

# Crystallography News

British Crystallographic Association



Issue No. 114 September 2010

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## ACA MEETING p12



**YOUR ECM  
WARWICK  
2013 LOGO  
HERE**



**BCA Spring Meeting p6**

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**ACA Meeting Reports p10**

**News from the Groups p16**

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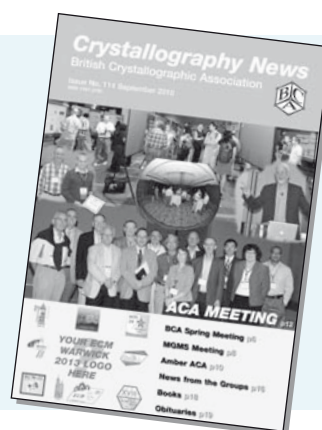
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## *This month's cover:*

*ACA photos by  
Peter Mueller,  
ECM28 logo  
competition*



# From the Editor



**ONCE** again this month's cover conveys an appeal to the creativity of our readers. Last time it was to design an information-rich poster illustrating the scope of the BCA. This time we need a logo for the 28th European Crystallographic Meeting to be

held at Warwick University in 2013: a simple, powerful image that symbolises the cachet of crystallography and the wonders of Warwick. Previous ECM logos are reproduced in colour on the cover and in black-and-white surrounding the detailed announcement on an inside page. This is not an inadvertent waste of paper: the new logo must look good in both styles of display. With some of us having just experienced ECM26 in Darmstadt and remembering how successfully the UK hosted the 1999 IUCr Congress in Glasgow (or should that be "Dramstadt") I hope that inspiration will be forthcoming. To remove any distraction the Puzzle Corner is suspended until next issue.

The issue also demonstrates the impact that crystallography is having on the scientific world. *Acta Crystallographica Section A* has achieved an impact factor of 49.9. Most of us would agree that this is simply a case of this journal at last claiming its rightful place in the scientific firmament. The details, which have something to do with SHELX, are reproduced in this issue. If only we could have persuaded **George Sheldrick** to send his magisterial article to Crystallography News...

This happy event finally disproves a hypothesis I formed a long time ago: the length of a journal's name correlates inversely with its impact. While my finest outpourings in the *Journal of the Chemical Society Perkin Transactions II* or *Acta Crystallographica* struggled to attain an impact factor somewhere near 2, this figure was effortlessly surpassed by shorties like *Science* (29.7), *Nature* (34.5), *Cell* (31.2) and *Gut* (9.4). I thought that if Freudian psychologists had founded journals called *Ego* and *Id*, they might have topped the tables, while *Journal of the Less Common Metals* never stood a chance.

We also celebrate our BCA Honorary Member and Nobel laureate **Venki Ramakrishnan**. At the recent meeting of

the American Crystallographic Association the beautifully illustrated plenary lectures given by him and his fellow Nobel laureates **Tom Steitz** and **Ada Yonath** made the structure and function of the ribosome clear even to non-MX specialists. They showed that this research has both practical and philosophical impact. Practically, we now understand where many of our most important antibiotics bind, and we can envisage targets for the design of new ones. Philosophically, we can begin to speculate about how this complicated machinery could have evolved from simpler precursors.

It is never easy for one person to summarise a vast meeting with parallel sessions like the ACA. I am most grateful to **Amber Thompson**, who was already busy with a lecture and two posters, for contributing a report. As well as summarizing the sessions she found most interesting, she has made some thought-provoking comparisons between the BCA and the ACA.

At the time I write this column, there is still another summertime treat in store, namely the European Crystallographic Meeting. However, it's not too soon to start thinking about our stimulating Group Meetings this autumn. We carry news of one meeting, organized by the Industrial Group, in the awe-inspiring surroundings of Diamond, and another, by the Chemical Crystallography Group, meeting in the elegant surroundings of the Royal Society of Edinburgh. Seeing another heading, "BCA Annual Spring Meeting", you might be expecting one last tardy report on the 2010 meeting. However, you would be wrong: the year is 2011! This is not just our Chair, **Arwen Pearson**, being admirably pro-active. The deadline for submission of abstracts to be presented orally at the main meeting is October 29, so if you prefer standing by a lectern instead of a poster, it's time to start writing!

I conclude by mentioning a change in my personal circumstances. After 38 years' service I have retired from Aston University. Therefore, please send all correspondence and e-mails to my home, as shown in my revised entry on the Council Page. I shall be taking up an honorary appointment with the Cambridge Crystallographic Data Centre, and I am very much looking forward to the intellectual stimulation that this will bring.

**Carl Schwalbe**



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

Full committee details on the BCA website [www.crystallography.org.uk](http://www.crystallography.org.uk)

Spring Meeting Registration and Subscriptions:

[www.crystallography-meetings.org.uk](http://www.crystallography-meetings.org.uk)

# From the President



**THE** lovely summer weather we have had in June and July appears to have temporarily deserted us, although I am just back from the ACA Meeting in Chicago, and it was certainly hot and steamy there. The ACA was a well attended and vibrant meeting, with many interesting talks and posters in all branches of crystallography. At the opening reception, I

was honoured to be photographed with Sine Larsen, IUCr President, and Judy Kelly, ACA President. While I long for the day when it will not be a notable fact that the IUCr, ACA and BCA Presidents all happen to be female, it seemed a juxtaposition worth recording for posterity. As well as some memorable sessions hearing new science, I very much enjoyed an evening spent (mainly dancing!) in Buddy Guy's Legends Club with a live band playing Blues, and ably hosted by Rayonix: a real taste of Chicago.

The European Crystallography Meeting (#26) in Darmstadt is the next big crystallography meeting on the calendar, and at the ECA Council Meeting there we will be reporting on our planning for ECM29 in Warwick in 2013. In fact, 2013 is being designated the 'International Year of Crystallography', so we will have a great opportunity to showcase our science to a wider audience, and I hope we can include some extra public outreach in the BCA activities that year. We will be discussing ways to go about this at our September 2010 Council meetings, and any ideas Members have will be most welcome (just send me an e-mail).

Following the ECM, the BCA/CCP4 Protein Crystallography Summer School will be held in Oxford from the 5th to 10th September. As well as taking participants through the 'pipeline' of macromolecular crystallography from protein preparation to crystallisation, and data collection and processing to structure validation, we will go on a 'field trip' to Diamond Light Source and have a social evening cruising down the Thames on a Salters Steamer. We are delighted that our after dinner speaker at the Summer School will be **Dr. Venki Ramakrishnan** from the MRC-LMB in Cambridge, Nobel Prize Winner in Chemistry in 2009 and newly an Honorary Member of the BCA in 2010. We are sure he will inspire our students!

For the 2010 School, we were staggered to receive over 130 applicants for the 45 places, with students interested in attending from every continent on the globe (except Antarctica!). In fact I am still receiving e-mails enquiring if there are any spare places. This level of interest in

the School underlines the vital role of such educational activities, and it is clear that we would have to run at least 3 such schools annually to satisfy the demand. Unfortunately this is just not a realistic proposition.

Planning for the BCA 2011 Spring Meeting, to be held at Keele University from 12th to 14th April (Young Crystallographers on the 11th/12th), is now well underway led by **Arwen Pearson**, and some details of the programme are already available later in this issue. I am happy to say that the 2010 Warwick Spring Meeting broke even, so we will be adopting a similar strategy for speakers expense reimbursement in 2011.

On 12th May I represented the BCA at the Royal Society's 100th anniversary celebrations of the birth of **Dorothy Hodgkin**. The afternoon and evening was a stimulating mixture of reminiscence and reports of ongoing/future science, with contributions from those who worked with Dorothy, her family members, past and present Royal Society Dorothy Hodgkin Fellows, and a final session (in which I spoke) on the Future of Dorothy's science. I am grateful to the BCA Group Representatives for each providing me material for my presentation on the crystallographic areas they foresaw as developing and engendering excitement in the 21st century. On reflection, a summary of these might make an interesting article for a future Crystallography News!

I had a wonderful excuse to delve more deeply into the life of Dorothy Hodgkin and read some details of her huge contribution to crystallography in the lead up to giving the annual Dorothy Hodgkin Memorial lecture organised by Somerville College and AWISE on 9th March in the Oxford University Museum to an eclectic mixture of the general public (including some school children), friends (among them 5 of my 1972 school leavers A'Level group) and assorted colleagues. This lecture aimed to explain protein crystallography and trace modern structure determination in comparison to the methods used by Dorothy Hodgkin in just 55 minutes... For those fortified with a good drink, it can be found at:  
[www.some.ox.ac.uk/2845/all/1/Dorothy\\_Hodgkin\\_Memorial\\_lecture\\_2010.aspx](http://www.some.ox.ac.uk/2845/all/1/Dorothy_Hodgkin_Memorial_lecture_2010.aspx)

On a personal note, I would like to close this letter by thanking all those of you who sent me messages of sympathy and condolence on the death from a brain tumour in July of my husband, John Barnett (see Times Obituary 20/8/10), and especially the Officers for their unflinching and much appreciated support over these last 9 difficult months.



# LUDO FREVEL SCHOLARSHIP

## Application Deadline: 29 October 2010

**TO** encourage promising graduate students to pursue crystallography oriented research, the International Centre for Diffraction Data (ICDD) has established the Ludo Frevel Crystallography Scholarship Fund. Multiple recipients are selected on a competitive basis, each receiving an award of \$2,500. Applications must be received by the ICDD by 29 October 2010.

Qualifications for the applicant: The applicant should be enrolled in a graduate degree program during the 2011 calendar year with major interest in crystallography, e.g. crystal structure analysis, crystal morphology, modulated structures, correlation of atomic structure with physical properties, systematic classification of crystal structures, phase identification and materials characterization. The term of the scholarship is one year. In order to broaden the geographic distribution of the scholarships, the committee will give special consideration to applicants in regions underrepresented in the past. These include Turkey, Africa & Middle Asia, China, India and Southeast Asia (Indonesia), Newly Independent States, and Latin America. We encourage applicants from all regions to apply.

Scholarship awards are made possible by donations from both private and industrial sectors. Donations can be directed to the Ludo Frevel Crystallography Scholarship at the address below.

Visit our web site at: <http://www.icdd.com/resources/awards/frevel.htm> for complete information on our new on-line application procedure.

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### BCA Corporate Membership

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

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

The cost of this membership is **£750.00** per annum. To apply for Corporate Membership, or if you have any enquiries, please contact:

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# BCA Spring Meeting 2011

## BCA Annual Spring Meeting University of Keele 11-14th April 2011

**I am delighted to invite you to the BCA Spring Meeting, to be held from the 11-14th April 2011 at the University of Keele, featuring 30 scientific sessions and 4 plenary lectures. After the now traditional Young Crystallographers' satellite meeting on Monday the 11th April the main meeting will run from 11:30am on Tuesday 12th April until 1:30pm on Thursday 14th April. We also welcome back the XRF community this year for the fourth time.**

Although this year no formal overarching theme has been given to the meeting, during the planning process it has become clear that there are an increasing number of scientific and methodological areas that are of broad interest across the groups of the BCA (Biological Structures, Chemical Crystallography, Physical Crystallography and the Industrial Group). This is reflected in the co-sponsorship of many sessions by multiple groups and we hope that you will be as excited as we are by the opportunity at this meeting to explore the interests we share as a crystallographic community. This year, as well as a series of workshops on sample preparation and calibration on the 12th April, the XRF sessions are also heavily integrated into the main meeting in joint sessions with the Industrial and Physical Crystallography Groups.

### Dates, Links & Abstract Submission

All the latest information about the meeting, including the programme, registration and abstract submission, can be found at the meeting website: <http://crystallography.org.uk/spring-meeting-2011>

### Deadlines:

Abstracts to be considered for oral presentations in the main meeting: 29th October 2010

Abstracts to be considered for oral presentations in the YC satellite meeting: 14th January 2011

Poster abstract submission deadline: 4th February 2011.

### YC Satellite 2011:

To all the Young Crystallographers out there: here are a few dates for your diaries! In style of previous years the YC Satellite will precede the main BCA Spring Meeting also

at Keele University. There will be three oral and one poster session starting midday on Monday, 11th, and closing by midday on Tuesday, 12th April 2011. These sessions are a fantastic opportunity to present and discuss your work in a friendly and relaxed atmosphere – difficult questions are simply not allowed. If you are a YC (grad student or postdoc within 5 years of graduation) all you have to do is submit your abstracts for oral contributions by 14th January 2011, and for posters by 4th February 2011 via the main meeting website. Best of all, the YC Satellite is free for those attending the whole BCA Spring Meeting (including accommodation and dinner on Monday). This year we will have the first Parkin Lecture given by a YC and we will finish our Satellite with a workshop on career development - so make sure you don't miss out!

**Susanne Coles (née Huth)**  
YCG Chair

### Currently Confirmed Sessions

	Groups
From molecular to supramolecular	CCG
MX and small molecule crystallography - a combined future	CCG/BSG
Structure/Property correlations in luminescent materials	CCG
Dynamic data, dealing with limited data	CCG/PCG
New Developments at Diamond	PCG/CCG
Local Structure	PCG
High pressure and energetic materials	PCG
XRF: New Developments	XRF
XRF: Applications	XRF/IG
Time-resolved structural studies	PCG/BSG/CCG/YC
Cultural Heritage	PCG/XRF
Materials Science - white beam methods	PCG/IG
Radiation damage in structural science	BSG/PCG/CCG/YC
Crystallization	IG/CCG
Stress-strain microstructures	IG/PCG
Materials Science - powder methods	IG
Getting more from diffraction data	CCG
XRF: Novel Techniques	XRF

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David Taylor (XRF)  
David Massey (Northern Networking)  
Elspeth Garman (BCA President)

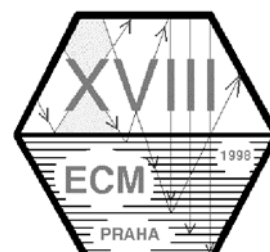


This number plate was photographed by a friend of Stan Nyburg on a visit to Malta last October. It seems plain that this must reflect the owner's interest in crystallography.



## Advance Notice of ECM28 Logo Competition

At the European Crystallographic Meeting in Istanbul last year, the BCA presented a successful bid to host the 2013 ECM at the University of Warwick. One of the things we have to do is choose a logo for the Meeting, and in keeping with tradition we will do this by running an open competition. Details will appear on the BCA website at <http://crystallography.org.uk>, and the winner will receive the prize of a free registration for ECM28. Some previous ECM logos are shown on this page and can also be seen at <http://www.ecanews.org/meetings.php>.



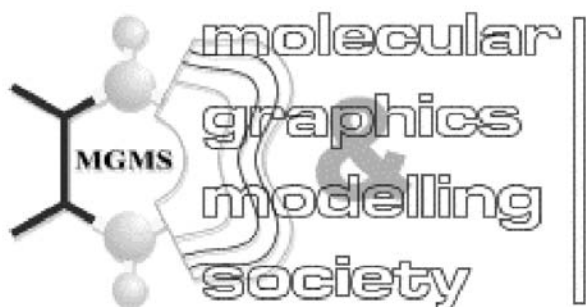
The ECM28 Organising Committee





# MGMS Meeting

## PROGRESS IN CRYSTAL STRUCTURE PREDICTION?



**CRYSTAL** structure prediction has been a major objective for the computational chemistry community and draws considerable attention from the entire crystallographic community due to both the academic challenge involved and the potential applications of such methods. Such applications range from polymorph screening and solid form selection during drug development in the pharmaceutical industry to the computer-aided design of novel materials. Understanding the packing of molecules into crystals and the energy and property differences between polymorphs also has important implications for gaining further insight into the nature of intermolecular interactions.

Notable progress has been made in this field over the past few years [1] and a meeting is being organised to discuss this progress and current research directions. This meeting, organised by the Molecular Graphics and Modelling Society (MGMS), is associated with the MGMS Silver Jubilee Prize. This annual Award, set up to mark the Twenty-Fifth Birthday of the Society, is to recognise the work of talented young researchers in the earlier stages of their careers. It was first awarded in 2008 and covers the area of computational chemistry and associated disciplines. The prize was recently awarded to **Graeme Day** (a Royal Society university Research Fellow in the Department of Chemistry, University of Cambridge), who was previously honoured with the BCA Chemical Crystallography Group CCDC prize for younger scientists in 2006 for his contributions to the field of crystal structure prediction.

The one day meeting will be held on 8 December, 2010, at the School of Oriental and African Studies (SOAS), Russell Square, London. The meeting will overview the latest in computational methods and their applications

for understanding and predicting the crystal structures of organic molecules. The results of the current blind test of crystal structure prediction, being organised by CCDC, will also be discussed. The programme for the meeting is outlined below. All BCA members are welcome to attend and should consult <http://www.mgms.org/diary.htm> for registration details. The organisers would particularly like to encourage poster presentations and free registration will be offered to the first 20 students who would like to present a poster.

10.20am Opening Remarks

10.30am **Dr Graeme Day** (University of Cambridge)  
MGMS Silver Jubilee Prize Lecture: "Progress in Crystal Structure Prediction?"

11.15am **Dr Neil Feeder** (Pfizer Global R&D)  
"The Emerging Application of Computational Methods to Pharmaceutical Solid Form Selection"

11.45am **Prof. Paul Raithby** (University of Bath)  
"Directed Assembly of Extended Structures with Targeted Properties - the new Chemistry Grand Challenge network"

12.00am Lunch and posters

1.30pm **Dr Peter Galek** (Cambridge Crystallographic Data Centre)  
"Getting to grips with potential crystal forms: Database-guided assessment of drug candidates"

2.00pm **Dr John Kendrick** (Institute of Pharmaceutical Innovation, University of Bradford)  
"The role of solid state density functional theory in predicting the crystal structures of organic molecules"

2.30pm **Prof. Jamshed Anwar** (University of Bradford)  
"Mode of Action and Design Rules for Additives That Modulate Crystal Nucleation"

3.00pm Refreshments and posters

3.30pm **Prof. Kevin Roberts** (University of Leeds)  
"Synthonic Engineering: from Crystal Engineering to Engineering Crystallography"

4.00pm **Prof. Sally Price** (University College London)  
"Why do we over-predict polymorphism?"

4.40pm Closing remarks

[1] Graeme M Day, Timothy G Cooper, Aurora J Cruz-Cabeza, Katarzyna E Hejczyk, Herman L Ammon, Stephan X M Boerrigter, Jeffrey S Tan, Raffaele G Della Valle, Elisabetta Venuti, Jovan Jose, Shridhar R Gadre, Gautam R Desiraju, Tejender S Thakur, Bouke P van Eijck, Julio C Facelli, Victor E Bazterra, Marta B Ferraro, Detlef W M Hofmann, Marcus A Neumann, Frank J J Leusen, John Kendrick,

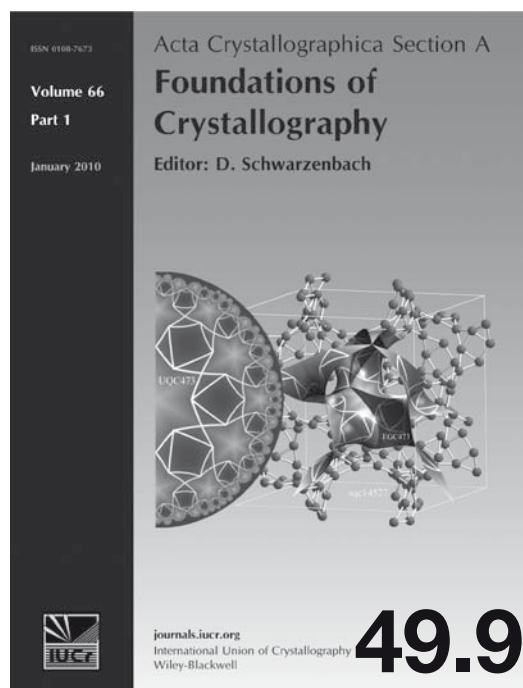
Sarah L Price, Alston J Misquitta, Panagiotis G Karamertzanis, Gareth W A Welch, Harold A Scheraga, Yelena A Arnautova, Martin U Schmidt, Jacco van de Streek, Alexandra K Wolf, Bernd Schweizer, Significant progress in predicting the crystal structures of small organic molecules – a report on the fourth blind test, *Acta Crystallographica*, B65, 107-125 (2009).

## SHELX makes an impact

**THE** recent release of Thomson Reuters' *Journal Citation Report for 2009*, reporting an impressive impact factor of 49.9 for *Acta Crystallographica Section A: Foundations of Crystallography*, has excited much comment amongst crystallographers. The primary cause of this high impact factor is a single feature article by George Sheldrick, *A short history of SHELX* [*Acta Cryst.* (2008). A64, 112-122]. Published in a special issue to celebrate 60 years of *Acta Crystallographica* and the IUCr, it gives an account of the development of the SHELX system of computer programs from 1976 to date.

The article has provided the crystallographic community with a citable reference when one or more of the programs, amongst the most widely used in structure determination, are employed in the course of a crystal structure study. Most citations have been made by small-molecule crystallographers, but citations have also come from articles reporting the structure of biological macromolecules. Until the publication of this article, the programs in the SHELX package were typically referenced by citing the unpublished computer programs themselves. The total number of citations in the Thomson Reuters statistics (6653 by the end of June 2009 - by any measure a significant achievement) is, of course, dwarfed when the total number of articles that have cited the unpublished programs is considered. A search of *Crystallography Journals Online* shows that over the years more than 43,000 articles published in IUCr Journals alone have referenced SHELX programs.

This article and its citations will be considered in the impact factor calculation for *Acta Crystallographica Section A* this year and next year. The journal impact factor that will be reported in 2012 is therefore likely to return to a more normal level of about 2.0-2.5.



Gernot Kostorz  
Brian McMahon  
Peter Strickland

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# ACA Meeting Reports

**THIS** was my first visit to an American Meeting and it was a real experience. Despite the cost of travelling and the very expensive accommodation, the UK and Europe were extremely well represented, and it was nice to see so many familiar faces. This was all the more so as it is true what they say, everything really is much bigger there. The meeting opened on the Saturday evening with Chicago style pizzas surrounded by exhibitors, but one of my over-riding memories of that evening will always be a conversation with two eminent scientists who were talking well over my head, quite literally! Some of the famous people I came across (many of whom had just been names before), included Bob Von Dreele, Ton Spek, Carol Johnson, I. David Brown, George Sheldrick, Brian Toby, Tony Linden, Peter Mueller, Wladek Minor, Tom Proffen, Håkon Hope, Judy Flippen-Anderson, Jenny Glusker, Sander van Smalen, Carol Brock and Hans-Beat Bürgi to name but a few.

The sessions began on Sunday morning, which at least had the advantage of being a lot drier than the day before, which had been hot and humid with thunderstorms and flash flooding. The morning included a session in memory of **Louis Delbaere**, the Canadian scientist who died suddenly last year. With the sad loss of Louis and, more recently, **Lachlan Cranswick**, Canadian crystallography has lost two of its leading figures; they will be greatly missed. There was also a general interest session including discussion of the fraudulent structures published in Acta Crystallographica Section E presented by **Tony Linden** (Zurich). One of the parallel sessions covered "Non-ambient Environments" and was dominated by UK scientists as it included **John Evans** (Durham), **Dominic Fortes** (UCL), **Russell Morris** (St. Andrews), **Craig Robertson** (Durham) and **Stephen Moggach** (Edinburgh), discussing everything from high pressure to low temperature and much else besides.

There were a number of excellent sessions, one of which took place on Sunday afternoon and was convened by **Joe Reibenspies** (Texas). It concerned Absolute Structure and focussed primarily on the validity of the Flack Parameter. I thought this had the potential to be an extremely controversial session, but the overwhelming conclusion seemed to be that the criterion given in Flack and Bernardinelli (J. Appl. Cryst., 2000) is too strict. The session was headed by **Simon Parsons** (Edinburgh) who discussed some careful experiments carried out on light atom structures and the application of quotient restraints, followed by **Martin Lutz** (Utrecht) who discussed the importance of standard uncertainties in data collection,

refinement and analysis. After the break, there were a number of people looking at samples with a weak anomalous signal concluding that even when the standard uncertainty is large, if the material is enantiopure it may be possible to draw a conclusion. Whether or not any of the proponents would publish such a conclusion is a different matter, however.

Monday was dominated by an all day session commemorating **Bob Bau** (University of Southern California) who died at the very end of 2008. Bob had been president of the ACA and had a particular interest in metal hydride complexes and neutron diffraction which were reflected in the session which was entitled, "The First Element". Although Bob was a US crystallographer, this session was well represented by UK and European speakers, including **Carl Schwalbe** (Aston) discussing salts of flubiprofen and **Chick Wilson** presenting neutron diffraction results as well as **Larry Falvello** (Zaragoza), **Alberto Albinati** (Milan) and **Hans-Beat Bürgi** (Berne). The "Data Collection Strategy" meeting that ran in parallel with this session was also very interesting with talks from **Mathias Meyer** (Oxford Diffraction), who spoke at the BCA back in the spring and **Simon Teat** who many of us will remember from Station 9.8 at Daresbury.

Tuesday featured two more superb sessions. The first of these was convened by **Peter Mueller** (MIT) and entitled "Blast from the Past: What was Old is New Again". It began with a truly superb talk from **Larry Falvello** (Zaragoza) on the precession method, a topic that was continued by **Carol Brock** (Kentucky). This is a notoriously difficult technique to understand from a book, but it laid out the diffraction data in a much more logical way, so much so, that synthesised precession photographs are still used today. **Jenny Glusker** (Fox Chase, Philadelphia) continued the session with a discussion of electron density maps and what they can tell us. **Bruce Foxman** (Brandeis) then gave an excellent discussion of comparing orientation matrices with examples where this is critical, and the session was closed by **Chuck Campana** (Bruker) and **Larry Dahl** (Wisconsin-Madison) discussing complex iron carbonyl clusters.

On Tuesday there was also an evening session, which was surprisingly well attended (although perhaps that was due to the alcoholic sponsorship from Oxford Diffraction...). This was unusual in that it consisted of people presenting "problem structures" with the title, "Would you Publish This?" This was an interesting session because it broached an awkward subject and unlike the Absolute Structure session two days earlier, it didn't feel like a consensus was



reached. This was exemplified by a structure presented by **Gary Nichol** (Arizona, formerly Newcastle), where the relative stereochemistry was desired, but the R(int) was extremely high even on the low data. Opinion was clearly divided between those that felt even the poor result was information and should be published with the rest of the data, and those that felt it may be faulty and was therefore unreliable.

Wednesday was the last day of the exhibition, so I spent much of it talking to the exhibitors, but personal highlights for me were the “Cool Structures” and “Precipitates and Voids” sessions that ran in parallel in the morning. The first of these had little to do with temperature and was really just a forum for people to present some of the weird and wonderful structures they had looked at; I was particularly taken with a talk on fullerene structures by **Marilyn Olmstead** (California), which covered some of the challenges associated with these materials. The second session included a range of techniques, including small angle scattering, X-ray spectroscopy, neutron diffraction, and resistivity. The UK was well represented by **Alex Graham** and **Peter Byrne** from Edinburgh, using high pressure crystallography to study MOFs and salicyladoxime complexes (respectively).

The conference dinner was held that night, but unfortunately was not as universally attended as those at the BCA conferences. The food was good though, with a main course of excellently cooked cow and a carrot! It was concluded with a short speech from **Bob Von Dreele**, the past president, who drew our attention to what we owe to an important and often forgotten part of the community. He summoned to their feet all those who had written a computer program in C, C++, Java, Python, FORTRAN (the vast majority of those standing) or any other language. He then asked the rest of us to thank these people for their contribution to our subject, as we couldn't do what we do without them. He is indeed right of course. The most concerning part however, is that the average age of those standing must have been at least sixty (if not more) reflecting how we, the younger generations, stand on the shoulders of giants. So, if we cannot find ways to support the old software, we will find it hard to continue to do what we do today.

The final day began with the presentation of Trueblood Award to **Ton Spek** who explained the genesis of PLATON and SYSTEM-S in **Professor Bijvoet's** “Crystal Palace”. People started to drift away after that with many people leaving immediately after the plenary. They were the unfortunate ones as they missed some excellent talks in

the morning including my personal favourite, a complicated discussion of “kryptoracemates” by **Carol Brock** (Kentucky). I personally had to slope off to the airport halfway through the afternoon session, but not before I had seen most of a session on handling disorder which included talks from **Luc Bourhis** and **Richard Gildea** (Durham) and **Peter Mueller** (MIT). Security at the airport was a barrel of laughs, including one security guard who seemed determined to joke about how my poster tube looked like a missile launcher, and didn't understand why I was reluctant to join in. At least it was an improvement on the static queue for check-in at Heathrow on the way out though...

So, what was my overall impression of my first US crystallography conference? Well, the people were all very friendly and seemed determined to make sure I wasn't left alone; a most hospitable bunch. The conference as a whole had a very, very different atmosphere to the BCA though: much more formal and dominated by the macromolecular/protein field. Compared with our own annual meeting, there were far fewer young scientists there and, certainly from the small molecule community, almost no students at all. Finance certainly played a very significant part in this. It was held in a hotel and was therefore an extremely expensive conference, in particular the accommodation, but also the registration. There is no doubt it was also a much larger conference, with some thousand attendees, more in line with the European Meetings or the IUCr, however, I feel there is another, more subtle reason. In the UK, service crystallography is still very much work carried out alongside the many vibrant research groups, whereas in the US many of the service personnel work distinctly in isolation, probably in a cellar. Perhaps this is also why there were so many crystallographers from the UK and Europe presenting work there too. On the other hand, maybe this is a testament to the quality of teaching in the UK and Europe which is epitomised by the Fankuchen award which this year went to our own **David Watkin** (Oxford). It was clear to me, however, that small molecule crystallography in the UK and Europe is in a much better state than in the US, and that we need to maintain the involvement of our young people at meetings, whatever the cost.

**Amber Thompson**  
University of Oxford

# ACA Meeting Reports...Cont.

**TO convey a visual impression of the exciting ACA meeting in Chicago we have a picture spread, nearly all of which has been supplied by Peter Mueller. We are very grateful to him for allowing us to reprint these photos.**

Following on from Amber's insightful description of this meeting, I shall try to give a complementary account. There is, however, one important gap in Amber's write-up of the session on "Absolute Structure Determination" which I must hasten to put right. Amber was too modest to mention her own lecture. As an introduction to the importance of stereochemistry she reminded us that D-limonene smells of citrus while L-limonene smells of turpentine. Then she really put the Flack parameter to the test on no less than 150 routine data sets from a CCD instrument. Initially she kept the Friedel pairs separate. After validation tests also with Bayesian (Hooft) analysis, which gave a similar but sharper distribution compared to the Flack parameter, she could reach an informed decision whether to merge the Friedel pairs.

In one of the first talks on the first day of the meeting (Sunday) **Joseph Reibenspies** really made the General Interest symposium live up to its name. Entitled "How Are We Doing?" his talk posed the question whether we are making progress in quality, quantity and completeness, based on trends in the CSD over the years. The quality does indeed look good, the recent mean and median R factor being 5.403 and 4.860 respectively. We are proud of the graph of the number of structures in the CSD versus time, with its ever-steepening slope. However, a different method of analysis suggests that we should yield the laurel wreaths to our crystallographic ancestors. The ratio of the number of structures known at the end of a 20-year generation to that at the beginning of the period is 13 for 1923-43, 16 for 1943-63, 12 for 1963-83, but only 5 for 1983-2003. If complexity is measured by unit cell volume, the average volume increased during the 1960's and 1970's but, surprisingly, began to decrease after 2000. However, if complexity is related to crystallographic challenges, it is clearly increasing: 1 in 4 of recent entries to the CSD has disorder, with 1.8% twinned.

This year's Transactions Symposium, entitled "The First Element", was in memory of **Bob Bau**, who by clever use of neutron diffraction had elucidated the structure of so many fascinating metal complexes containing hydrogen. Bob had also been an unselfish contributor to the crystallographic community, on a personal level by giving so much

encouragement to so many postgrads and postdocs, and on an institutional level by serving as president of the ACA and on panels preparing bids for new national facilities. His greatest such triumph was to get funding, from a government not well known for its interest in basic science, to build the Spallation Neutron Source (SNS) at Oak Ridge. It is good to know that Bob lived to see the start of the commissioning process. Speaker after speaker paid heartfelt tribute to him.

**Tom Koetzle** gave the first talk, describing 25 years of collaboration between Tom's group at Brookhaven National Laboratory and Bob's group at USC on the structure of transition-metal hydrides with ligands in a variety of places. Important trends were discovered, such as the variation in M-H distance with H coordination number. **Xiaoping Wang** reported good progress in commissioning the TOPAZ single-crystal neutron diffractometer on the SNS. **Paula Piccoli** described a new high point in the quest for ever higher coordination numbers. Working on the principle "big metal—small ligand", she and her colleagues have prepared a 15-coordinate  $\text{Th}(\text{H}_3\text{BNMe}_2\text{BH}_2)_4$  complex, the highest observed to date. Talks by **Dwayne Miller** and **Nobuo Niimura** broadened the subject to include macromolecules, and **Garry McIntyre** described polarized-neutron Laue diffraction. I gave the first talk after lunch. I assume that during the lunch break someone must have installed a highly intelligent expert system with a short attention span on the projection system computer. The first half of my talk went very smoothly, but then the system must have decided it was bored with flurbiprofen structures and froze up. After some rapid random button-pushing the system remained frozen, and I started to freeze up inside. Fortunately one of the conference staff in distinctive red T-shirts came forward and restarted the system. The rest of my talk passed without incident. Presentations by **Larry Falvello**, **Alberto Albinati**, **Muhammed Yousufuddin** and **Joel Miller** introduced us to more fascinating complexes with interesting shape changes, dynamics and magnetic properties. If participants returning from the coffee/tea break had not had enough stimulation from caffeine, **Chick Wilson** gave a typically entertaining lecture showing how high-throughput neutron diffraction can elucidate proton migration and many other fascinating phenomena. **Dean Myles** applied high-resolution neutron diffraction to rubredoxin from the wonderfully named *Pyrococcus furiosus* to explain how hydrogen bonding and hydration help to endow this protein with exceptional stability even in boiling water. **Michael O'Keefe** told us about the study of MOF's by neutron diffraction, and **Hans-Beat Bürgi**

showed how neutron radiation may also be used to interpret diffuse scattering.

Another useful symposium was entitled “What Can Your Beamline Do For You?” This consisted of a series of presentations about facilities, mostly in the United States and featuring two presentations about Oak Ridge by **Dean Myles** and **Ken Littrell**. Since collaboration is also welcomed from outside North America, would-be users are well advised to consult the abstracts. I found that the presentation by **Brian Toby** from Argonne National Laboratory not only provided an introduction to the many and varied beamlines available

at the APS at Argonne but also gave valuable generic advice that would help scientists intending to use any such facility anywhere in the world. I am grateful to Brian for the opportunity to reproduce some of this advice in the box accompanying this report. When I discussed these points with **Dave Allan**, he mentioned one more thing to bear in mind. Beamlines normally are provided with laboratories for sample preparation. However, if your sample requires unusual apparatus or reagents, ensure that they can be made available.

**Carl Schwalbe**

## From the presentation “Harness Advanced Photons at their Source to Further your Research” by Brian Toby.

### New Users Challenge: Finding a beamline

With ~30 teams, some internal to the APS and some external, covering a very wide range of science, there is no single place to get technique-specific questions answered.

- Use “beamlines” resources on APS web page ([www.aps.anl.gov](http://www.aps.anl.gov)) to learn about techniques and facilities.
- Contact a beamline staff member to ask about the appropriateness of that beamline for your experiment.

### Beamline techniques web page

- Lists ~65 techniques available at APS
- Look at pages for individual beamlines to see how the instruments differ.
- Submitting a proposal with an impossible measurement does not help your review.
- If you are really not sure where to start, contact the APS User Office: [apsuser@aps.anl.gov](mailto:apsuser@aps.anl.gov).

### PLAN AHEAD!

#### See the APS web site for new user info:

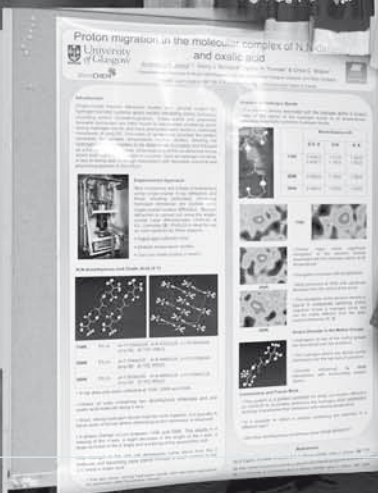
How to Become an APS User for prerequisites.

- There are three proposal deadlines per year. Expect >4 months between proposal submission and experiment.
- If your proposal is sound but does not get a good enough score, keep asking again for time in subsequent cycles: resubmission causes the score to improve.
- Non-citizens (including green-card holders); also US citizens born in sensitive countries:
  - Please apply well in advance to get on-site; DOE security reviews cannot be rushed.
- User Agreements:
  - These are non-trivial contracts– if needed, start well in advance.





# ACA MI







# EETING





# News from the Groups

## BCA Industrial Group Autumn Meeting



**Applications of Synchrotron Radiation  
Diamond Light Source**

**Harwell Science and Innovation Campus  
3-4 November 2010**



Our autumn meeting this year will take place at the Diamond Light Source. Set over two days at the Harwell Science and Innovation Campus there will be a variety of lectures by Diamond beamline scientists as well as academic and industrial application scientists. Confirmed speakers include Bill David (ISIS), Chris Frampton (Pharmorphix), Gemma Newby (ESRF), Emyr MacDonald (Cardiff) and Dave Rugg (Rolls-Royce). Further details on the programme will be published in due course. There will also be an opportunity to tour

inside the Diamond ring and to see selected beamlines during the meeting.

The meeting fee includes registration, overnight accommodation, conference dinner and lunch on the final day and is £180. For non-residents the fee for registration, conference dinner and lunch on the final day is £100. There are no concessions fees but there are a limited number of free student places available and these will be allocated on a first come first served basis. There is an optional lunch available for all on the first day for an additional £5.

Registration for this event is now open and places are limited so sign up now!

### Agenda

#### Wednesday 3rd November

- 12:00 Arrival and lunch in Diamond House
- 14:00 Welcome to Diamond
- 14:15 I11 – X-ray Powder Diffraction
- 14:45 I19 – Small Molecule Crystallography
- 15:15 Macromolecular Crystallography at Diamond
- 15:45 Coffee break
- 16:15 I07 – Surfaces & Interfaces
- 16:40 I12 – Joint Engineering, Environment and Processing
- 17:05 I22 – Non-crystalline Diffraction
- 17:30 X-ray Absorption Spectroscopy at Diamond
- 18:00 Wine reception and posters in Diamond Atrium
- 19:00 Dinner

#### Thursday 4th November

- 09:30 Tours of Diamond
  - Linac, booster & storage ring
  - beamlines
- 11:00 coffee available in Diamond Atrium
- 11:30-12:30 applications of diffraction
- 12:30 Lunch
- 13:30-17:00 applications of diffraction and other synchrotron techniques
- 17:00 Close

Meeting organiser: **Matthew Johnson**



## CCG Autumn Meeting, UNDERSTANDING the Solid State, Royal Society of Edinburgh, Wednesday 17th November 2010

10.30-11.15 Registration

11.15-12.00 **Dr Terry Threlfall**, Southampton "First and Second Order Transformations: A Re-appraisal"

12.00-12.30 **Jonathan Foster**, Durham "Changing old habits in new mediums: influencing crystal growth using supramolecular gels"

12.30-14.00 Lunch

14.00-14.30 **Dr Carole Morrison**, Edinburgh "Bananas, Pears (and other fruitful discussions)"

14.30-15.00 **Dr Craig Robertson**, Durham "Solid State Properties of Organic Neutral Radicals"

15.00-15.30 Tea/Coffee

15.30-16.00 **David Millar**, Edinburgh "The Power of Pressure: Energetic Materials at Extreme Conditions"

16.00-16.30 **Professor Russell Morris**, St Andrews "The structure and medical applications of 'toxic' gases adsorbed in metal organic frameworks and zeolites"

16.30 Close

## Follow-Up from Previous Issues

The article on Beevers-Lipson strips included a demonstration. "In the example given the  $k = 0$  row has F values on an arbitrary scale 124, 69, -31, -6, 0 (typed by mistake with the adjacent key as 9), 3 for  $h = 1$  to 6." This is the reason why no strip for 9 has been placed in the illustration.

The collection of X-ray tubes curated by Dr Grzegorz Jezierski has a website: [www.xraylamp.webd.pl](http://www.xraylamp.webd.pl)

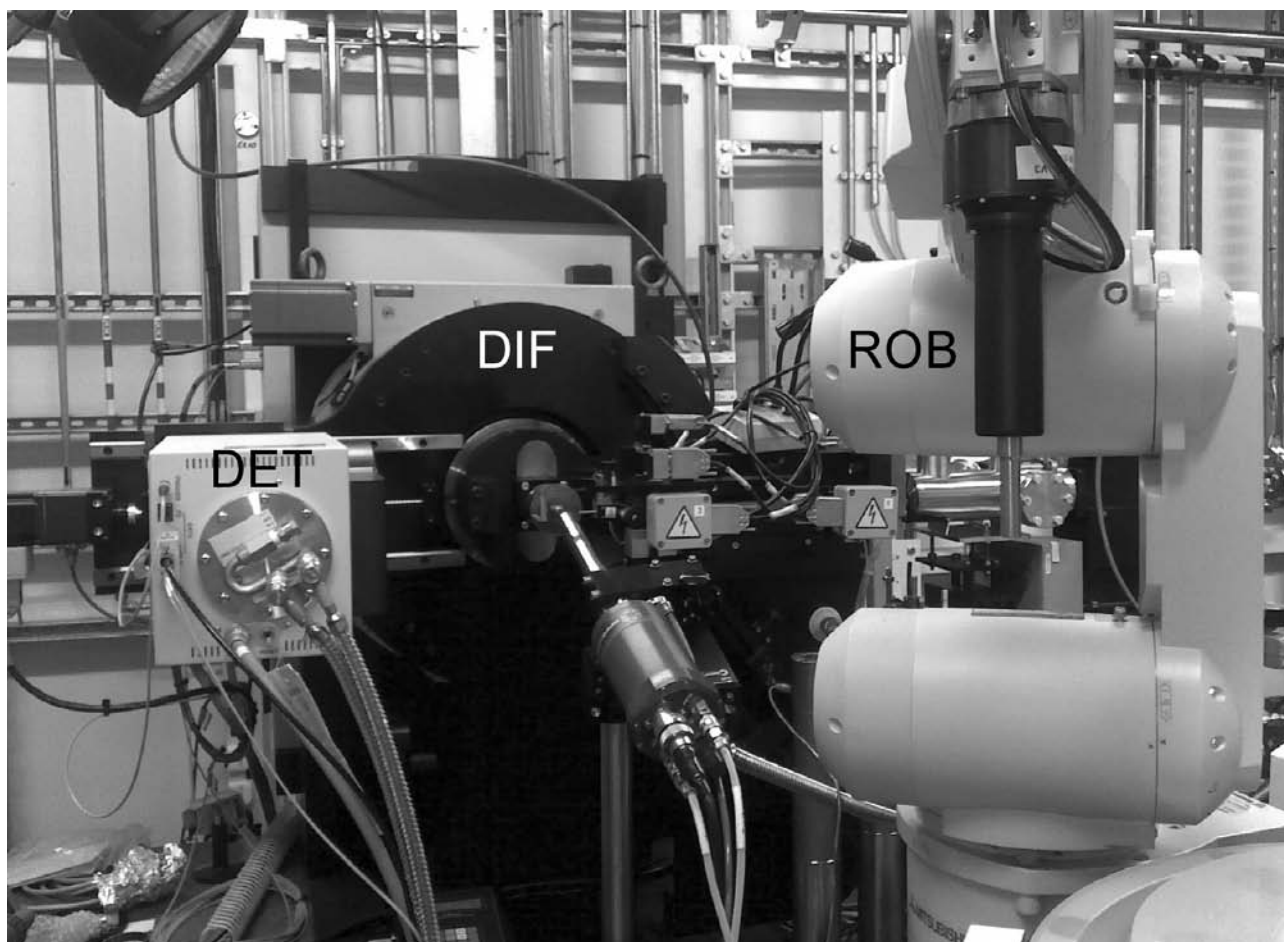


# Central Facility News...

After accepting **Carl Schwalbe's** request to write a piece for *Crystallography News* that would provide an update on crystallography facilities at Diamond Light Source and ISIS, it dawned on me that there would be a lot of material to cover and I, sadly, couldn't write something quickly in one afternoon. Certainly there would be too much for one issue and given the level of activity at both facilities I thought it might be appropriate to contribute a series of short updates covering different scientific areas – this would also give me the chance between each article to catch up with what's going on and to speak to those involved. With this in mind, I thought it would be easier for me to start off close to home at Diamond with two beamlines which are, probably, of most immediate interest to the chemical crystallography community. I will then provide updates on the protein crystallography beamlines before branching off into other aspects of physical crystallography and news from TS1 and TS2 at ISIS. To stay more firmly in my comfort zone, I start off with the small-molecule single-crystal diffraction beamline, I19, at Diamond which I am responsible for, as principal beamline scientist.

## Beamline I19: Small-Molecule Single-Crystal Diffraction

The design of the beamline builds on the experience of the operation of stations 9.8, and latterly, 16.2, at SRS Daresbury Laboratory. My predecessor in the role of principal beamline scientist, **Simon Teat**, was involved in the earliest days of 9.8 from its design and construction phases, when it was initially a Newcastle-Daresbury project (headed by **Bill Clegg**, The University of Newcastle), and through most of its operation before he started at Diamond. Simon is now running the small-molecule single-crystal diffraction beamline (11.3.1) at The Advanced Light Source and I took over responsibility for I19 in October 2006, just before construction got underway. **Harriott Nowell**, the beamline scientist, has been involved with I19 over virtually the entire period from initial design through to current user operations and **Sarah Barnett**, the beamline support scientist, was appointed towards the end of the construction phase. We were joined by the beamline PDRA **Kirsten Christensen** just after the beamline became operational. The design ethos for I19 essentially follows a



*The four-circle diffractometer (DIF) housed in experiments hutch 1 of beamline I19. The arm of the robotic sample changer (ROB) is in the foreground and the Rigaku Saturn 724+ CCD detector (DET) is on the left of the image.*

similar pattern to that of station 9.8: i.e. the instrumentation and software should be easy to use and have similar functionality to the options available for a university-based laboratory setup. Additionally the beamline would have an expanded capability and offer users the option of conducting experiments with bulky sample-environment cells, such as a closed cycle cryostat and have in-built capabilities for time-resolved studies. With the scientific remit outlined by the user working group (chaired by **Paul Raithby**) it was clear that two experiments hutches would be required: the first experiments hutch (EH1) would house a small, versatile, high-throughput diffractometer which would be equipped with a robotic sample changer; and the second experiments hutch (EH2) would contain a much larger diffractometer capable of carrying much heavier sample-environment equipment.

It is a happy coincidence that the September 2010 issue of *Crystallography News* marks the second full year that I19 was made available for user operation. The past two years have proved to be a busy time and, as well as completing the installation and commissioning of all the major beamline components, we have hosted over 80 user visits. Over the period, the beamline has 14 reported user publications, with many more in progress, and these include a paper in *Science*, and a *Nature Chemistry* publication from work conducted during the beamline's first month of operation. The majority of users have carried out what could be described as relatively conventional structural chemistry studies, albeit on extremely challenging systems, but the beamline has also been used for photo-crystallography experiments and a growing number of high-pressure structure determinations. Much of this work has been carried out in the first of the two experiments hutches, which supports a small 4-circle kappa geometry diffractometer, but within the last few weeks we were able to accept users for the second much larger diffractometer in the second experiments hutch. This marks an important milestone in the development of the beamline as we progress towards full operation. We have also made considerable progress in the commissioning of the optics and undulator with the aim of offering full flexibility in wavelength selection. In the coming few weeks we will be working towards making the robotic sample changer available to users and the progressive introduction of additional sample environment equipment such as the Helix open-flow sample cooler, the gas capillary cell and, now that the EH2 diffractometer is operational, the closed-cycle cryostat. In the more medium term we will also introduce facilities for time-resolved studies. The major items are already on site and are being tested prior to installation.

*Top Right: The large four-circle diffractometer housed in experiments hutch 2 of beamline I19. The Oxford Diffraction Atlas CCD detector (DET) is mounted on a very large 2 $\theta$  arm (set at an angle of 90° in the image).*



### Beamline I11: Powder-Diffraction

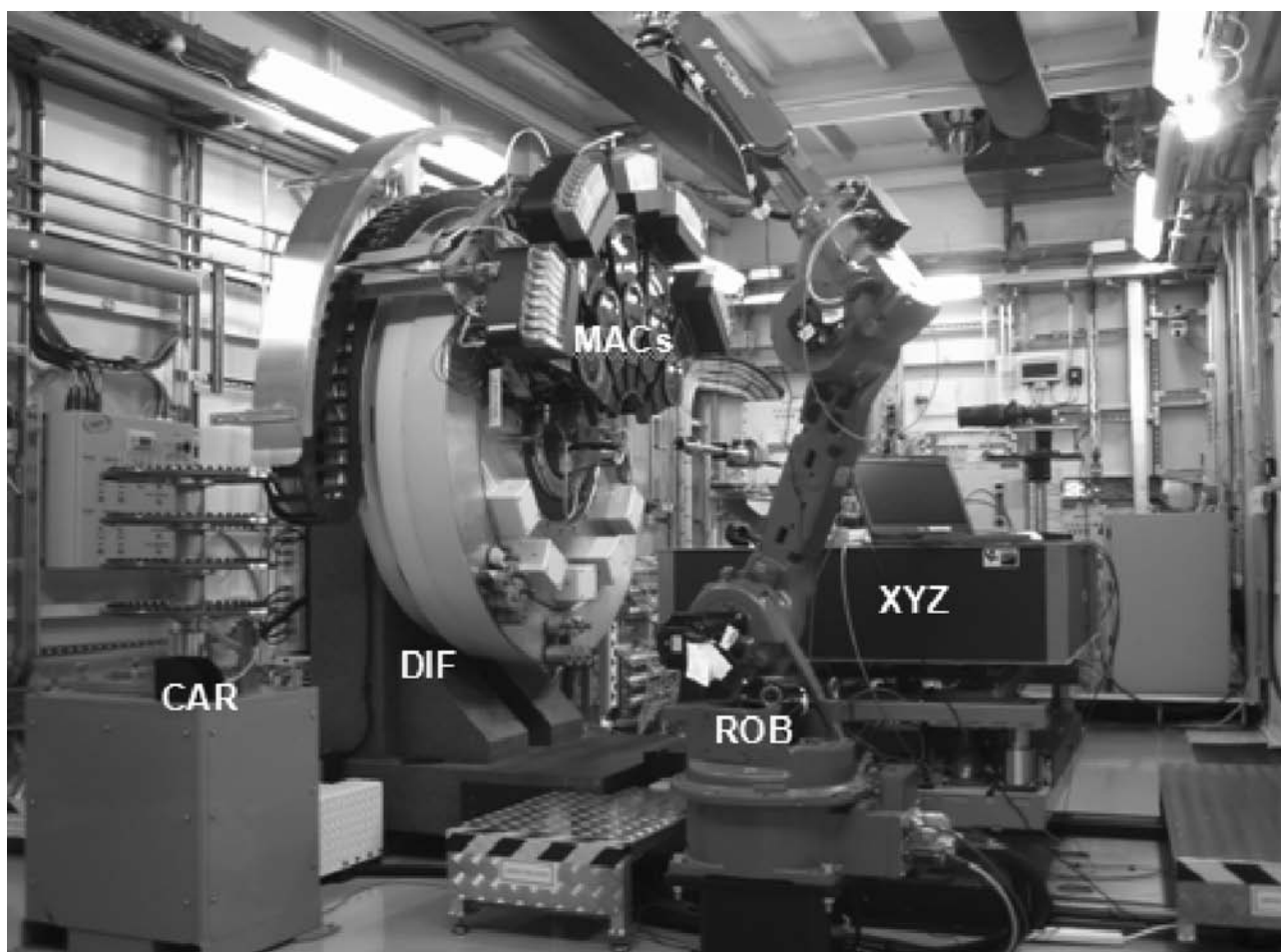
Powder-diffraction was catered for at SRS Daresbury laboratory in 1983 after the opening of station 9.1, with **Peter Hatton** acting as the first station scientist. This instrument was further developed by **Bob Cernik** during the high brightness lattice development in 1987. He also designed and built a second powder-diffraction facility on station 8.3 (with **Mike Hart, Phil Pattison** and **Andy Fitch**), this was subsequently transferred to station 2.3 some two years later. The two HRPD stations were further developed by **Graham Bushnell-Wye** and **Chiu Tang**. Very early on it was realised that a dedicated facility for energy dispersive diffraction was necessary so station 9.7 was converted for this purpose by **Simon Clark**. There were eventually a number of stations made available for powder-diffraction techniques including monochromatic methods on a further two stations, 9.5 and MPW6.2 (**Alistair Lennie** and **Chris Martin**). Diffraction from single grains (single crystals) was recognised as an important part of structure solution for a wide range of applications and, as already mentioned, station 9.8 was built over the site of the old 9.7 by **Bob Cernik** and **Bill Clegg**. The energy dispersive diffraction was transferred to station 16.4 where it remained until the end of the lifetime of the SRS. With the closure of SRS, high-resolution powder-diffraction methods have moved to beamline I11 at Diamond

# Central Facility News...Cont.

which has been operational since June 2008. The principal beamline scientist **Chiu Tang**, who started his career in synchrotron powder-diffraction methods at SRS on station 9.7, moved to Diamond in 2004 and was responsible for the design, construction, commissioning and eventual operation of I11. **Steve Thompson**, who also started his synchrotron career at SRS Daresbury became the beamline scientist on I11 in 2005. The scientific team was completed by **Julia Parker**, the beamline support scientist, who was appointed in 2007, and with the appointment of **Alistair Lennie**, who many of us know from his time as a station scientist at SRS Daresbury, as a PDRA just over a year ago.

Perhaps the most striking feature of the I11 experiments hutch is the large 3-circle diffractometer ( $2\delta$ ,  $2\theta$  and  $\omega$ ) which, at least at first glance, appears to have an unusual design as it is constructed around what could be described as a  $2\theta$  detector wheel rather than the more familiar  $2\theta$  detector arm geometry. Mounted radially on the upper segment of the wheel are five high-resolution detector modules each composed of 9 detector elements, with the individual elements each containing their own multi-analyser

crystal (MAC). This high-resolution mode has been running reliably for more than two years which has allowed I11 to support more than 70 user experiments with remarkably little loss of beamtime. Occupying the lower segment of the diffractometer is the  $90^\circ$  position-sensitive detector (PSD) built using Mythen2 silicon modules for time-resolved studies. This is supported on the  $\delta$  detector wheel, which lies within and is concentric with the  $2\theta$  detector wheel, and allows the PSD to be scanned separately from the MAC. Although the PSD has a more limited resolution than the MAC ( $\Delta\delta \sim 0.05^\circ$  compared to  $\Delta 2\theta \sim 0.002^\circ$ ), it is possible to collect complete powder-diffraction patterns in less than 1 second with smaller beam and sample sizes. The PSD has been operational for about a year and can be used simultaneously with the MAC if required. Apart from the diffractometer itself, it is impossible not to notice the extremely large robotic sample changer (the arm can extend to over 2 metres) with its associated carousel, which can hold up to 200 samples contained in capillaries. This has been operating reliably since the beamline became operational. Recently, an upgrade project has been completed to achieve micro-focussed beam. A set



*The experiments hutch of beamline I11 showing the powder-diffractometer (DIF) and the robotic sample changer (ROB). The sample carousel (CAR) is in the foreground and the motorised optical table (XYZ), for supporting sample environment equipment, is shown to the right of the diffractometer.*



of compound refractive lenses on an alignment table in the experimental hutch has been commissioned to provide small beam sizes ranging from 10 to 100  $\mu\text{m}$  over the 15 - 25 keV energy range. This additional capability is particularly useful for studies of single micro-polycrystalline particles with nano-domains or for experiments which require a small beam for high spatial resolution. In this mode an optical table is placed downstream of the diffractometer which supports a MAR image plate reader and a range of motorised stages for the sample holder and a series of collimators and pin-holes. This set-up would be very familiar to users of station 9.5 at SRS Daresbury after its conversion to support microbeam powder-diffraction techniques. The beamline now offers a wide range of sample environments: cryostats and cryostreams (5 – 500 K), a hot-air blower (295 – 1273 K), capillary and flat-plate furnaces (295 – 1700 K). Over the period of operation the users, together with in-house staff, have already published over 18 papers and many of these are published in high impact journals, such as *Nature* and *Journal of the American Chemical Society* (JACS).

The I19 and I11 beamline scientists are happy to discuss any queries you may have about the beamlines and their peripheral laboratories including the range of sample preparation facilities that they offer. The Diamond web site ([www.diamond.ac.uk](http://www.diamond.ac.uk)) has links to the beamline pages. In the next issue we will walk round to the other side of the storage ring to catch up on some of the recent developments on the macro-molecular beamlines.

I'd like to thank **Chiu Tang, Paul Raithby, Bob Cernik, Harriott Nowell** and **Sarah Barnett** for their assistance in the preparation of this short article.

David Allan



A close-up view of the powder-diffractometer on beamline I11. The high-resolution (MAC) detectors are mounted to the upper section of the diffractometer on the  $2\theta$  axis while the position sensitive detector, shown in the lower region of the photograph, is mounted on the  $\delta$  axis which can be driven independently of  $2\theta$ .



## Protein Crystallography

### A Concise Guide

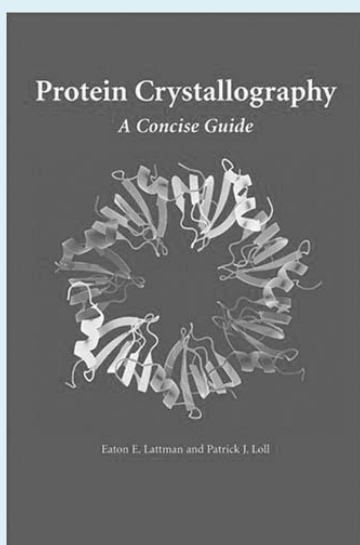
By Eaton E. Lattman and Patrick J. Loll

Johns Hopkins University Press

| 2008 | 136 pages |

isbn-13: 9780801888083 |

isbn-10: 0801888085



**Any academic, aspiring or established, will feel a small frisson of excitement when acquiring a new text. What will it contain? How will the subject be delivered? What potential does it promise to unlock in the reader? The power of the book is a well established matter of historical fact, and in this age of ceaseless electronica there is**

**surely something comforting about a physical book that can be wholly owned and held by the reader.**

All the more fascinating is the slim volume with the word 'concise' in the title, on a specialist subject promising, as in this case, a fine distillation of all that is relevant in that subject. Certainly this is a laudable and worthy aim for the author(s), and seductive to the buyer/reader. Here then a word of caution; for the author(s) a most difficult approach; to the reader do not conflate the notion of concise brevity with some arcane way of acquiring knowledge and understanding on the cheap.

The authors here do tend to suddenly introduce terms which may be unfamiliar, so unsettling, to readers with only basic physics or maths; emphasising the fact that a good understanding of the method is not casual or to be had on the cheap. On a number of occasions I did ask "where are we off to now?" only to find that the progression was reasonable if a little abrupt, e.g. happy with the model so far? Wait a moment... did you really think that atoms stood still while being photographed!...leading to a clear explanation of the effect of thermal motion, and disorder,

on diffracted intensity.

The style is a little different but, on reflection (pun intended), is pedagogical in its manner of leading the reader through the text, inviting them to pose questions to which the answers are then supplied. The journey from elastic scattering by a single electron in an oscillating field to the Huygens light model describing diffraction, and ultimately a 3D crystallographic model forms a core introduction. I particularly enjoyed being reminded of the basics of cosine summation as a fundamental model of image formation. The transition from a single object to a crystalline solid containing many copies of the same object is well handled and, to my mind, a vital part of the story. The phase problem and its solution occupies nearly half the book; three whole chapters; underlining the importance of this part of the method. A final chapter on crystallographic refinement nicely concludes the book. Now the reader will either be keen to delve deeper or, at least, feel more comfortable in discussion with a crystallographer.

The authors have deliberately avoided including any discussions on the practical aspects of the method. This is a subject in its own right and easily separated from this presentation. An end of chapter summary to consolidate learning, and further reading (with comments) provides added value. The comprehensive glossary also adds to the usefulness of this well crafted concise volume. Interestingly the use of recycled material in its production not only adds to a sense of virtue in the purchaser but (to my eyes anyway) enhances the reading experience by eliminating the glare that sometimes results from a glossy page.

As our technique becomes ever more routine there has been some concern expressed in the community regarding the loss of the classic 'crystallographer' to powerful pipeline methodology, often requiring little user intervention and background knowledge. Whilst this process seems inevitable and normal to progress it would be a pity to neglect a general appreciation of the underlying principles so well presented in these few pages. Not an easy read, especially for those lacking the maths/physics background but, with some application, this book is rewarding and great value for money.

**Patrick K. Bryant**  
University of Manchester

## Lachlan Cranswick. Crystallographer Extraordinaire



**LACHLAN'S sudden disappearance in January immediately caused real concern amongst his colleagues. It was so out of character that they could only believe the worst. In June we learned that Lachlan had indeed drowned.**

Lachlan appeared on the UK crystallography scene in 1998, rather like the hero-to-be walking towards the camera out of the heat haze of the Australian desert. He was largely unknown to the UK community, but his appointment to CCP14 (the EPSEC Collaborative Computing Project 14) was to change that. **Bob Cernik**, the Principal Investigator at the time, has since written to me "I don't remember exactly where I met him first but I learned of his interest in crystallographic software and collared him at a conference in Budapest (EPDIC 6). I talked to him for a while before I convinced him that the position might interest him. He was worried that he would get tied down in a programming role. The rest is history, he really made CCP14 his own."

Lachlan did not get bogged down in programming - he rose well above it. His task in the CCP14 project was to mediate between practicing crystallographers and people developing software, to help ensure that the users knew what was available, and that the developers knew what users wanted. His regular visits to laboratories in the UK and the rest of the world convinced him that fewer and fewer users had much idea of what was going on inside the programs they used, nor even of the full scope of the software they did use. His mission became to make CCP14 a centre of knowledge for non-macromolecular crystallographic computing. He not only made a wide range of software easily available, he also used the software himself, producing User Guides for beginners and experts, and suggesting to developers improvements which would make the programs more accessible. I don't know if he coined the phrase, but he was well aware of the

importance of "eye candy" to lure folk into trying something new. He had a big influence on the development of user-interfaces in crystallography, see for example CRYSTALS, and via the "Age Concern" project, OLXE2.

Although he only worked at CCP14 for 5 years, his influence on modern crystallographic software was profound and on-going. Lachlan was much more than just a scientist. He was interested in economics, philosophy, sociology, religion in a wide sense, music, history and poetry. This enabled him to take a broad view of how crystallography was changing, and to become very concerned with growing trends. In particular he was concerned that knowledge was being lost, and that there were no mechanisms to ensure continuing funding of software developments. As secretary and then chairman of the IUCr Computing Commission he continually worked to promote crystallographic computing. His Software Fayres have become an integral part of all big meetings, and to help people unable to get to the meetings and without good internet access, he produced his regular NeXus CDs, which contained the latest copies of freely available software. His departure from CCP14 to Chalk River left a gap which was impossible to fill.

As editor of the IUCr Computing Commission newsletter, he cajoled programmers to contribute articles covering new developments, and users to contribute novel uses for existing programs. He well understood the importance of setting science in its context, and searched out items of historical interest. These newsletters deserve to be more widely read since they contain lots of otherwise unpublished material of interest to all crystallographers: <http://www.iucr.org/resources/commissions/crystallographic-computing/newsletters>

Apart from being a tireless emissary for crystallographic computing, Lachlan was also good fun to be with. Even though he knew something about almost everything, he was still always keen to try new things. During his time in London, he became impassioned with Early Music, and took every opportunity to go to the many church concerts. He loved museums, books, libraries, and was always up for any new eating-experience, however weird the menu. I feared that his move from the hustle of London to the quiet of Chalk River might not really suit him, but I was quite wrong. He simply re-channelled his enthusiasm to the wealth of new out-door activities available.

Lachlan was a good friend, and had a big influence upon me as a scientist. I miss the amicable arguments, and the occasional e-mails asking if I had read such-and-such, which might be anything from a current crystallographic paper to a

# Obituaries

recently digitised 19th century book. A loss to us all.

See also:

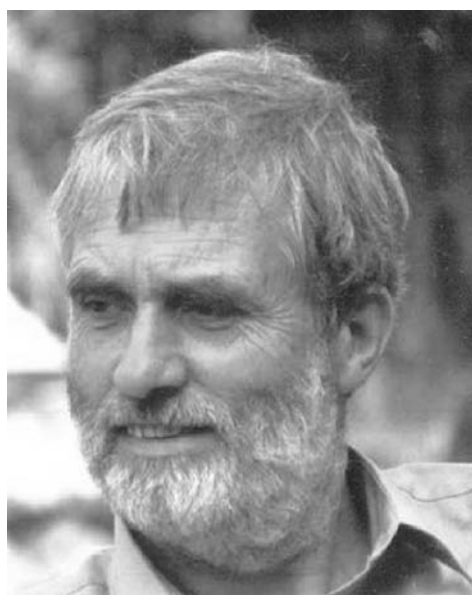
<http://www.magma.ca/~drcanrt/100623identity.html>

<http://tech.groups.yahoo.com/group/sdpcd/message/2481>

P.S.: I never saw Lachlan drink alcohol, but this never inhibited him from joining post-lecture sessions where much unpublished crystallography was discussed.

**David Watkin**

## John Stewart Rutherford (1938-2009)



**JOHN STEWART RUTHERFORD**, passed away in September 2009 at the age 70 years in the aftermath of a stroke from which he had suffered in May. Remembering John for his achievements in teaching and research falls short of characterizing the entirety of his contributions to the scientific community which is equally indebted to him for the energy and effort he spent in helping institutions of higher learning in emerging countries to uplift their teaching and research programs.

After graduation from Glasgow University in 1959 and an interlude at an ordnance establishment in Scotland John joined the group of the late **Crispin Calvo** at MacMaster University in Hamilton, Ontario, where in 1967 he received his PhD with a thesis on the crystal structure of selenourea. John then went on to the Department of Crystallography at

the University of Pittsburgh to study the structure of anti-cancer drugs. Back in Great Britain he investigated the crystal structure of phosphorus-nitrogen ring compounds at the University of Essex, after which he returned to MacMaster for low-temperature diffraction studies. This was followed by a two years' engagement at the Northern Electric Company in Bramalea, Ontario, after which John joined the University of Regina, Saskatchewan, where he investigated the crystal structures of disulfonates. Back in his beloved Scotland John applied his teaching skills at a high school in Linwood until 1979. This year marks a break in John's career, because from now on we see him in Africa and the Arabian Peninsula until the end of his active engagement in 2003. The first station is the University of Swaziland (1980-1982), followed by the University of the Transkei (1983-1984), the Sultan Qabos University in Oman (1995-1996), and finally the National University of Science and Technology in Bulawayo, Zimbabwe (1998-2003), where he stayed until re-tirement. All these institutions are indebted to John for his assistance in their quest towards academic excellence. John created or revised curricula, taught chemistry courses, participated actively in the administration, acting as head of the Department of Chemistry and assuming other functions which are too numerous to be listed here.

After retirement in 2003 he moved back to his native Scotland, where the newly gained freedom from administrative duties enabled him to resume and further develop his research on theoretical crystallography, from 2005-2008 as member of the IUCr Commission on Mathematical and Theoretical Crystallography which he had joined since its foundation as an informal international work group in 2002. He continued his investigations on the application of number theory - one of the most fundamental areas of mathematics - to problems involving crystal lattices.

The cover of *Acta Crystallographica* A62 (2), a special issue on Mathematical and Theoretical Crystallography, is taken from his article Some algebraic properties of crystallographic sublattices. In later years he became increasingly interested in the applications of graph theory to problems of crystal chemistry. Here John made substantial contributions to a monograph on Graph Theory in Crystallography and Crystal Chemistry. His passing prevented him from finishing this important task, which will nevertheless be brought to completion and will represent a most fitting homage to his memory.

John is survived by his wife Sasha and two daughters by a previous marriage.

**Wilfrid E. Klee, Baden-Baden**

Reprinted from ECA News

## Gordon Leslie Squires (1924-2010)



**GORDON LESLIE SQUIRES, one of the pioneers of neutron scattering in the postwar period, passed away peacefully on Saturday 10th April 2010 in Cambridge, England. While Gordon is known to all neutron scatterers as the author of**

**Introduction to the Theory of Thermal Neutron Scattering, not so many are aware of his role in the 1940s and 1950s. When he was hired into the Cavendish Laboratory, Neville Mott referred to our field as “a funny mix of nuclear and solid-state physics”. The Squires group from Cambridge then established itself at Harwell, long before any formal user program, sharing a time-of-flight beam line with Peter Egelstaff’s group, originally on the world’s first liquid hydrogen cold source at the BEPO reactor and later on the cold source at the DIDO reactor.**

An undergraduate in Cambridge during the Second World War, Gordon then worked at the Royal Aircraft Establishment, followed by PhD research back in Cambridge immediately afterwards with J. M. Cassels (Rutherford’s last PhD student) using a cyclotron-driven neutron source, before moving to Harwell and doing experiments on the first British Reactor BEPO. He spent two years in the USA, at University of Chicago and Princeton University, before moving back to Trinity College Cambridge and the Cavendish Laboratory in 1956, where he remained ever since. He was a wonderful teacher and mentor, with a deep love of experimental physics. For instance he believed strongly in Rutherford’s tradition that every graduate student should “build their own piece of scientific apparatus”, something that is increasingly difficult in these days of large-scale facilities.

Gordon made a number of original scientific contributions, including measurements of the ortho- and para-hydrogen cross-sections (with A T Stewart in 1953), the first observation of critical scattering with neutrons (1954), and a series of studies of the lattice dynamics of elements. But it is perhaps how Gordon built on his pioneering research days to become an outstanding research supervisor and gifted university teacher in the years that followed that will equally contribute to his enduring legacy. Alongside his textbook *Introduction to the Theory of Thermal Neutron Scattering*, which emerged from his lecturing and teaching to quickly become, and has remained, a canonical text in the field for the last thirty years, Gordon nurtured a long line of graduate students who have remained deeply involved in the development, progression and widening of the neutron scattering technique across the world.

As a university lecturer and Director of Studies for many years at Trinity College he also oversaw the education of many generations of undergraduates in physics, writing a highly successful book, *Practical Physics*, for use with senior undergraduate laboratory courses. A particular passion of his was the teaching of quantum mechanics through tutorials and lectures that quickly became renowned as models of clarity and elegance in university teaching. His undergraduate text *Problems in Quantum Mechanics (with Solution)* and an article on quantum mechanics for the *Encyclopaedia Britannica* also ensured that a wider audience were able to enjoy his skill in conveying the physics behind this fascinating subject.

In recent years, Gordon had been the curator of the small museum within the Cavendish Laboratory, looking after and displaying its unique collection of artefacts from its history in physics, including the equipment used by James Chadwick to demonstrate the existence of the neutron itself. Gordon’s enthusiasm for this subject led him to write several articles and become a regular guest speaker on the historical characters and experiments they performed at numerous neutron schools and meetings. Typically modest, he was often surprised at the large audiences his talks attracted but never failed to delight them with his deep knowledge and insights into some of the defining experiments in physics.

Gordon is survived by his wife Shoshana, and two sons, Adam and Dan.

**Gordon’s former graduate students around the world  
Reprinted from *Neutron News***



# Meetings of interest

**FURTHER** information may be obtained from the websites given. If you have news of any meetings to add to list please send them to the Editor, [c.h.schwalbe@aston.ac.uk](mailto:c.h.schwalbe@aston.ac.uk). Assistance from the IUCr website is gratefully acknowledged.

## 5-7 September 2010

BACG 2010. British Association for Crystal Growth, Manchester.

<http://www.bacg2010.org/>

## 5-9 September 2010

Diamond 2010. 21st European Conference on Diamond, Diamond-Like Materials, Carbon Nanotubes, and Nitrides, Budapest, Hungary.

<http://www.diamond-conference.elsevier.com/>

## 5-10 September 2010

BCA/CCP4 Summer School XV, Oxford.

<http://crystallography.org.uk/bca-ccp4-summer-school-2010>

## 8-10 September 2010

17th International Workshop on Industrial Crystallization (BIWIC 2010), Halle (Saale), Germany.

<http://tvt.iw.uni-halle.de/biwic2010/>

## 9-11 September 2010

4th International SAXS / GISAXS Workshop, Leoben, Austria.

## 10-16 September 2010

13th International Conference on the Crystallisation of Biological Macromolecules (ICCBM13), Dublin, Ireland.

<http://www.iccbm13.ie/>

## 13-17 September 2010

E-MRS 2010 Fall Meeting, Warsaw, Poland.

[http://www.emrs-strasbourg.com/index.php?option=com\\_content&task=view&id=334&Itemid=1](http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=334&Itemid=1)

## 14-16 September 2010

BCA Industrial Group PANalytical Tube Factory Visit, Netherlands

<http://sites.google.com/site/bcaindgrp/meetings/14-16-sept-2010>

## 15-17 September 2010

ILL 2020 Vision. Future directions in neutron science, Grenoble, France.

<http://www.ill2020-vision.eu/>

## 16-17 September 2010

Neutrons for Catalysis: A Workshop on Neutron Scattering Techniques for Studies in Catalysis, Oak Ridge National Laboratory, TN, USA

<http://neutrons.ornl.gov/conf/NandC2010/index.shtml>

## 19-23 September 2010

Structure Under Extreme Conditions of Pressure and Temperature Gatlinburg, TN

<http://neutrons.ornl.gov/conf/IUCr2010/>

## 19-24 September 2010

IWN2010. International Workshop on Nitride Semiconductors, Tampa, FL, USA.

<http://www.iwn2010.org/>

## 20-22 September 2010

17th Bruker Users' Group Meetings 2010 Single Crystal X-ray Diffraction, Karlsruhe, Germany.

## 20-23 September 2010

XTOP2010, the International Conference on High-resolution X-ray Diffraction and Imaging. University of Warwick, UK.

<http://www2.warwick.ac.uk/go/XTOP2010>

## 20-24 September 2010

10th International Symposium on Ferroic Domains and Micro- to Nanoscopic Structures, Prague, Czech Republic.

<http://palata.fzu.cz/isfd10/>

## 26-29 September 2010

Neutrons for Global Energy Solutions, Gustav-Stresemann Institute, Bonn, Germany.

[http://www.iucr.org/news/notices/meetings/meeting\\_2009\\_270](http://www.iucr.org/news/notices/meetings/meeting_2009_270)

**26 September - 2 October 2010**

International School on Aperiodic Crystals, Carqueiranne, France.

<http://www-xray.fzu.cz/sgip/isac2010/isac2010.html>

**27 September - 2 October 2010**

HSC12: Synchrotron Radiation and Neutron for Extreme Conditions Studies, Grenoble, France.

<http://www.esrf.eu/events/conferences/HSC/HSC12>

**28-29 September 2010**

2010 Annual Meeting of the Mineralogical Society. Nuclear Waste Management: Research Challenges for the Future, Cambridge.

<http://www.minersoc.org/pages/meetings/nuclear/nuclear.html>

**29 September - 1 October 2010**

6th International Workshop on Sample Environment at Neutron Scattering Facilities Herrsching, Germany.

<http://www.frm2.tum.de/en/aktuelles/events/se-workshop/index.html>

**4-7 October 2010**

Nuclear Materials 2010, Karlsruhe, Germany.

<http://www.nuclearmaterials2010.com/>

**4-7 October 2010**

JCNS Workshop 2010 "Trends and Perspectives in Neutron Scattering: Magnetism and Correlated Electron Systems", Bernried, Germany.

[http://www.jcns.info/Workshop\\_Magnetism/](http://www.jcns.info/Workshop_Magnetism/)

**11-14 October 2010**

IXS2010. 7th International Conference on Inelastic X-ray Scattering, Grenoble, France.

<http://www.esrf.eu/events/conferences/ixs2010>

**11-26 October 2010**

X-ray Methods in Structural Biology, Cold Spring Harbor, NY, USA.

<http://meetings.cshl.edu/courses/c-crys10.shtml>

**12-14 October 2010**

Specimen Preparation for X-ray Fluorescence, ICDD Headquarters, Newtown Square, PA, USA.

<http://www.icdd.com/education/spec-xrf-workshop.htm>

**13-16 October 2010**

Murnau Conference on Structural Biology – The modern RNA world, Murnau, Germany.

<http://www.murnauconference.de/2010/>

**18-20 October 2010**

Basic Rietveld Refinement & Indexing, ICDD Headquarters, Newtown Square, PA, USA.

<http://www.icdd.com/education/rietveld-workshop.htm>

**21-22 October 2010**

Advanced Rietveld Refinement & Indexing, ICDD Headquarters, Newtown Square, PA, USA.

<http://www.icdd.com/education/rietveld-workshop.htm>

**21-23 October 2010**

SENSE 2010 Superconductivity explored by Neutron Scattering Experiments, ILL, Grenoble, France.

<http://www.ill.eu/news-events/events/sense2010>

**25-26 October 2010**

Neutron reflectometry: the next generation and beyond, Grenoble, France.

<http://www.ill.eu/news-events/events/superadam>

**25 October - 1 November 2010**

EMBO Practical Course: Solution Scattering from Biological Macromolecules, EMBL, Hamburg, Germany.

[http://www.embl-hamburg.de/training/courses\\_conferences/course/2010/SAXS/](http://www.embl-hamburg.de/training/courses_conferences/course/2010/SAXS/)

**27-29 October 2010**

68th Annual Pittsburgh Diffraction Conference, Pittsburgh, PA, USA.

[http://www.pittdifsoc.org/PDC\\_2010/index.htm](http://www.pittdifsoc.org/PDC_2010/index.htm)

**3-4 November 2010**

BCA Industrial Group Autumn Meeting, Diamond Light Source, Harwell.

<http://sites.google.com/site/bcaindgrp/meetings/3-4-nov-2010>

**9-10 November 2010**

Advances in Protein Crystallography, Florence, Italy.

<http://www.selectbiosciences.com/conferences/APC2010/>

**10-11 November 2010**

Synchrotron radiation in Earth, Space & Planetary Science - Exploiting the UK's newest facility, Didcot.

[http://www.diamond.ac.uk/Home/Events/EE\\_village\\_workshop.html](http://www.diamond.ac.uk/Home/Events/EE_village_workshop.html)

**15-16 November 2010**

PCG-SCMP Winter Meeting, "Current Research in Physical Crystallography", The Coseners House, Abingdon

[http://www.pcg-scmp.org/Main\\_Page](http://www.pcg-scmp.org/Main_Page)

**17 November 2010**

CCG Autumn Meeting, "Understanding the Solid State", Royal Society of Edinburgh.

<http://ccg.crystallography.org.uk/>

**29 November - 3 December 2010**

MRS Fall Meeting, Boston, MA, USA.

[http://www.mrs.org/s\\_mrs/sec.asp?CID=16777&shy;&amp;DID=216967](http://www.mrs.org/s_mrs/sec.asp?CID=16777&shy;&amp;DID=216967)

**8-10 December 2010**

8th International Conference on X-ray Investigations of Polymer Structure, XIPS 2010, Wroclaw, Poland.

<http://www.xips2010.ath.bielsko.pl/>

**14-16 December 2010**

Condensed Matter and Materials Physics (CMMP10), Coventry.

<http://www.cmmp.org.uk/>

**26 March - 3 April 2011**

13th Intensive Teaching School in X-ray Structure Analysis - Durham.

<http://www.dur.ac.uk/durham.x-ray-school/>

**11-14 April 2011**

BCA Spring Meeting, Keele University.

<http://crystallography.org.uk/spring-meeting-2011>

**10-14 May 2011**

ICSG 2011 International Conference on Structural Genomics, Toronto ON, Canada.

<http://www.sgc.utoronto.ca/ICSG2011/>

**21-26 May 2011**

American Crystallographic Association Meeting, New Orleans, LA, USA.

<http://www.amercrystalasn.org/content/pages/main-annual-meetings>

**2-12 June 2011**

The Power of Powder Diffraction, Erice, Italy.

<http://www.crystalerice.org/Erice2011/2011pd.htm>

**2-12 June 2011**

Electron Crystallography: New Methods to Explore Structure and Properties of the Nano World, Erice, Italy.

<http://www.crystalerice.org/Erice2011/2011ec.htm>

**22-29 August 2011**

IUCr2011. XXII Congress and General Assembly, Madrid, Spain.

<http://www.iucr2011madrid.es/>

**25-29 August 2013**

28th European Crystallographic Meeting, University of Warwick.

<http://www.crystallography.org.uk/>



# EMPYREAN

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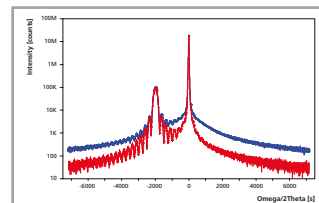
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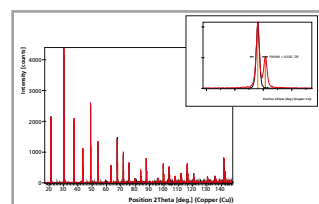
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- Unmatched area detector dynamic range, linearity and resolution
- See inside your samples with the world's first 3D detector

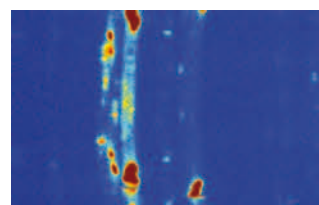
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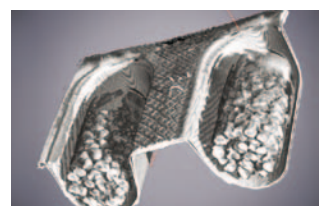
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# AlphaBiotech Introduces the New MPCS Plug Maker™ – for Next Generation Micro Batch Style Crystallization, from Emerald Biosystems



AlphaBiotech Ltd., a leader in crystallization instrumentation in the UK, is proud to announce the release of the new MPCS PlugMaker™ from Emerald Biosystems. Based on lab-on-a-chip micro-fluidics the PlugMaker has several key features:

- Low sample volume: 5-10 nL/experiment; up to 800 experiments / 4 uL protein
- No dead-volume, therefore no loss of protein sample
- Enables systematic assessment of optimal protein 'crystallization slot' through optimization screens
- Crystals directly amenable to X-ray diffraction experiments with standard equipment
- Crystals can be readily extracted for traditional cryo-preservation
- Low cost per experiment

**For Further Information Please Contact: [enquiries@alphabiotech.co.uk](mailto:enquiries@alphabiotech.co.uk)**



*Date for your Diary*  
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# Enhance Productivity

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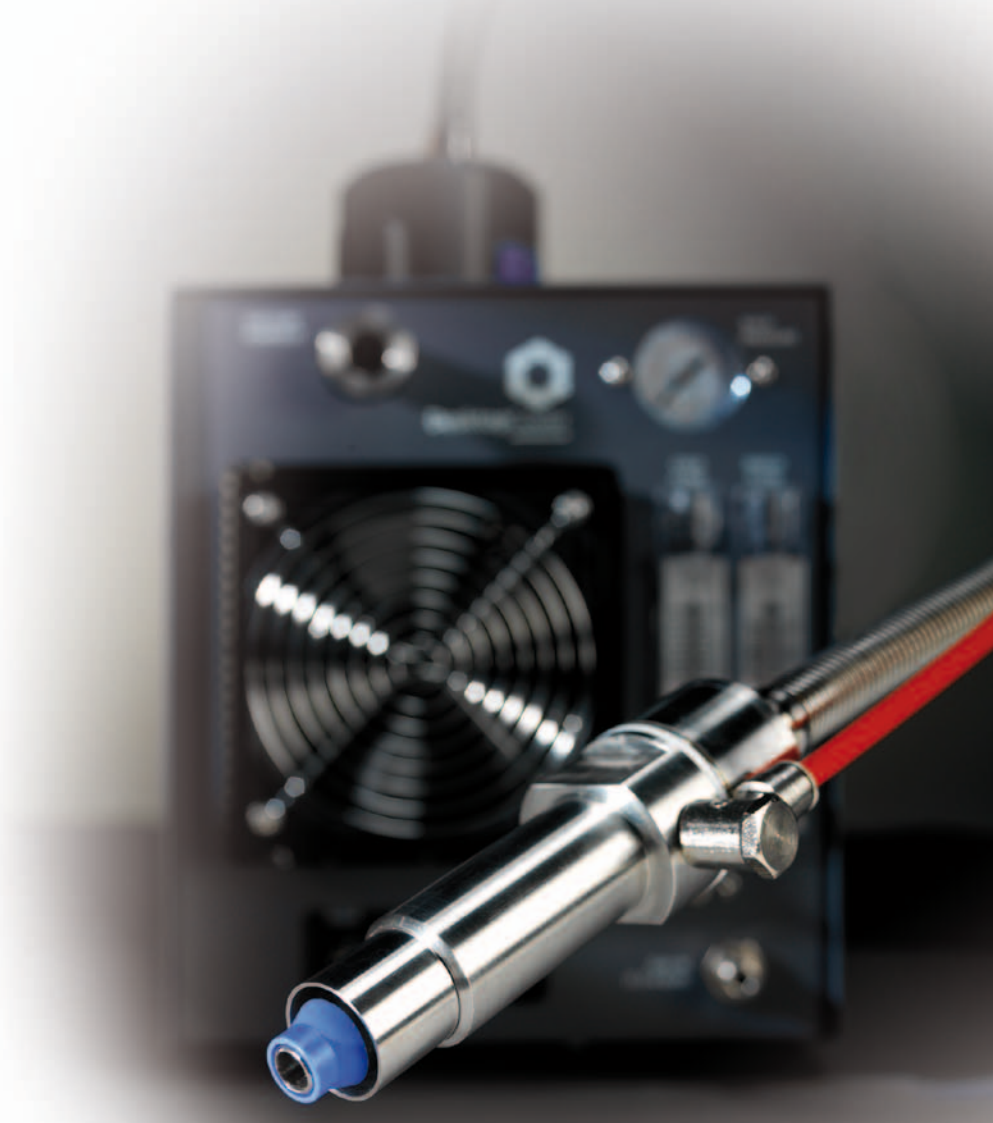
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**Allow us to introduce the DTC.**

For uncomplicated sample cooling, the Desktop Cooler (DTC) is hard to beat. The DTC refrigeration unit and a dry air source; that is all that's required to deliver a cold gas stream with a temperature range of 170 Kelvin to room temperature.

The mechanical cooler does not require a separate helium compressor, which means that cooling water is not required and maintenance is reduced to virtually zero. The DTC is simple to set up and control and can be left running for weeks at a time.

Certainly, for those working within this temperature range, the DTC offers convenient and simple cooling at an attractive price.

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For further information on the DTC visit [www.oxcryo.com](http://www.oxcryo.com)