collection of Bragg archives held at the RI, and that also formed the touchstone for these biographical works. The nature of the father and son work and relationship is described particularly in the recent book by **John Jenkin** (5) and disagrees with some interpretations in ref (4). That WHB spoke highly of his son,

Fig 2
From ref 2 - with the permission of The Science Museum London

WLB, and that WLB admired his father, is abundantly clear but the question of recognition of WLB's work independent of his father remained and is a matter of much written analysis. Recall that WLB was a Trinity College Cambridge undergraduate and then first year postgraduate when the inspiration for his 'Bragg's Law' struck his mind while 'walking on the Cambridge backs'. WHB was an established Professor of Physics at Leeds University. It was WHB who attended the 1913 Solvay Conference on Physics, held in October 1913, without WLB, but who received a postcard signed by Sommerfeld, Curie, Laue, Einstein, Lorentz, Rutherford et al congratulating him for 'advancing the course of natural science' (5). WHB and WLB are the only father and son joint recipients of the Nobel Prize for Physics, and WLB is still the youngest recipient. The Jenkin book, and biographical research, on father and son and their work is just waiting to be turned into a movie script in my view!

WHB was born in Cumbria in 1862; and when his mother died when he was only 7 years old, he was moved to Market Harborough to live with the family of his uncle, also called William. WHB was educated as a boarder at the King William's College in the Isle of Man (a fact commemorated on an Isle of Man stamp). He went from there to Trinity College, Cambridge to study maths, graduating as a 'wrangler' ahead of the mathematician Whitehead (5). J J Thompson, Head of the Cavendish, proved influential in WHB's appointment as a very young Professor of Maths and Physics at Adelaide University, 'learning physics on the boat on the way out to Australia'. WHB was twenty-three years there, married and had a family of two sons and a daughter. When WLB, the eldest son, was 16 years old he entered Adelaide University to study, mainly, maths and physics, but also chemistry, and was 18 years old when WHB accepted the appointment as Chair of Physics at Leeds University in 1908, 'in order to be more at the centre of things' (5), including by then his scientific friend and correspondent, Rutherford, based in Manchester. WLB then also, like his father, entered Trinity College Cambridge and graduated with 1st class honours in physics (5). How did WHB get to know of the Munich X-ray diffraction experiment? Jenkin states (5) that 'not highlighted before, there was a letter sent by a Norwegian, Lars Vegard, to WHB who knew of WHB's strong interest in the nature of X-rays, and who included a copy, with Laue's blessing, of an X-ray diffraction photograph, and who explained various details of the work'. Father and son discussed the work in detail, including during that summer holiday in 1912 at Cloughton, near Scarborough (5).

WLB himself makes clear the sequence of events in his own lifetime look back book (6) The Development of X-ray Analysis, involving repeating the 'Laue diffraction experiment' but on crystals of NaCl, KCl, KBr and KI in the Cavendish and repeating the work on his father's X-ray spectrometer, which was 'more powerful'. WLB's paper in 1913 (1) is under his own name, W L Bragg BA (i.e. without a doctorate at that point), includes the raw data comprising the 'Laue diffraction' photos (modern terminology) and also some of the X-ray spectrometer scans. The paper (1) is written without an address, is communicated by his father Prof W H Bragg FRS and is received at The Royal Society June 21st 1913 and read June 27th 1913. WHB's description of the 'X-ray spectrometer' is under his name and published in Nature (2). There are various joint papers in this period; I will highlight one in particular at the end of this short article.

After World War I, when their science work resumed, WHB at UCL concentrated on organics whilst WLB at Manchester concentrated on inorganics in general and silicates in particular. For WLB this included the X-ray crystal structure of calcite and explaining the optical property of birefrigence, as well as understanding the absolute intensities based on X-ray atomic scattering factors, with **Douglas Hartree**, presumably both to the appreciation of his physics department colleagues.

In this short article many details, including very significant ones, are left out. The respective obituary notice and biographical memoirs of The Royal Society give separate comprehensive summaries of the lives and scientific outputs of WHB and WLB (7,8). I commend to you to read at least the references I cite. You will find details on the influential role of WHB in British science and society 'between the wars', as measured by his Order of Merit, one of only 24 persons at any one time selected by the ruling King or Queen, and being President of the Royal Society.

For WLB his important role in WWI as a key 'science and technical person' from the British side, in association with the French, for developing sound ranging to pinpoint German gun emplacements, led to his rank of Major and the award of the Military Cross (5). Jenkin cites the written evidence which points to sound ranging being as important as the introduction of tanks by the allies in concluding the war. Alongside this was the family tragedy of the death of Bob Bragg, WLB's younger brother, basically in the same military operation as took the life of Harry Moseley. WHB was 52 when the death of Bob happened. As a parent you expect to die before one's own children. As a father myself who has lost a son I can relate to the overwhelming pain and anguish that such a loss brings.

WLB went from Manchester, via a short time (a year) as Director of the National Physical Laboratory (all that admin was not for him) before succeeding Rutherford again as Head of the Cavendish Laboratory. Under WLB's direction came the solution of the first protein crystal structures by **Max Perutz** and **John Kendrew** as well as the double helix by **Frances Crick** and **James Watson**, with **Rosalind Franklin** and **Maurice Wilkins**, who were based at Kings College, London. During his term as Director of the RI **David Phillips** and colleagues solved the first enzyme crystal structure. I would observe that WLB had at the end of WWI been in charge of 40 sound ranging stations of 50 persons each. Thus management and leadership, learnt in WWI, were also further developed and applied by WLB in these scientific roles as Director.

Both WHB and WLB were fine expositors of science to the public and to school children, especially through the Adelaide (WHB) and the Royal Institution periods (WHB and WLB both giving sets of RI Christmas Lectures). They both evidently had a great way of explaining complex things simply and by analogy. An example for WHB is his book (9) *The Universe of Light* based on his RI Christmas Lectures of 1931, which is superbly illustrated. For WLB see for example his Scientific American article on X-ray crystallography (10). Joel Bernstein and I were teaching at a crystallography school in Como recently and he told me of hearing a lecture by WLB at Yale University in the 1960s; he vividly recalled that WLB described a crystal as a 'symphony of electrons'- a beautiful thought.

I entered University in 1971 so I never met WHB or WLB. I have read much about them and much of their work. I learnt more during my term as Chair of the Bragg Lecture Fund Committee (my final report delivered here in this *Crystallography News* in Issue 110 September 2009). As the University of Manchester W L Bragg Lecturer on the occasion of the University's 150th Anniversary I wrote up my lecture for the Manchester Literary and Philosophical Society, reproduced in Z Krist (11), where I investigated much detail of WLB's time in Manchester (1919 to 1937), references cited therein.

As a final aspect to this article let's revisit their joint article (12). This was 'received on April 7th and read on April 17th 1913'. WHB's address is the Department of Physics, University of Leeds and WLB's was Trinity College Cambridge University. Its first reference is to WLB presenting the interpretation of Laue diffraction photographs by means of 'reflection of X-rays in such planes within the crystal as are rich in atoms' (at the Cambridge Philosophical Society

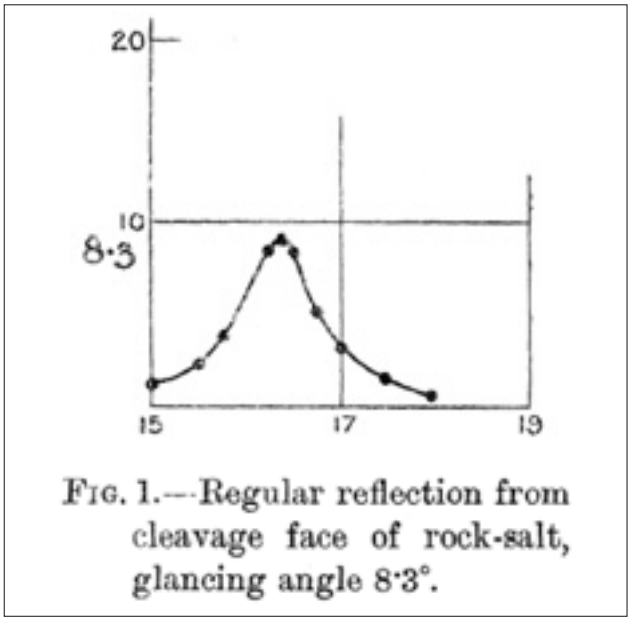


Fig. 1.—Regular reflection from cleavage face of rock-salt, glancing angle 8·3°.

From ref 12 - the caption shown is the original.

November 11th 1912). Their Figure 1 is reproduced here with permission of The Royal Society. On page 436 is the footnote that "We learn that Messrs. Moseley and Darwin have lately been making similar experiments to some of those recorded here. Their results, which agree with ours, have not been published." The end of the article in its concluding paragraph includes the statement "The effect which we have been describing is clearly identical in part with that which Prof Barkla (using an X-ray sensitive photographic plate) has described…in an abstract. But it seems probable that the ionisation method (see Figure 2) can follow the details of the effect more closely than the photographic method has so far been able to do." Evidently there was a close running competition between Leeds, Manchester and Liverpool Universities. The rest, as they say, is history.

Prof John R Helliwell
University of Manchester

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International School of Crystallography, Erice

AT the beginning of June this year I was fortunate to attend the 45th International School of Crystallography, entitled: present and future methods for biomolecular crystallography. The conference was held in the truly spectacular medieval mountaintop town, of Erice, Sicily. Under the direction of Vladimir Lunin, Randy Read and Alexandre Urzhumtsev a stimulating program of 60 lectures, 11 workshops and 90 poster presentations were presented over the course of 10 days. Surmising such a myriad of content is truly a challenge. Nevertheless, I will attempt to share my highlights and experiences from the meeting.

The program started rather unusually on validation, a topic often left to the end of conferences. **Jane Richardson** provided a fascinating talk on the use of MolProbity to identify the many common errors within our structures and how to alleviate such issues. **Martin Caffrey** provided a demonstration of the methodology and application of the lipid cubic mesophase for crystallisation of membrane proteins. His talks demonstrated the power of this technique, in allowing structure determination for a β2-adrenergic receptor complex, which was described in *Nature* last year.

There was an exciting presentation on the development of X-ray free electron lasers (X-FEL), in solving the structure of nanocrystals. Petra Fromme presented a solution of a photosystem 1 structure from nanocrystals using X-FEL radiation. The talk included data from last year's *Nature* paper, the progression since as well as what the future holds. We were then brought back to reality by **Sean McSweeney**, reminding us that this is not the end of synchrotron radiation for crystal structure solution, far from it. At the same time the community should be encouraged to make appropriate use of facilities available at synchrotron sources.

Kay Diederichs presented his recent *Science* paper documenting the advantages of correlation coefficients as a measure of data quality, in what has been described as "the death of R-merge". He also presented potential methods to optimise resolution cut-offs in refinement, in order to achieve the best possible model to your data. This inevitably brought forward some interesting debates on resolution cut-offs in refinement and the importance in defining a consensus for comparison of structure resolution, important in validation.

On a more sombre note, there was a special dedication to **Lodovico Riva di Sanseverino**, **Herbert Hauptman** and **David Sayre** who sadly passed away recently. This provided my highlight of the conference, with the live submission of the first Wikipedia article dedicated to David Sayre, by his former student **Pierre Thibault**.

Away from the lecture theatre there was time to explore the beautiful Town of Erice and take in the spectacular views. In addition there were excursions to sites of historical and cultural significance, with a trip to Mothia Island and local temples, including a dinner overlooking the magnificent temple and amphitheatre at Segesta. There was also an option for the sun lovers to visit local beaches including the picturesque San Vito Lo Capo beach. Evening entertainment ranged from local folk dancing displays, to discussion, singing and dancing aided by the freely flowing Marsala wine.

I have returned from Erice truly inspired. The atmosphere generated by the participants was friendly and encouraging, with students, postdocs and PI all mingling together. This brief summary barely scrapes the surface of content of the meeting and I can only recommend that you experience it for yourself in the future.

Richard Birkinshaw
University of Bristol

Honorary BCA Membership for Prof Jack Dunitz

PROF Jack D. Dunitz was awarded a certificate marking his appointment as an honorary member of the BCA at the Cambridge Crystallographic Data Centre's annual research symposium. The immediate past president of the BCA, Prof Elspeth Garman presented Jack with his award during the symposium.

Professor Jack Dunitz receiving his award from Elspeth Garman

Professor Dunitz (born Glasgow 1923), started his scientific career at the University of Glasgow, where he began research under the direction of **J. Monteath Robertson** and became familiar with the work of **Dorothy Hodgkin**. He subsequently took a position at Oxford as a postdoctoral researcher under Hodgkin's supervision, where he determined the crystal structure of a calciferol derivative, one of the most complex structures to have been determined at that time through x-ray crystallography.

After three years at Caltech, with **Linus Pauling** and **Verner Schomaker**, Dunitz returned to Oxford where he established the sandwich structure of ferrocene, before taking up further research positions at Caltech, NIH and the Royal Institution in London, then under the direction of **Sir Lawrence Bragg**. Here, Dunitz continued to collaborate with **Leslie Orgel** in the development and application of crystal-field theory.

On joining the ETH in Zurich in 1957, Dunitz began work on the conformations of medium-ring compounds, the structures of ionophores and their mode of action, relationships between crystal and chemical systems, phase transformations, polymorphism, and x-ray crystallographic methods. One of his best known achievements was the estimation of the angle of nucleophilic attack on a carbonyl group (known as the Bürgi-Dunitz trajectory). This work introduced the concept of 'structure correlation' to the scientific community.

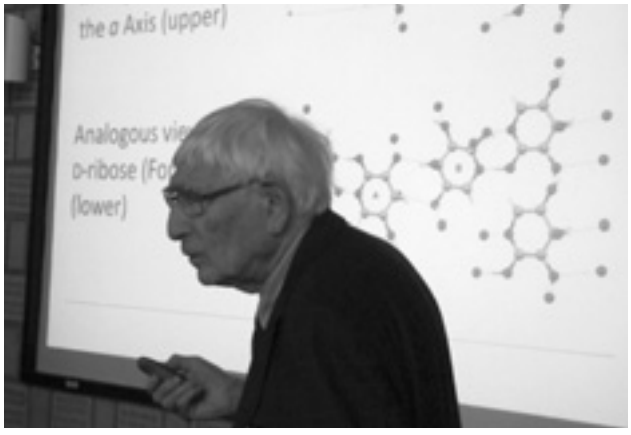
His contributions to science in general, and to chemical crystallography in particular, have been seminal and he has written or edited two monographs that have been crucial to the development of these subjects: X-ray Analysis and the Structure of Organic Molecules (Cornell University Press, 1979), and (with **H.-B. Bürgi**) the two volume multi-author set entitled Structure Correlation (VCH Weinheim, 1994).

Prof Dunitz has published nearly 400 scientific papers. His works and notebooks form one of the special collections at Oregon State University: **http://osulibrary.oregonstate.edu/specialcollections/coll/dunitz/index.html** .

Prof Dunitz has also contributed to the BCA in the most significant way possible, being one of its Founder Members; indeed Elspeth showed a slide of one of the first pages of the BCA AGM Minutes book of 1982, with his signature amongst the 43 names.

It was most fitting for the award to be made at the CCDC, given that Jack has been an avid user and supporter of the Cambridge Structural Database. As well as being a founder member of the BCA, he also served as an inaugural Governor of the CCDC from 1987-1999.

Following the award, Prof Dunitz gave a fascinating presentation on the crystal structures of D- and DL-ribose, including an account of a solid-state nmr study of the glass-crystal transition of these materials. Despite over half a million crystal structures of organic molecules being published, this fundamental molecule had hitherto evaded the efforts of crystallographers.



Neutron Scattering and NATO Science

On the Cucumber Tree: Scenes from the Life of an Itinerant Jobbing Scientist

By Peter Day

The Grimsay Press/Zeticular 2012
Price GBP 12.95
ISBN-13 978-1-84530-119-4
or **1845301196, xiv + 221 pages**

PETER Day used neutron scattering in his studies of mixed valence compounds and became Director of the Institut Laue-Langevin (ILL) from 1988 to 1991. He might have been expected to continue for two more years but returned from Grenoble to London to be Director of the Royal Institution (RI) until 1998.

Day's memoir is broadly chronological, from Kentish schooldays to relaxing at his holiday house near Andorra. However, as the subtitle suggests (the title apparently means 'on the climb'), he incorporates frank explanatory reflections on hierarchies and relationships impinging on science, scientific institutions and scientists. These range from the Oxford collegiate and tutorial system to European research collaboration. For his first appointment at Oxford in the 1960s, like later ones to the ILL and the RI, the successful candidate seemed to emerge without the formalities of advertisement or interview. Day was a strong advocate of the amply funded NATO Science Fellowships, collaborative grants, and Advanced Study Institutes in the 1960s and 70s; there is an implied contrast with the bureaucracy of European Commission funding programmes and what he refers to as Soviet-style five-year plans.

Interest in mixed valence compounds and the colours associated with low-energy electronic transitions stemmed from Oxford where his tutor was **R J P Williams**, and was encouraged, straight after Part II, during early research in **Klixbull Jorgensen**'s ('idyllic') Cyanamide fundamental research institute near Geneva. Day's 20 years at St John's was interrupted by nine months, 1966-7, collaborating with **Melvin Robin** at the Bell Telephone Laboratories (BTL); this led to the Robin-Day classification. He later advised several speculative multidisciplinary research groups in the US supported by commercial companies. Back in Europe, there was a long series of neutron scattering experiments at Harwell and Grenoble on, e.g., chromium ferromagnetics and high-temperature superconductors, so that Day was on the SRC Neutron Beam Research Committee. (He claims to have helped the merger into the SERC.)

From 1988, when he became Director, Day soon became aware that the ILL was a Societe de Droit Civile, a French not-for-profit company with a French majority in its staff. Accordingly, rules of employment, planning, etc were those of the region; the management had protracted wage negotiations with the unions, here more political than trade. In 1991, cracks in the reactor were reported to the Safety Authority so that ultimately the reactor was to be out of action for three years. Since the ISIS spallation pulsed neutron source at RAL (and funded only by the SERC) had recently been commissioned, **Mark Richmond**, the new SERC Chairman, was unsympathetic to substantial support of another neutron source. This meant that the proposed troisieme soufflé modernization programme, possibly financed by increasing the number of 'scientific member' partners, had to be postponed. After a Richmond visit to ILL, **Jane Brown**, retired in 2011 from the ILL but earlier at AERE, commented tersely on Richmond's remarks. In the event, a relatively small economy in the Research Council budget proved disproportionally expensive in loss of both beam time and goodwill at ILL. From 1991, Day would normally have contracted to be Director for a further two years but there was some disillusionment at the inflexible attitude of the unions and at the tendency of some members of the Steering Committee of an international facility to pursue national advantage. Further, the Director of the RI had indicated to Day that he was soon going elsewhere. Day writes that two more years at the ILL could lead afterwards only to the apparently 'uninviting prospect of a senior administrative position such as a University Vice-Chancellor'. Instead, he went to the RI.

In the absence of an assured income stream, the RI's Directors and Treasurers have often had cause for concern at the Institution's precarious financial state. To this the new Director Day found had to be added the crumbling state of the Albemarle Street building, including its elegant façade, and the chaotic internal organization of the staff (numbering 50, one-tenth of the ILL staff). Proposed deviations from tradition continued to be opposed by his predecessor, another solid-state chemist but centred on catalysis, who kept a toehold in the RI for several years. Day devoted much of 1996-98 to planning substantial internal reconstruction of the building (illustrated in his book by plans and sections) that would also find space for the British Association (BA), an organization similarly committed to furthering the public understanding of science. To Day's intense disappointment, the Millennium grant to accomplish this transformation was not forthcoming. A partial refurbishment was achieved by his

successor with Lottery funding but at some personal and financial-security cost. (The BA, later the British Science Festival, went to the Science Museum.)

This personal account is enjoyable and well written (the author hints that he nearly chose English and History over Chemistry and Physics at school). The 63 photographs, although only moderately well reproduced, help to make it accessible to the general reader with some scientific interest. It has a special appeal for neutron users in that it gives an insider's appreciation of the problems of running an international laboratory in France while continuing negotiations with SERC.

Derry W Jones

International Year of Crystallography

The United Nation General Assembly,

Recalling Economic and Social Council resolution 1980/67 of 25 July 1980 on international years and anniversaries and General Assembly resolutions 53/199 of 15 December 1998 and 61/185 of 20 December 2006 on the proclamation of international years,

Recognizing that humankind's understanding of the material nature of our world is grounded, in particular, in our knowledge of crystallography,

Stressing that education about and application of crystallography is critical in addressing challenges such as diseases and environmental problems by providing protein and small molecule structures suited for drug design essential for medicine and public health as well as solutions for plant and soil contamination,

Considering that the impact of crystallography is present everywhere in our daily lives, in modern drug development, nanotechnology and biotechnology, and underpins the development of all new materials from toothpaste to aeroplane components,

Considering also the significance of the scientific achievements of crystallography, as illustrated by twenty-three Nobel Prizes awarded in the area, and that crystallography is still fertile ground for new and promising fundamental research,

Considering further that 2014 marks the centenary of the beginning of modern crystallography and its identification as the most powerful tool for structure determination of matter,

Being aware that 2014 provides an opportunity to promote international collaboration as part of the sixty-fifth anniversary of the founding of the International Union of Crystallography,

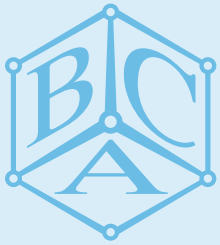
Noting the broader welcome by the crystallographic community worldwide of the idea of having 2014 designated as the International Year of Crystallography,

Recognizing the leading role of the International Union of Crystallography, an adhering body of the International Council for Science, in coordinating and promoting crystallographic activities at the international, regional and national levels around the world,

1. Decides to proclaim 2014 the International Year of Crystallography;

2. Invites the United Nations Educational Scientific and Cultural Organization, mindful of the provisions of the annex to Economic and Social Council resolution 1980/67, to facilitate the implementation of the International Year of Crystallography, in collaboration with Governments, the International Union of Crystallography and its associated organizations throughout the world, relevant organizations of the United Nations system, the International Council for Science, as well as other relevant non-governmental organizations, also invites the United Nations Educational Scientific and Cultural Organization to keep the General Assembly informed of progress made in this regard, and stresses that the costs of all activities that may arise from the implementation of the present resolution above and beyond activities currently within the mandate of the lead agency should be met from voluntary contributions, including from the private sector;

3. Encourages all Member States, the United Nations system and all other actors to take advantage of the Year to promote actions at all levels aimed at increasing awareness among the public of the importance of crystallography and promoting widespread access to new knowledge and to crystallography activities.



British Crystallographic Association Industrial Group

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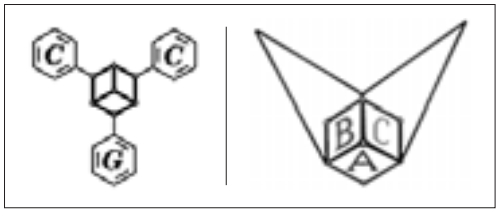

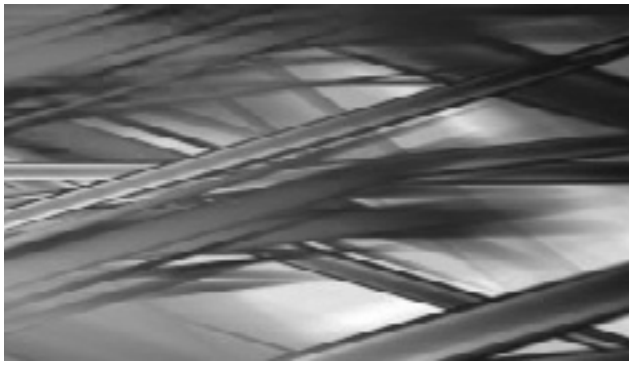

THIS year the CCG and IG groups will be joining forces for their annual Autumn Meeting, which will be on the topic of "Perspectives on Crystallisation for Chemical and Industrial Crystallographers". A plenary session will provide an overview of the role of crystallisation in control of the solid form and the influence this has on the manufacturing process with the main speaker being **Dr Simon Black** (Astra Zeneca). This will be followed by two themes based around predictive tools for crystallisation and an education session explaining the science of crystal growth and practical hints on how to grow better crystals. The meeting will be held at the Paragon Hotel, Birmingham on 14th November - so please save the date as we look forward to joining you for an exciting day which is assured to have something new to learn for everyone!

Simon Coles, **Cheryl Doherty** and **Elizabeth Shotton**

CCG-IG Autumn Meeting 2012*

"Perspectives on Crystallisation for Chemical and Industrial Crystallographers"

Wednesday 14th November 2012, The Paragon Hotel Birmingham

10:30	Registration (COFFEE/TEA)
	Session 1 *(Chair: Simon Coles)*
11:00	**Simon Black** (AstraZeneca)
11:45	**Alastair Florence** (University of Strathclyde)
12:30	LUNCH
	Session 2 *(Chair: Cheryl Doherty)*
14:00	**Sally Price** (University College London)
14:30	**Cambridge Materials Chemistry Group** (University of Cambridge)
15:00	COFFEE/TEA
	Session 3 *(Chair: Elizabeth Shotton)*
15:30	**T.B.A.**
16:00	**Kevin Roberts** (University of Leeds)
16.30	CLOSE

***** *sponsored by **Rigaku** and **Pfizer***

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.

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

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

2-6 September 2012
ECSCRM2012. 9th European Conference on Silicon Carbide and Related Materials, Saint Petersburg, Russia.
https://www.ecscrm-2012.org/

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

3-7 September 2012
CMD-24, ECOSS-29, ECSCD-11 and CMMP-12. European Condensed Matter Conferences, Edinburgh, UK.
http://www.cmd-24.org/Home

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

11-14 September 2012
Mc Phase School 2012, Grenoble, France.
http://www.ill.eu/news-events/events/mc-phase-2012/

13 September 2012
First Annual Open Day of the EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation, University of Strathclyde, Glasgow, UK.
www.cmac.ac.uk

13 September 2012
Macromolecular Structure: 25th Anniversary Meeting of the NCMH, Nottingham, UK.
http://www.nottingham.ac.uk/ncmh/25th-anniversary/index.html

14-15 September 2012
Applications of Precession Electron Diffraction, Manchester, UK.
http://www-hrem.msm.cam.ac.uk/events/Precession_Meeting/main.xhtml

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

16-19 September 2012
MOF2012. 3rd International Conference on Metal-Organic Frameworks and Open Framework Compounds, Edinburgh, UK.
http://events.dechema.de/en/mof2012

16-21 September 2012
50th EHPRG Meeting, Thessaloniki, Greece.
http://www.ehprg.org/meetings/

17-19 September 2012
Neutrons for Energy; Advanced Materials for Energy Storage, Delft, The Netherlands.
http://tnw.tudelft.nl/en/about-faculty/departments/radiation-radionuclides-reactors/research/research-groups/fame/workshops-conferences/neutrons-for-energy/

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

17-21 September 2012
HSC14: Neutrons and Synchrotron Radiation in Materials for Energy, Grenoble, France.
http://www.esrf.eu/events/conferences/HSC

17-21 September 2012
E-MRS 2012 Fall Meeting, Warsaw, Poland.
http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=500&Item=172

17-22 September 2012
Nanomaterials: Application and Properties, Alushta, Ukraine.
http://nap.sumdu.edu.ua/index.php/nap/nap2012

19 September 2012
Crystal Growth - Point Defects, Lyon, France.
http://www.afc.asso.fr/index.php?option=com_content&view=article&id=159:croissance12&catid=45:les-colloques&Itemid=85

20-21 September 2012
A Celebration of the 50th Anniversary of the Diode Laser, Coventry, UK.
https://www.eventsforce.net/iop/frontend/reg/thome.csp?pageID=90978&eventID=233&eventID=233

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

24-26 September 2012
NOBUGS 2012: New Opportunities for Better User Group Software, Rutherford Appleton Laboratory, Didcot, UK
http://nobugs2012.org/

24-28 September 2012
SR Summer School 2012, Oxford and Didcot,Oxon, UK.
http://www.diamond.ac.uk/Home/Events/SR-Summer-School-2012.html

26-27 September 2012
13th Ad Hoc Workshop on Jana2006: Powder Diffraction, Prague, Czech Republic.
http://jana.fzu.cz/w013.html

26-27 September 2012
Workshop on Transient and Ultrafast Processes in X-ray Excited Matter, Hamburg, Germany.
http://conferences.cfel.de/transient_2012/

30 September - 2 October 2012
70th Annual Pittsburgh Diffraction Conference, Menlo Park, CA, USA.
http://www.pittdifsoc.org/PDC_2012/index.htm

1-3 October 2012
Basic Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA
http://www.icdd.com/education/rietveld-workshop.htm

3-5 October 2012
A Symposium in honour of Joe Zaccai's Career: Structural Dynamics and Dynamical Structures, Grenoble, France.
http://www.ill.eu/sdds2012/

4-5 October 2012
Advanced Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA.
http://www.icdd.com/education/rietveld-workshop.htm

7-9 October 2012
ICRS-9. Ninth International Conference on Residual Stress, Garmisch-Partenkirchen, Germany.
http://www.mf.mpg.de/en/abteilungen/mittemeijer/icrs9/index.htm

7-11 October 2012
MS&T12: Materials Science & Technology 2012 Conference and Exhibition Pittsburgh, PA, USA.
http://www.matscitech.org/

10-12 October 2012
40 Years D11 - Status & Perspectives of Small Angle Scattering at ILL, Grenoble, France.
http://www.ill.eu/news-events/events/40-years-d11-status-perspectives-of-small-angle-scattering-at-ill

14-18 October 2012
2012 AAPS Annual Meeting and Exposition, Chicago, IL, USA.
http://www.aaps.org/annualmeeting/

14-18 October 2012
Weak Protein-Ligand Interactions: New Horizons in Biophysics and Cell Biology - Biophysical Society Thematic Meeting, Beijing, China.
http://biophysics.org/2012china/Home/tabid/2984/Default.aspx

14-18 October 2012
2012 American Association of Pharmaceutical Scientists Meeting and Exposition Chicago, IL, USA.
http://www.aaps.org/annualmeeting/

14-19 October 2012
IWN2012. International Workshop on Nitride Semiconductors, Sapporo, Hokkaido, Japan.
http://iwn2012.jp/

15-16 October 2012
14th Ad Hoc Workshop on Jana2006: Magnetic Structures, Prague Czech Republic.
http://jana.fzu.cz/w014.html

16-18 October 2012
Handheld XRF Workshop, Newtown Square, PA, USA.
http://www.icdd.com/education/handheld-xrf-**workshop.htm**

17-19 October 2012
SYNEMAG2012: Synchrotron and Neutron Applications of High Magnetic Fields Grenoble France.
http://www.esrf.eu/events/conferences/synemag-2012

17-20 October 2012
Murnau Conference on Structural Biology of Molecular Transport, Murnau, Germany.
http://www.murnauconference.de/2012/index.html

17-24 October 2012
EMBO practical course on Solution Scattering from Biological Macromolecules, Hamburg Germany.
http://events.embo.org/12-sas/

18-19 October 2012
International Symposium - "Quasicrystals Today", Grenoble, France.
http://qcgrenoble2012.grenoble.cnrs.fr/

20-27 October 2012
BioCrys2012. Fundamentals of Modern Methods of Biocrystallography, Oeiras, Portugal.
http://www.febs.org/index.php?id=652

22-26 October 2012
Crystal structure prediction using the USPEX Code, Lausanne, Switzerland.
http://www.cecam.org/workshop-0-635.html

26 October 2012
A Life of Refinement - 50 Years of Neutron Scattering: Colloquium in Honour of Alan Hewat, Grenoble France.
http://www.ill.eu/news-events/events/alan-hewat-colloquium

27-28 October 2012
Satellite of EPDIC13 - Accuracy of Crystal Structures Obtained from Powder Diffraction Data ILL, Grenoble France.
http://www.accuracy2012.sav.sk/

28-31 October 2012
EPDIC13. 13th European Powder Diffraction Conference, Grenoble, France.
http://epdic13.grenoble.cnrs.fr/

28-31 October 2012
7th International Workshop on Modeling in Crystal Growth (IWMCG-7), Taipei, Taiwan.
http://iwmcg7.ntu.edu.tw/

4-7 November 2012
2012 Geological Society of America Annual Meeting & Exposition, Charlotte, NC, USA.
http://www.geosociety.org/meetings/2012/

6-8 November 2012
Workshop on Advanced Diffraction Data Collection with Multi-Axis Goniometer and Single-Photon Counting Detector in Protein Crystallography, Paul Scherrer Institute, Villigen Switzerland.
http://indico.psi.ch/conferenceDisplay.py?ovw=True&confId=1753

11-13 November 2012
20th PDSI: Protein Structure Determination in Industry 2012 Chantilly Forest, Paris France.

14-16 November 2012
Advances and Frontiers in Chemical Spectroscopy with Neutrons Abingdon, UK.
http://www.isis.stfc.ac.uk/news-and-events/events/2012/advances-and-frontiers-in-chemical-spectroscopy-with-neutrons13154.html

18-22 November 2012
11th International School and Workshop on Macromolecular Structure of Biological and Non-biological Materials, Hurghada, Red Sea, Egypt.
http://www.iucr.org/news/notices/meetings/meeting_mm_structure_11

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

19-20 November 2012
Polymorphism & Crystallization: Chemical Development Issues - 10th International Conference and Exhibition, Prague, Czech Republic.
http://www.scientificupdate.co.uk/conferences/conferences-schedule/details/89-Polymorphism-and-Crystallization.html

21-23 November 2012
SFBBM-SFB 2012: Molecular Mechanisms and Integrated Life Processes Grenoble France.
http://sfbbm-sfb2012.u-strasbg.fr/index.php?_lang=uk

25-30 November 2012
Symposium VV: Advanced Materials Exploration with Neutrons and Synchrotron X-Rays - 2012 MRS Fall Meeting & Exhibit Boston, MA, USA.
http://mrs.org/f12-cfp-vv/

26-27 November 2012
Workshop on the Science and Technology of 4th Generation Light Sources Based on Superconducting Technology, Stockholm, Sweden.
http://agenda.albanova.se/conferenceDisplay.py?confId=3489

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

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

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

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://www.crystallography.org.uk/

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

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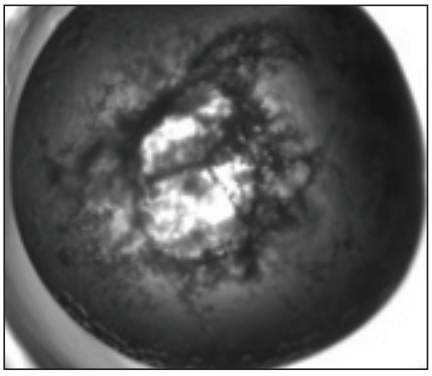
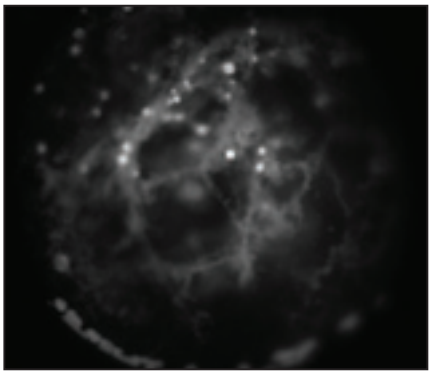


Visible image



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