Crystallography News

British Crystallographic Association

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Convivial Crystallographers

Next BCA Spring Meeting: April 2014

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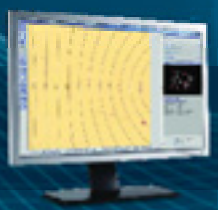

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Contents

This month's cover:

Our Etter Prize winners at the ACA; Erice and Durham (courtesy of Horst Puschmann, OlexSys) School photos

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Please ensure that items for inclusion in the December 2013 issue are sent to the Editor to arrive before 25 October 2013.

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From the President

ONE of the challenging things about my role is that you are always planning for another event. This means that you can find yourself thinking about a key meeting that is two years in the future whilst planning for various events next year and with this year's major meeting still to take place. However, it is exciting to see each event take shape right from its inception as different groups come together to form each meeting. And it allows you a longer period of anticipation... This has certainly proved to be the case over the past few weeks where I have been thinking about the BCA Spring meeting in 2015 in York, helping plan the programme for the BCA Spring meeting in 2014 in Loughborough and – at least as I write this – ECM28 is still to take place next month!

Taking the most imminent of these events first, I'm encouraged that **Sandy Blake**, the ECM28 Chair of the Local Organising Committee and Programme Committee, remains cheerful – as well he should since the excellent looking programme is nearly complete and we have a good number of attendees already registered. It should be a fantastic meeting that we can be justifiably proud to have hosted. It will also be enhanced by the Two Braggs Exhibition, which is running in parallel with ECM28 (see www2.warwick.ac.uk/fac/sci/physics/events/twobraggs). I spent an enjoyable day in Warwick two weeks ago with **Mike Glazer** (Oxford), **Pam Thomas** (Warwick), **Charlotte New** (RI) and others looking through the vast range of possible artefacts available to us for this exhibition. There was so much that we could have used and I am sure that the distillation that will appear will definitely be worth a visit. There is much to see and many original documents, some of which have only been available for public viewing in the last ten years. For those of you who did get to go to ECM28 and/or the Two Braggs Exhibition, I hope that you have enjoyed your time in Warwick as much as I am anticipating doing so now.

We are also currently looking to see whether some of the Two Braggs exhibition can be further distilled into a small display for our Spring Meeting in 2014. For insurance reasons this will most likely exclude the museum exhibits, but we hope that a flavour will be available – most likely through copies of the original documents – for those who were unable to make the Two Braggs exhibition but will be at our Spring meeting next year. This leads me very neatly on to our plans for Spring 2014 in Loughborough. **Lee Brammer** is the Programme Committee chair for this meeting and we had our first Programme Committee meeting in Loughborough earlier in July. Preliminary details of the meeting are given later in this issue of *Crystallography News* and I am confident that we have the usual vibrant collections of speakers and sessions to look forward to and that the Loughborough venue – that many of you will remember – having undergone a significant revamp, will give us more space and a much more attractive meeting space. Finally, while on the subject of meetings, our 2015 Spring Meeting will be held in York and **John Helliwell** has agreed to chair the Programme Committee. Thank you to Sandy (and Elspeth as ECM28 co-Chair), Lee and John for taking on these important tasks on our behalf.

John Helliwell also gets an additional mention because he has just been given the 2014 ACA Patterson Award "for his pioneering contributions to the development of the instrumentation, methods and applications of synchrotron radiation in macromolecular crystallography" (see www.ecanews.org/hotnews and later in this issue of *CN*. He recently emailed me to say that he is extremely grateful for all that the BCA has done for him and his PhD students over the years and that he could not have won the Patterson Award without the BCA. We are very grateful for the acknowledgement but nonetheless we all congratulate you, John, for your much-deserved award!

You will probably have seen that there has been a change in the Education and Outreach Coordinator with one becoming three. **Ross Harrington** is making a career change and will formally step down from the role in August and the job is being transferred to the triumvirate that is **Claire Murray**, **Lynne Thomas** and **Anna Warren**. It was felt that the role, in these key centenary years, was too large for one person and Claire, Lynne and Anna were keen to take it on collectively. Thank you to them and to Ross for their work over the past year and in the future. Please see their article for details of what public engagement events are planned for the future. I have also been really impressed with the variety of events that have already taken place through the efforts of our community to celebrate the Bragg Centenary. Since I last wrote there have been further radio programmes and I am looking forward to the Radio 4 programme "Bragg on the Braggs" later in August that I hope you have managed to hear (if it is still available then details should be still available from www.bbc.co.uk/mediacentre/proginfo/2013/33/r4-bragg-tues.html or by searching on iPlayer). To pick a few other examples, the Royal Institution is adding crystallographic content to their Ri Channel as part of an STFC-funded grant to coincide with the Bragg Centenary, Leeds university continues to host a wide variety of events and the copper sulphate encrusted London flat created by **Roger Hiorns** has been transferred semi-permanently to the Yorkshire Sculpture Park (see www.ysp.co.uk/exhibitions/roger-hiorns-seizure). We aim to announce these events and keep a record of past events on our website under the Bragg Centenary 2013 tab. Please take a look there for further information; clearly even more events will be happening worldwide as part of the 2014 International Year of Crystallography next year.

I hope that you have enjoyed your summer season of vacations, conferences and catching up on interesting research over the summer, and that you enjoy reading this issue of *Crystallography News*.

David Keen

BCA Council 2013

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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**

From the Editor

I have entitled our cover page "Convivial Crystallographers" because of the cheerful photographs. One, from the American Crystallographic Association, emanates from a typical meeting where crystallographers get together to discuss interesting results and learn from each other without showing off or point-scoring. Even better, of the Etter Prize Lectures at this meeting awarded by the ACA's subject groups for the best abstract in their subject area submitted by a student, two were given by UK crystallographers. The happy pair pictured on the cover are Andrew Cairns and Karim Sutton, both from Oxford. The group pictures, from the Durham and Erice Schools, demonstrate the willingness of eminent crystallographers to give up a large chunk of precious time to educate the next generation of crystallographers, and the keenness with which such education is received. Reports on these events are featured in this issue.

That meeting of the American Crystallographic Association in Honolulu was very significant. The fascinating science will be covered later in this issue, but here I want to mention a couple of items from the business meeting. Yes, the business meeting at 5 PM on Tuesday after a long day of lectures, attended only by apparatchiks with iron bottoms! Two items jolted me out of a state of profound reverie. The first was the treasurer's report of a balance well above a million dollars. This is a flattering figure since the registration fees for the Honolulu meeting had been collected but most of the expenses had not yet been paid. Even so, this should dissuade anyone from calling the BCA Treasurer "moneybags". Like the BCA, the ACA has experienced a slow decline in membership. It is energetically trying to attract new members from related scientific disciplines. The other exciting item was a report on the ACA's plans for the upcoming International Year of Crystallography. **Martha Teeter**, the Vice-President, is leading the effort, aided by about a dozen members from regions of the USA and Canada. They are producing a multi-faceted website that will present crystallography to school pupils, university students, fellow scientists and the general public. Other initiatives aimed at schools include crystal-growing competitions. Interaction with schools is designed to match both the "bottom-up" US system, where teachers have a lot of room to exercise initiative, and the more centrally directed "top-down" Canadian system. I was left with the impression that there is a lot of common ground between the ACA's and BCA's efforts, and collaboration would be beneficial. As usual, there were several parallel scientific sessions at the meeting with a lot of interesting information being imparted in each one. Therefore I am pleased to include a report by **Lauren Hatcher** along with my own. Lauren was part of a high-powered delegation from Bath, led by **Paul Raithby**. Unlike your Editor, in a display of iron-willed self-discipline Paul flew to Honolulu for the meeting and flew straight back afterwards. On the other hand, Joan and I spent a week on the Windward Coast of O'ahu before the meeting. I am sure you will believe that the main purpose of this extra week's stay was to unwind 11 hours of time difference so that I became alert enough to produce an accurate record for *Crystallography News*.

The event that will be of greatest significance to the majority of BCA members is in prospect as I write this column but will be fresh in everybody's memory when this issue is sent out. The European Crystallographic Association meeting at Warwick University is our chance to welcome our European colleagues. Judging by the information available on the website, this meeting will excite and enthuse them as well. The Young Crystallographers' satellite meeting before the main meeting is further encouraging evidence of the growing links among Europe's younger scientists – links which may spark friendships and collaborations lasting an entire scientific career.

Two articles provide additional good news for early career crystallographers. Again in 2013-14 PANalytical will be providing extra support to the research efforts of a promising crystallographer, who may have status up to but not including that of Professor. Students can look for support from the International Centre for Diffraction Data by way of a Ludo Frevel Scholarship. Last year's PANalytical Award was won by a British crystallographer, Dr **Thomas Bennett**, University of Cambridge; but I do not recall any recent British winner of a Ludo Frevel award (apologies if I have missed you), and 2014 would be an excellent year to start. Please note the respective deadlines: 30 November and 23 October.

I conclude with an appeal to the Bragg-ologists among you. While Joan and I were in North Carolina last May, we passed close to the big Army base of Fort Bragg. On our recent tour of northern California following the Honolulu meeting we drove through the town of Fort Bragg. Both of these Fort Braggs were named for the Civil War Confederate general **Braxton Bragg**. Ironically, he deserves some credit for the ending of slavery in the United States. He is considered to have been one of the least effective Confederate commanders, veering inconsistently between aggressive attacking strategies and passive retreat and alienating his subordinate commanders. Furthermore, in Louisiana before the outbreak of war, he and **P. G. T. Beauregard** appointed their friend **William Tecumseh Sherman** as the first President of the Louisiana State Seminary and Military Academy (which later became Louisiana State University). Having resigned his Army commission some years previously and then presided over the failure of a bank, Sherman had become deeply depressed; but his success in the Louisiana post restored his confidence. Subsequently, Sherman became a ruthlessly effective Union commander, his March through Georgia doing much to break the Confederacy. Does anyone know if Braxton is any relative of our Braggs?

Carl Schwalbe

Puzzle Corner

FOR each clue, provide the answer with the indicated number of letters. Then transfer each letter to the space in the grid bearing its number. A quotation from W. H. Bragg will be revealed.

Co-discoverer of insulin
__ __ __ __
6 33 13 14

Isle frequented by yachtsmen
__ __ __ __ __
19 2 3 15 23

God of element 90
__ __ __ __
5 24 21 7

Emit visible radiation
__ __ __ __ __
11 4 28 17 18

Big source of visible radiation
__ __ __
32 12 27

Most intense X-ray source (initials)
__ __ __
22 16 1

Point-and-click software access (initials)
__ __ __
10 26 8

Fe bridge across this river
__ __ __ __ __ __
20 25 29 30 31 9

	1	2	3	4	5	
6	7	8	9	10	11	
12	13		14	15	16	
17	18	19	20		21	22
	23	24	25		26	27
28	29	30	31	32	33	

In recognition of the fact that many readers have been fully occupied with preparing their abstracts for ECM28 and marking exams, the answer to the June puzzle will be held over until December.

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 and includes the following benefits:

- Up to 10 free BCA memberships for your employees.
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- Corporate Members will be listed in every BCA Newsletter and on the BCA Web Site with links to your corporate site.

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Benefits of Individual BCA Membership:

- The professional organisation for crystallographers in the UK
- A broad range of meetings organised by the BCA and its subject groups
- Preferential members' rates for such meetings
- Eligibility of students and postdocs for an Arnold Beevers Bursary award
- A copy of Crystallography News every quarter
- Optional E-mail notifications of news items and meeting information
- Influence on the development of crystallography and the BCA

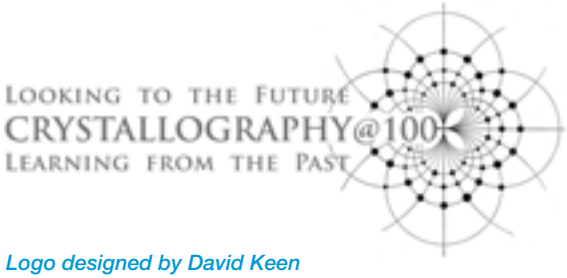
For current rates, and to join, please see **www.crystallography.org.uk/membership**

BCA Annual Spring Meeting – University of Loughborough 7-10 April 2014

"Crystallography @ 100: Looking to the future, learning from the past"

NEXT year's Spring Meeting will follow the successful format used in recent years with the traditional Young Crystallographers' satellite meeting on Monday 7 April, followed by the main meeting starting at lunchtime on Tuesday 8 April with the final session finishing at lunchtime on Thursday 10 April.

Crystallography as a field of research has reached its centenary and 2014 has been designated by UNESCO as the International Year of Crystallography. The theme of the meeting is in tune with these milestones and will be **"Crystallography @ 100: Looking to the future, learning from the past."** The meeting logo incorporates an image of the X-ray diffraction pattern of NaCl reported by **W. L. Bragg** in the charmingly titled 1913 paper "The Structure of Some Crystals as Indicated by their Diffraction of X-rays" (*Proc. R. Soc. Lond. A.* **1913**, 89, 248-277; doi:10.1098/rspa.1913.0083). We are grateful to the Royal Society for permission to include this image.



Logo designed by David Keen

Awards and Plenary Lectures

THE meeting will be the first to include a new schedule of plenary lectures recently agreed by BCA Council. Thus, the 2014 meeting will open with the Lonsdale Lecture, which will now be an annual lecture. The meeting will also include the Bragg Lecture, which will conclude the presentations on the middle Wednesday of the meeting. The Bragg lecture will be scheduled in future on a triennial basis in a cycle along with the Hodgkin lecture and the President's lecture, also known as the BCA Prize lecture. Formal descriptions of these award lectures feature on the BCA web site (http://crystallography.org.uk/prizes/).

In addition to the two award lectures, there will be four other plenary lectures associated with the Biological (BSG), Chemical (CCG), Physical (PCG) and Industrial (IG) subject groups. The Young Crystallographers' satellite meeting will also include two separate plenary lectures.

Prize Lectures

THE meeting will also include a prize symposium devoted to early career scientists on the morning of the middle Wednesday (April 9). This session will include four lectures as well as prize presentations. These are the established Chemical Crystallography Group prize, sponsored by the Cambridge Crystallographic Data Centre, the Physical Crystallography prize, sponsored by the Institute of Physics, a new Biological Structure Group Prize, and the IG/YCG Prize. The latter is selected from presentations made at the YCG satellite meeting, whereas the former three will require nominations to be submitted (details forthcoming on the BCA web site, with approximate deadline dates in January 2014).

The meeting will also include a number of poster prizes.

Dates, Links & Abstract Submission

ALL the latest information concerning the meeting, including the programme, registration and abstract submission, can be found at the meeting website: http://crystallography.org.uk/spring-meeting-2014.

Deadlines

As in 2012, there will be a single common abstract deadline for oral and poster abstract submissions including submission for the YCG Satellite Meeting. ***All submissions must be received by 17 January 2014***. If your oral abstract is not accepted, you will be invited to submit the abstract as a poster abstract instead. ***This deadline cannot be postponed*** due to the tight schedule surrounding printing the abstract book.

Currently Confirmed Award and Plenary Speakers

Bragg Lecture – **Prof. Judith Howard**, FRS
Lonsdale Lecture – TBC

Plenary lectures:

BSG: TBC
CCG: TBC
PCG: Prof. Malcolm McMahon
ICG: TBC

Currently Confirmed Symposia

The overall theme of the meeting is very forward looking and focuses on the development of crystallography away from purely structure determination towards crystallography under non-ambient conditions, crystallography at different timescales, combining crystallography with other diffraction and non-diffraction techniques (e.g. spectroscopy, computation), and applications of structural science.

Symposium Title
Non-ambient Diffraction
Crystal Engineering
Neutron Diffraction in Chemical Crystallography
Getting a Job in Industry
Magnetic Structure Determination
Dynamic Processes and Reactions
XRD in the Pharmaceutical Industry
Complementary Diffraction Methods
Complementary Non-Diffraction Methods
Pushing the Limits: Faster
Pushing the Limits: Slower
Pushing the Limits: Larger
Pushing the Limits: Smaller

Non-ambient diffraction: including crystallography at different temperatures, pressures and under different gas atmospheres.

Complementary diffraction methods: combining X-ray, neutron and electron diffraction.

Complementary non-diffraction methods: use of spectroscopic and computational modelling methods instead of, or in combination with, crystallography to obtain structural information (e.g. SS-NMR, IR/Raman/UV/Vis, EM, EELS, XAFS).

Pushing the limits: a sequence of symposia focussed on biological macromolecules, but with overlap of techniques of interest to a broad crystallographic audience. (***Faster*** – FELs & single-shot synchrotron; ***Slower*** – the X-ray limits: neutrons, CryoEM, SS-NMR; ***Larger*** – viruses, complexes; ***Smaller*** – micro/nano-focus beams).

Applications: chemical, physical and industrial crystallography (crystal engineering, dynamic processes & reactions, magnetic materials, XRD in pharma).

Careers: There will be a symposium which will include presentations and round-table discussion – ***Getting a Job in Industry***.

Programme Committee

- Lee Brammer (2014 Programme Chair)
- Peter Moody (BSG)
- John Schwabe (BSG)
- Hazel Sparkes (CCG)
- Lynne Thomas (CCG)
- Emma McCabe (PCG)
- Ivana Evans (PCG)
- Judith Shackleton (IG)
- Anthony Phillips (YCG)
- Anna Warren (YCG)
- John Helliwell (2015 Programme Chair)
- David Keen (BCA President)
- Dave Allan (BCA Vice-President)
- Claire Wilson (BCA Secretary)
- Nicola Peel (HG3)

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New Education and Outreach Team

THE BCA council has appointed three Education and Outreach coordinators to continue the fantastic work of Ross Harrington. He is a very hard act to follow, and his outstanding work leading up to and during the Big Bang Fair has really raised the profile of the BCA and taught more than 30,000 people aged 4 and above about crystallography!

You may think three people is quite a lot to replace one person, but our growing portfolio of outreach events and activities requires a lot of planning and coordination, so we are sharing the work between us! We are all lucky enough to be able to celebrate the centenary of our science, and hope that by promoting crystallography to the general public we can continue to awaken their curiosity and excitement about our fantastic science.

For the coming months we have quite a few activities planned that you may like to get involved with. First up is the British Science Festival in September. We will be running hour long workshops (3 per day) from Monday 9 – Thursday 12 September aimed at school children aged 16. It is still based on 'The Structure of Stuff is Sweet' like at the Big Bang Fair, but instead of a stand for students to come and look at, it will be held as a workshop where we explain particular aspects of crystallography to small groups, including a tour of the Newcastle crystallography department.

For many years now the MRC Laboratory of Molecular Biology at the University of Cambridge have been running a very successful crystal growing competition in Cambridge. We will be helping with a similar activity in March with the Oxford Science Festival, supported by STFC, Diamond Light Source, the Museum of the History of Science and the Natural History Museum Oxford. It will culminate in the display of crystals grown by local schoolchildren in a public area in Oxford. We would love to get volunteers to visit schools and explain some of the science behind diffraction and crystallography. Each session should run for no longer than one afternoon, and is a great opportunity to get schoolchildren interested in science and crystallography. If you are interested please do contact us on the email address provided below – even if you have never done this before we have lots of worksheets and materials available to support you, so please do have a go!

We are also talking with the STFC and other organisations about the different science fairs around the country that we could visit with our stand from the Big Bang Fair. We will send out details as soon as we decide, and we would very much appreciate any time that you could volunteer. The success of these events relies entirely on the enthusiasm and energy of all our volunteers so we need you!

We do have an Outreach mailing list, so if you are interested in getting involved or have ideas for outreach events please email us to let us know: education@crystallography.org.uk

We have also just started tweeting – follow us @Whatsinacrystal for updates on our activities over the next few months!

Anna Warren, Claire Murray and Lynne Thomas


Anna Warren


Claire Murray


Lynne Thomas

The BCA Industrial Group XRF Meeting

XRF Meeting Report 24 April 2013

A joint BCA/RSC Atomic Spectroscopy Group Meeting at University of Leicester.

The meeting was sponsored by: *Analysco, Bruker, Claisse, Datech Scientific, NitonUK, Olympus, PANalytical, SciMed, Socachim, Specac, Spex CertiPrep and Thermo Scientific*

Morning Session

THE first session of the meeting was a practical demonstration by Oliver Meyer and Rainer Schramm, of Fluxana, of techniques for the preparation of solid samples for XRF without using a fusion. In many cases, fusion is the best option, but it is not the simplest. Loose powder samples can give good results, but all too often do not, because of variable packing and/or particle-size effects. Pellets can sometimes be pressed without a binder (like the KBr discs often used for infrared), but in general, a binder is needed. The binder produced by Fluxana is a wax, typically used at 20 % m/m. With pressed pellets, particle size can be an issue, especially if the sample is only ground to 100 µm or so, because this dimension can be similar to the penetration depth for light elements. They also mentioned a number of other useful tips:

- Liquid samples tend to outgas; this can be prevented by ultrasonicing (or any of the other tricks used to outgas HPLC samples!)
- Inhomogeneous liquids can be mixed with a binder – Fluxana supply a cellulose for this purpose, used at 33 % m/m – to form a paste which is then put into a liquid sample cup.
- "Sticky mess" samples can be dealt with by pressing a pellet which has a depression in one side; this requires a special die. This depression is filled with sample, which is smoothed off with a microscope slide and covered with a piece of film (e.g. polypropylene).

The second practical session was led by **Frédéric Davidts** of Socachim. This dealt mainly with fusions, using either gas or electric furnace. For method development, he prefers working with the gas fusion machine because he can see what is going on. The electric furnace is fully enclosed and therefore laboratory staff are protected from hot material and from all moving parts. He also demonstrated how an awkward sample like wood chips can be ground with a planetary ring mill, with a binder/grinding additive, to form a satisfactory pellet, from which all the air occluded in the wood has been extracted. He pointed out that all mills contaminate the sample with small amounts of themselves.

continued overleaf

Morning Session demonstrators and speaker, *from left to right: Oliver Meyer, Ros Schwarz (Chair), Allan Finley, Frederic Davidts, Anne-Catherine Breton, Rainer Schramm and Margaret West (Chair)*

After the coffee break, **Anne-Catherine Breton** from Claisse spoke about the development of a procedure for the XRF analysis of iron ore samples. The present method, ISO9516-1:2003, covers a fair range of elements (not including iron), but over calibration ranges which are often inadequate. The first calibration used standards made with pure oxides and a comparison was made with a second calibration using CRMs as standards. The new method includes iron and widens the calibrated range for almost all elements. The 29 standards used are 20 iron ores and 9 other materials. The XRF analysis uses the LiF (200) crystal wherever possible; count times are designed to give the required accuracy and precision. Sample preparation is a fusion using a borate flux - a different mixture of lithium metaborate and tetraborate to the ISO procedure – at 1050 °C in a 95Pt/5Au crucible. Ammonium nitrate (rather than sodium nitrate, which precludes Na determination) is added as oxidant, and ammonium iodide as non-wetting additive. Copies of a leaflet on this process were available from the Claisse stand.

The final talk of the morning session was **Ros Schwarz**'s introduction to the participant sample. Portions of this were distributed to any participant who wanted it. This is intended to act as an aid to methods development and training, and is not a proficiency test or Round Robin. Participants are asked to determine as many elements as they wish by any suitable XRF method or other technique, and to return the results by 30th September 2013. The origin of the sample was not disclosed in detail, but it is a composite from more than one brownfield site. Accessory minerals include sand and clays.

David Beveridge

Afternoon Session

FORTIFIED by a good lunch we enjoyed two papers offering good advice for delegates who had collected their "participant sample" from Ros.

Afternoon Session speakers, *from left to right: Garry Smith, David Beveridge (Chair), Chris Calam, Colin Slater, Steve Davies and Dave Taylor (Chair)*

Being in the audience for **Steve Davies**'s original talk on *Specimen Support Films* back in 1995 it was interesting to note that not much had changed. Using 3 international standards for oil applications (ASTM D6443, ISO 20884 & IP503) Steve showed that hydrocarbon films were "cleaner" than those bearing O_2 and benefited from better transmission per unit area. The chemical resistance data showed that the films hadn't changed but in the petrochemical industry the samples are different. Fuels now have increasing O_2 bearing additives and samples containing hydrocarbon mixed products should not be placed on hydrocarbon films. For oil samples 3.5 μm Mylar was recommended. For those outside the petrochemical industry interested in standardless analysis, hydrocarbon films are cleaner and have better transmission. Whichever film is selected, the analyst was advised to test before use as leakage may have an adverse effect on the service support costs.

Colin Slater's talk on *Standardless Analysis* gave us useful advice when charged with answering the time old question "What is in my sample?" When no standards are available, we now have fundamental parameters at our disposal. Colin steered through challenges such as matrix effects and showed that any XRF FP data is as good as the information that is known about the sample. Using an Aldrich molecular sieve, analytical data was shown to improve as more facts concerning the sample were introduced into the software package. For water/ethanol/oil based samples, the Rh Kα Compton ratio technique was offered as a valuable way to deal with very low density materials. Finally, Colin gave examples of how to analyse layer thickness in samples.

Margaret West

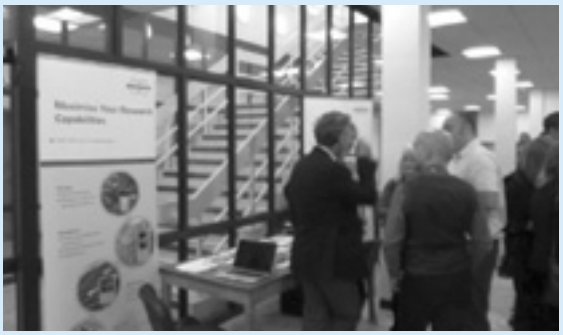
After our break for tea (and yummy cake!), **Garry Smith**, XRF Application Specialist with SciMed, discussed the difficulties inherent in carrying out *Liquid Waste Analysis*. He highlighted the general problem caused by the presence of two phases in these samples; suspended solids and immiscible liquids, which will start to settle out and separate as soon as the sample is poured into an XRF cup. He emphasized how difficult this makes it to fulfil the basic requirement that the analysis should be representative of the bulk material, because the radiation from each element in the sample will have a different penetration depth. Penetration depth increases with increasing photon energy, but decreases with average atomic number of the matrix and sample density. With light matrix liquid samples the penetration depths can be dramatically different on the scale of a sample cup. For example Cr Kα radiation will come from up to 4.33mm in oil or 1.44mm in water, but Cl Kα will come from the bottom 0.36mm in oil or only 0.17mm in water. He showed graphs of an oil and water mix with the Cl predominately in water and Cr predominately in oil where over ten minutes the Cl signal increased by about 70% and the Cr signal decreased by 33% as the water layer separated to the bottom of the cup. He then mentioned two options to tackle the problem; separating the phases by centrifuging or filtration before analysis; or using a solid binder to immobilise the phases. He suggested binders such as graphite powder or activated alumina for this purpose.

The final talk of the day, given by **Chris Calam** from Thermo Scientific Portable Analytical Instrumentation, took us out of the laboratory into the African bush, away from any sources of power. His talk on *Field Portable Sample Preparation Tools for Mineral Analysis in Remote Location* discussed the challenges of surveying for ore bodies. Field Portable (FP)-XRF is used to detect elements such as Cu, traces of which can reach the surface above an exploitable deposit. In the first instance, FP-XRF is used on a transect to look for a “Cu anomaly”; levels significantly above background. Chris showed us plots demonstrating how well FP-XRF can detect Cu anomalies with no sample preparation at all (compared to laboratory results for samples from the same transect analysed by XRF and ICP-MS). However, when the exploration moves on to resource estimation and reliable quantitative analysis is required, sample preparation is needed as figures from FP-XRF can vary markedly over one piece of a heterogeneous rock. Comparing FP-XRF field and laboratory XRF and ICP-MS measurements graphically illustrated the improvement in correlation obtained when some sample preparation was carried out in the field. For example, the relative standard deviation of results for nickel improved from 0.797 to 0.961 and for Mg improved from 0.417 to 0.950; also emphasizing how particularly important this is for light elements. The battery-operated sample preparation tools he suggested included a direct rock sampler which grinds material from the surface of an outcrop into a collection tube and a portable mill. Other preparation equipment was human-powered, such as a crusher with a large hammer and a sample press, also operated by sharp blows with a hammer (up to about 10 tons). These items are marketed in a kit.

We ended the meeting by expressing our thanks to the local organisers from the University of Leicester, **Nick Marsh** and **Cheryl Haidon** and to the members of the XRF committee.

Ros Schwarz

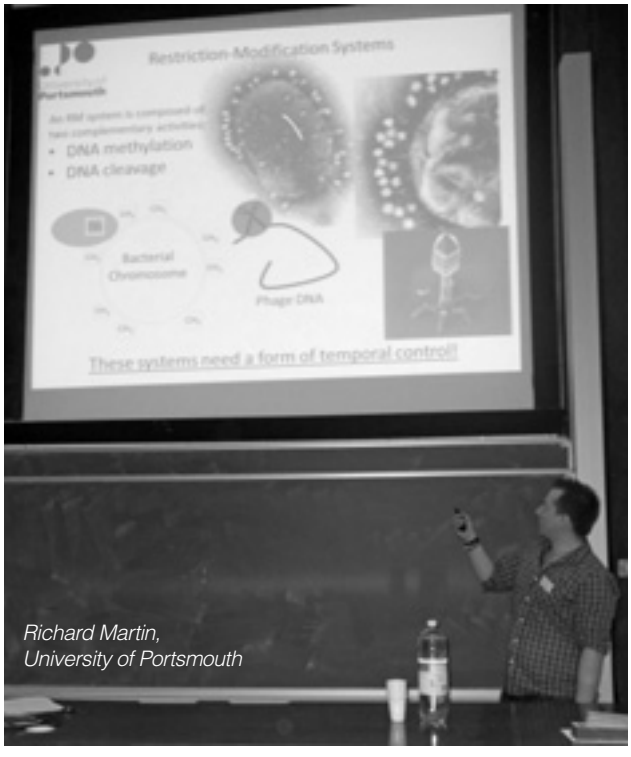
Informal images taken in the Exhibition area



Southwest Structural Biology Consortium

THE South West Structural Biology Consortium holds an annual meeting aimed at bringing together researchers from across the South West region with an interest in structural biology. This year's meeting was held on 1-2 July, hosted by the University of Bristol and organised by Paul Race, Alice Robson, Matt Crump and Jim Spencer. With over 150 registered delegates, this was the most extensive meeting in the consortium's 12-year history.

We were treated to three exciting talks from plenary speakers who are world leaders in the field of structural biology. Firstly, Dr **Ray Owens** from the Oxford Protein Production Facility UK gave an interesting overview of the work his group are doing trying to solve the structures of glycosylated eukaryotic proteins, which are hugely underrepresented in the PDB. He described the systems that his group have developed to overcome the difficulties in working with such proteins and a number of examples of success at solving structures by x-ray crystallography. Secondly, Prof **Steve Matthews** from Imperial College London gave a fascinating insight into how his group are using NMR to study precise binding interactions within large protein complexes. He exemplified this with a study into the interaction between a phage protein and the bacterial transcription machinery. Finally, Prof **Bryan Krantz** from University of California, Berkeley presented his work on protein translocation through the anthrax toxin translocase. He explained how he uses a combination of structural biology techniques, electrophysiology and biophysical methods to shed light on the mechanism by which proteins are threaded through the pore, driven by a proton electrochemical gradient.



Richard Martin, University of Portsmouth

The SWSBC has a history of being a platform for younger researchers to present their work and network with other scientists across the region. There were 10 talks from junior researchers and 45 poster presentations. Congratulations to **Eyram Adjogatse**, a graduate student from University College London, who won the Agilent Poster Prize for his poster on the structure and function of L-threonine dehydrogenase.

The conference dinner was held at local microbrewery Zero Degrees; after an excellent meal many delegates sampled the variety of beers on offer!

The meeting is made possible by ongoing generous sponsorship from CCP4 and the Biological Structures Group of the BCA. In addition, participation of commercial exhibitors has always been a major part of the conference and this year we were overwhelmed by the generous support of 14 different companies. Representatives from 4 of these companies gave talks during the main sessions, giving us updates on the latest developments in technologies relating to structural biology.

The extremely high quality of talks and posters, particularly from younger researchers, was very encouraging and demonstrated that the field of structural biology is thriving and developing in the region. We look forward to next year's meeting, which will be held at the University of Bath.

Alice Robson
University of Bristol

The 14th BCA/CCG Intensive Teaching School in X-ray Structure Analysis, Durham

THE 14th BCA/CCG Intensive Teaching School in X-ray Structure Analysis was held at Durham University from the 6th-14th of April this year. The theoretical course combines a mixture of lectures and tutorials in tutor groups alongside a few relaxed social evening events. The programme is very intensive and saw the 81 students, 10 tutors and 6 lecturers working very hard throughout. The participants were predominantly PhD students or PDRAs, either working in crystallographic groups or using crystallography to assist their research. The students were able to form links to scientists both in the UK and from abroad with participants coming from a range of countries including Brazil, Chile, Finland, France, Germany, Ireland, Portugal, Russia, Slovenia, Saudi Arabia and the UK.

The lectures and tutorials cover crystallographic theory and are designed to give the participants a good understanding of all aspects of crystallographic data collection and refinement along with data interpretation. The content of the course is kept up to date with new developments in technology or software incorporated as they arise, and this year's course was no exception including the following topics: relevant mathematics, symmetry, data collection from instrumentation to data collection strategies, structure solution methods, refinement, derivation of results, errors, twinning, structure validation, disorder and databases. In addition there were short presentations on incommensurate structures and synchrotrons and neutrons; despite being optional these were attended by almost all the participants. This year we welcomed two new members to the teaching staff, Dr **Richard Cooper** (Oxford) joined the lecturing staff and Dr **Mark Warren** (Diamond) joined the tutoring staff. I would like to thank all of the lecturing and tutoring staff for their hard work both before and during the course as this contributed to the overall success.

The evening events included a partly crystallographic bar quiz, group presentations on a crystallographic topic and the course dinner. The bar quiz held on the first Sunday of the course was good fun and a great opportunity for the tutor groups to socialise together; it required crystallographic and general knowledge including an 'identify the space group' picture round and a Disney films round! The group presentations, as with previous years, were of a very high standard providing both amusement and an educational content; this year the groups' presentation titles were based on James Bond film titles modified to have a crystallographic twist, such as 'Coldfinger' and 'On Her Majesty's Twinning Service'. As with previous years the lecturers were cast in

several of the presentations, including an excellent rendition of a twinned **Bill Clegg** and excerpts of **Simon Parsons**' famous twinning lecture with London Bricks before he had chance to deliver it the following morning! The course was rounded off with the course dinner on the final Saturday night, during which prizes for the quiz and group presentations were made and thanks were expressed to all of the staff.

The feedback from the students on this year's course was very good with the general feeling that, although it was hard work, it was both enjoyable and hugely beneficial to their research. As usual the lecturers and tutors scored highly along with the overall organisation, and students particularly appreciated having so much contact with expert crystallographers in a friendly atmosphere. All of the students worked very hard and with a positive collegial attitude which helped to create a pleasant and enjoyable school.

Finally we would like to thank our sponsors for financial support of the course which makes a huge difference enabling us to support students to attend the course; this year's sponsors were Agilent Technologies, Bruker, CCG, CCDC, Diamond, ECA, ISIS, IUCr, Oxford Cryosystems and Rigaku.

Hazel A. Sparkes (ISIS)

Erice School – The 46th International School of Crystallography, Sicily

THE 46th International School of Crystallography entitled 'The Future of Dynamic Structural Science' was held from the 30th of May to the 8th of June 2013 at the Ettore Majorana Foundation, Erice, Sicily. The main objective of the course was to increase the knowledge of younger scientists in the required crystallographic and spectroscopic techniques that are essential to work successfully in the field of dynamic structural science. To this end the programme included presentations by world leaders in the fields of time-resolved crystallography and spectroscopy and the course feedback indicated that mixing experts and talks in these two areas was felt by participants to have been hugely beneficial.

Crystallographic lectures covered both chemical and biological studies ranging from slow through to faster timescales as the week progressed. Topics covered included metastable species, linkage isomerism, dynamics under pressure in both chemical and biological species,

single crystal to single crystal transformations, X-ray scattering from liquids, photo-excited species, magnetic properties, challenges for studying irreversible reactions, how to study biological processes during which radiation damage occurs, time resolved synchrotron experiments, use of pulsed X-ray beams and mechanical choppers, X-ray Coherent Diffraction Imaging, timing tools and XFEL. Time-resolved spectroscopic techniques discussed included Raman, XAFS, fluorescence spectroscopy, absorption and emission spectroscopy. Approximately a third of the lecturers also gave demonstrations and / or workshops of relevant software in order to introduce the participants to available analysis programs.

Alongside the lecturing program, 10 students were selected from the submitted abstracts to give short 25 minute presentations on their research. These talks covered the range of topics presented during the course and were of a very high standard. In addition, all of the participants presenting a poster gave a two minute talk to the rest of the participants to encourage people to visit their poster. One particularly memorable presentation featured **Ben Bax** (GSK, UK) using bread sticks and his hands to illustrate, very effectively, the catalytic behaviour of a conformationally flexible enzyme.

During the course two half-day excursions were made; the first to Mozia Island, which has ruins alongside a small museum that, despite its small size, contained a large number of fantastically well preserved artefacts including pots, grave items, jewellery and games all of which had been excavated on the island mostly by the Whitakers. The second trip took in Selinunte and Segesta which both contained Greek ruins including temples, city remains and an amphitheatre; the huge size of the temples was breath-taking given the tools that were available to build them. For those participants who preferred a relaxed afternoon there was the opportunity to go to the beach with all participants meeting up again for traditional Sicilian food in the evenings.

Poster prizes were awarded to **Maike Joester** (Germany) and **Ahmed Mabied** (Egypt) for the best two posters presented during the meeting, and we commended three others: **Joshua Hill** (Oxford, UK), **Nikita Marchenkov** (Russia) and **Franziska Pinker** (France), as the standards were really excellent and the poster prize judges had a tough time selecting the winners. The Lodovico prize is awarded in memory of **Lodovico Riva di Sanseverino** who founded the crystallographic courses in Erice and died in 2010. It is awarded to a younger scientist(s), who make(s) a significant contribution to the meeting particularly during the lectures and was shared this year between **Elenora Conterosito** (Italy), **Matthew Robinson** (Edinburgh, UK) and **Alexander Theodossis** (Melbourne, Australia).

No mention of Erice would be complete without mentioning the contribution of the 'orange scarves' who work very hard to ensure the smooth running of the course, from preparations behind the scenes registering participants and making local arrangements to meeting participants at the airport, setting the IT up and keeping it operational through the course, running around during the course and always being there to help participants with local information. A huge thank you is due to all of the orange scarves, but in particular **Annalisa Guerri** (Florence, Italy) and **Paola Spadon** (Padova, Italy).

In spite of unseasonably cold weather at the start to the course, which saw many people sporting newly purchased sweatshirts, the course was thoroughly enjoyable and provided an excellent opportunity for scientists from around the world to mix and form new multi-disciplinary collaborations across the fields of time-resolved crystallography and spectroscopy. The high standard of lectures, demonstrations and workshops provided participants with an excellent overview and increased understanding of all aspects of this developing field. We would like to thank the lecturers for their hard work preparing their material and the participants for their enthusiastic contributions throughout the course which made it both and educational and pleasurable course.

Finally, we would like to thank NATO, the ECA, the IUCr, OPCW and PANalytical for sponsorship without whom the course would not have been as successful.

Hazel A. Sparkes (ISIS) and
Judith A. K. Howard (Durham)

American Crystallographic Association Annual Meeting

AS usual, the start of scientific sessions at the main meeting on Sunday, 21 July, was preceded by a set of workshops the day before, designed to impart "how-to-do-it" information in various areas of crystallography: WK.01 Biological Small Angle Solution Scattering – Theory and Practice, WSK.02 GSAS-II Workshop, WK.03 Get the Most out of the Cambridge Structural Database System. My colleagues from the CCDC tell me that their workshop had a good attendance by people eager to sharpen their skills with the database, and I'm sure the same is true of the other workshops. That evening, all meeting participants were treated to an Opening Reception which was noteworthy for two things. The supply of food and drink was generous and kept us happily sipping, munching and chatting until the security people reminded us that it was closing time. It was evident that a good number of crystallographers from Australasia were present, presumably because the ACA met them halfway across the Pacific.

Bright and early at 8 AM on Sunday morning a large number of participants overcame any desire for a lie-in after their evening activities and attended the **Robert Bau** Award Lecture. This lecture commemorates the life and work of Bob Bau, whose untimely death deprived us of a brilliant scientist and a generous research collaborator. Fittingly, it was given by Bob Bau's long-time friend and coworker, **Thomas Koetzle**. In a wide-ranging description of neutron diffraction facilities and results as they advanced over the years, Tom demonstrated the capabilities of neutron diffraction as he paid tribute to Bob and to **Walter Hamilton**, his mentor who also suffered an untimely death. From simple beginnings with studies of amino acid structures that unambiguously determined their protonation state the biological applications of neutron diffraction advanced to the elucidation of the stereochemistry of alcohol dehydrogenase by discriminating between H and D in the chirally deuterated product. Neutron diffraction revealed the fascinating structures of numerous types of metal hydrides, of relevance both to an understanding of chemical bonding and to technology needed for a hydrogen economy.

Among the five parallel sessions that followed, the one on "Improving Structural Models through Computational Tips & Tricks" drew a crowd, particularly the first lecture by **Anthony Spek** about the SQUEEZE tool. One might have thought that this method had reached its final state, but we learned about exciting new developments. Over 10,000 entries in the Cambridge Structural Database report the use of SQUEEZE. The original approach identified regions of disordered solvent, calculated the contribution of their electron density and subtracted it before continuing with normal refinement using the modified .hkl file. This modification of the data file drew criticism from some crystallographers who deplored any tampering, and it was not clear how to handle twins. SQUEEZE has now been adapted to work with SHELXL2013, and it runs under Louis Farrugia's GUI. The use of more files has eliminated the need to modify the data file. SHELXL2013 accepts a fixed solvent contribution to F(calc), and the method now can handle twins. Requirements are: no residual unresolved density in the discrete model region, no inconsistent filling with solvent, sufficient resolution and completeness, no issues about charge balance.

The next lecture by **Julien Jorda** on "Crowdsourcing the phase problem in protein crystallography" started out along familiar lines. We know about attempts to solve problems requiring massive amounts of computation by using otherwise idle time on large numbers of personal computers. Julien's method for solving the phase problem uses a genetic algorithm, in which each phase is a gene and the phase set is a genome. Fitness is driven by an estimator. At intervals a tournament is held among the two fittest individuals plus a random sample of others. As proof of principle, estimating fitness by the weighted RMS error gave rapid convergence to the correct solution. Of course, this estimator requires knowledge of the correct phases, i.e. the structure must already be solved. Next, the skewness of the electron density distribution, which needed no prior knowledge, was tried as an estimator, but it did not work. Now the computer owners as well as their computers were put to work. By dressing up the method as a multi-player game and giving some training about the features of correct and incorrect electron density maps, even non-crystallographers could select the most reasonable-looking map as an estimator of fitness.

Amy Sarjeant showed how crystallography and modelling could work together. She studied the structure of a carborane-based MOF which existed in three forms: (1) hexagonal tablets, for which the structure could not be solved, (2) rectangular plates, which could be solved with difficulty, and (3) hexagonal prisms, which were solved easily. There was enough similarity between (1) and (2) that the latter could be taken as a trial structure for (1), but refinement stuck at R = 34%. *Ab initio* modelling with Materials Studio failed to produce any useful results. However, "bootstrapping" the modelling with the trial structure moved the atoms just enough to initiate a successful refinement.

As usual, the displays of the commercial exhibitors, with or without delicious free lunches, and the talks given by some of their delegates, were most impressive. For me the biggest surprise came in a General Interest talk by **Bjorn Hansson**. In the development of X-ray sources over the last century one of the greatest fear factors has been melting of the anode. Microfocus and rotating anode generators have worked around this limitation but still could not avoid it. The obvious solution is to use an anode that is already in the liquid state, but the issue is how to control its geometry. An X-ray source now operates reliably in which a jet of gallium containing a little indium about 200 μm across moves without turbulence through a vacuum chamber at about 75 m s^{-1}. The GaKα radiation generated has a wavelength of 1.3 Å. The rapid motion of the jet spreads the heat loading,

enabling a very intense beam to be produced. The fear factor now is vaporisation of the anode!

Monday's session on "Structure Validation" began with a characteristically thought-provoking talk from **Bernhard Rupp** provocatively entitled "The Road to Scientific Serfdom" and subtitled "Sociology, epistemology and systemic human factors in the emergence of over-interpretation of crystallographic models". In every era of the development of science it has been difficult to deal with negative results. Modern projects in macromolecular crystallography often have as their objective the discovery of suitable ligands. Thus a fervent wish may arise to find a ligand even when its presence is ambiguous or lacking. Binding sites want to bind something, so they "suck up stuff", which may or may not be the ligand of interest. With the mass of a ligand typically being 1/1000 that of the protein and high B-factors and partial occupancy being common, the correct or incorrect fitting of a ligand has very little effect on the overall measures of quality. Local indicators are needed. The procedure of ligand fitting is addressed in the paper by C. X. Weichenberger, E. Pozharski and B. Rupp entitled "Visualizing ligand molecules in twilight electron density" in *Acta Cryst.* (2013). F**69**, 195-200.

In the Etter Early Career Award Symposium **Aurora Cruz-Cabeza** clarified the concept of conformational polymorphism. She introduced 5-methyl-2-[(2-nitrophenyl)amino]-3-thiophenecarbonitrile, nicknamed ROY because it has red, orange and yellow polymorphs. To date 7 forms of ROY are known, all with more or less different torsion angles. Which of these are genuine conformational polymorphs is clarified by plotting their values on a graph of conformational energy in the gas phase. It then becomes clear whether the gas-phase minimum-energy conformation has merely adjusted somewhat in the crystalline state or whether a new minimum is occupied. In fact, 5 polymorphs of ROY are near one minimum and 2 are near another. Aurora generalised her analysis to the polymorphic subset of the Cambridge Structural Database. Of 1297 molecules represented by 2770 crystal structures, 63.8% have just one conformer, and only 11% of rotatable bonds change. This proportion varies widely with bond type: it is 27% for C-C-N-C but only 1% for ester bonds.

This is just a small selection of the excellent talks that were presented. In addition, three very informative poster sessions were aided by the provision of drinks and snacks. I should have remembered what was on offer at previous ACA meetings; but I didn't, and therefore I ended up with beer and cookies one day and wine and pretzels the next. Still, I met some very interesting people and increased my level of knowledge.

Carl Schwalbe

YOU might think that, being in Hawaii, there was more surfing than science to be done at this year's ACA Annual Meeting, but it was apparent from the first day that the sessions would be well attended despite the lure of sparkling sun and sea outside!

By Monday morning the meeting was in full swing, and a particularly interesting session on "Cool Structures" caught

my attention. The session consisted of nine short talks, each presenting a structure that had some aspect that might be considered rather neat, at least to the crystallographic audience assembled! I particularly enjoyed two exemplary talks given by fellow young scientists, both recipients of Margaret C. Etter Student Lecturer Awards this year. Firstly, **Andrew Cairns** from Oxford presented his work with systems undergoing the interesting phenomenon of giant negative linear compressibility, the ability of a system to expand along at least one axis whilst the crystal is actually being placed under pressure. Secondly, **Christopher Rackauckas** from Oberlin College described his work understanding the structure of an incommensurately modulated phase of "H-acid", a highly useful material in manufacturing, obtained by variable temperature experiments. Chris's talk included one of the more accessible explanations of modulated structures I think I have come across, which was particularly helpful on a topic that very often goes way over my head!

Running throughout the meeting was the Transactions Symposium, this year focussed on the role of Neutron and Synchrotron sources in crystallography, and a huge volume of very interesting and progressive work was being presented. In addition to a number of sessions dedicated to MX topics, where synchrotron work is so far advanced, a few of these sessions focussed also on the central facilities available for inorganic and chemical crystallography studies. A number of talks presented materials with interesting potential applications, as well as showcasing the power of these high intensity facilities for this type of work. In TR04, **Bill Clegg** gave insight into the process that went about setting up the first chemical crystallography beamline in the UK at Daresbury, which was both a captivating history and no doubt instructive for new projects looking to achieve similar ends in the future.

By the last day Waikiki beach still hadn't claimed all delegates, and the final sessions were still well attended until the last. The meeting was ended with the conference dinner at the spectacular Royal Hawaiian Hotel next door to the conference. The "Pink Palace", as it is sometimes known, was one of the first hotels to be established in Waikiki and it is certainly one with some character. A beautifully cooked dinner followed a drinks reception overlooking Waikiki beach at sunset, making a fitting end to what had been a great conference in such a beautiful part of the world.

Lauren Hatcher
University of Bath

Available Awards

ICDD Awards – Ludo Frevel Crystallography Scholarships

Honoring Ludo K. Frevel
(1910-2011)

A gentleman and scientist, Ludo joined The Dow Chemical Company Spectroscopy Laboratory in 1936 and until retirement, was one of Dow's top scientists. In fact, he was the first Dow scientist to have the title 'Research Specialist'. He held 60 patents and co-authored 446 technical papers, publishing his most recent paper at age 95. Ludo was co-author with Hanawalt and Rinn on the famous 1938 paper, *"Chemical Analysis by X-ray Diffraction"*, was a world expert in catalysis, and was known for several innovations in the field of powder diffraction. He also wrote some of the first computer automated material identification software utilizing X-ray powder diffraction data. Ludo served as ICDD Chairman of the Board of Directors from 1990-1992.

TO encourage promising graduate students to pursue crystallographically oriented research, the International Centre for Diffraction Data (ICDD) has established a Crystallography Scholarship Fund, known as the Ludo Frevel Crystallography Scholarship Fund. While the Ewald Prize is awarded every three years to an internationally recognized crystallographer, little effort has been made by science departments to cultivate aspiring crystallographers. Convinced of the beneficial, scientific impact of the proposed scholarships for crystallographically oriented research, the ICDD has solicited funds from private and industrial sectors to support this program.

The ICDD has awarded 148 scholarships since 1991. The 2013 Scholarship Awards were in the amount of $2,500 each. Since the scholarship's inception in 1991, $347,250 has been awarded to aspiring crystallographers. Applications for the year 2014 awards must be received by ICDD no later than **23 October 2013**.

All applications are to be submitted via the ICDD web site. Please follow the instructions below. The preferred method of application is via the web; however, if you require an alternate method, please contact *Lisa ONeill* – E-mail: oneill@icdd.com or Tel: **+610-325-9814**.

The on-line application will request you to upload the following information in the form of two separate PDF documents. The on-line application will also request you to provide the contact information for your primary research advisor. An e-mail will be sent to this advisor seeking a letter of recommendation on your behalf. Please note the recommendation letter is due on or before the deadline of **23 October 2013**.

Please prepare the following in advance of applying on-line.

1. **A description of the candidate's proposed research (limit 2 pages) including:**

- Purpose and rationale for the research
- Proposed methodology to be used in the study
- References and/or descriptions of the scientific background for the proposed research

2. **A curriculum vitae including:**

- Educational preparation (institutions, dates, degrees obtained and in progress, and particularly pertinent coursework)
- Awards, honors received
- Any research publications and/or presentations given
- Any work experience (dates, employers, positions)
- Professional activities, memberships

ICDD®
International Centre for Diffraction Data

PANalytical Award 2013 / 14

THE success of the first PANalytical Award 2012 / 13 (won by Dr Thomas Bennett, University of Cambridge) has encouraged us once again to embark upon the exciting enterprise to reward young researchers that have demonstrated innovative thought to their research when using an X-ray analytical technique. The winner of this award will be rewarded with a €5,000 prize.

The project is an opportunity to advance scientists that are presently establishing their research careers. These early-career researchers are most affected by the reduced government research spending in many regions due to the prevailing economic climate.

In establishing the award, PANalytical provides substantial support, but more importantly a meaningful injection of encouragement to the career of an outstanding scientist. Researchers that have never held a professorship and that use laboratory-scale X-ray equipment as their primary analytical technique are eligible to apply for the award. No restriction is placed on the manufacturer of the X-ray equipment.

The winner of the award would have demonstrated the most exceptional groundbreaking thinking in a topical field to a committee of established scientists. In order to do so, the assessment is based on a single research publication that would form the basis of the submission to the selection committee.

The publication needs to have been published in the period from 1 January 2012 until 30 November 2013. Submissions have to be in the English language, or alternatively the applicant would supply an English translation where this is not the case. For articles with more than one author, the award is made to the first author listed on the publication.

Applying for the award is designed to be as easy as possible, and an online application at www.panalytical.com/award will be made available for the purpose. The online application form will be available from 1 August 2013. Correspondence or questions about the award can be addressed to award@panalytical.com. Most questions should be answered in the Statutes file, which is also available on the PANalytical Internet.

Applications will be open from 1 August, closing on 30 November 2013.

PANalytical

Images from the ACA Annual Meeting *Hawaii*

Two poster prize winners, Lauren Hatcher and Mathew Bryant, both from the University of Bath

Andrew Cairns and Karim Sutton relax in true Hawaiian style

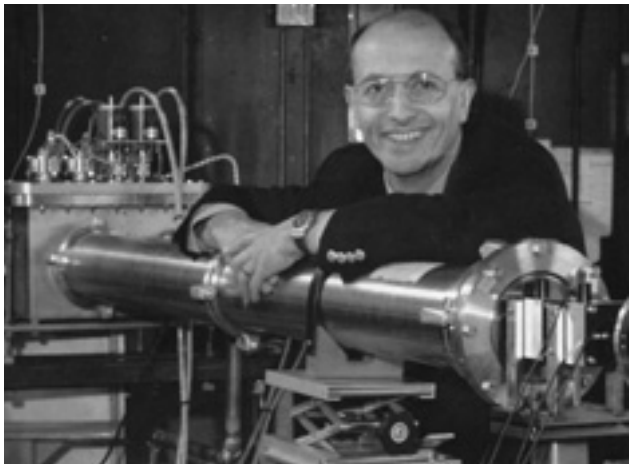
2014 ACA Patterson Award to John Helliwell

THE Patterson Award, named for one of the greatest pioneers of crystallography, is one of the highest honours that the American Crystallographic Association can award and is only given every three years. Its remit is "to recognize and encourage outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information." It has just been announced that John Helliwell will receive the 2014 ACA Patterson Award at the meeting next May in Albuquerque for his pioneering contributions to the development of the instrumentation, methods and applications of synchrotron radiation in macromolecular crystallography.

John has achieved distinction as Professor of Structural Chemistry at the University of Manchester and has provided supervision and help to a cadre of students and postdocs who have themselves achieved renown as crystallographers. Among his many achievements is to show that the seemingly impossible task of locating protons in proteins, so informative about their mechanism of action, can indeed be accomplished by using a combination of ultra-high-resolution synchrotron and neutron data. Plainly this is an innovative application of diffraction methods to the elucidation of biological phenomena. John has generously contributed time and effort to the improvement of synchrotron and neutron facilities worldwide. In the UK he has been a long-time Joint Appointee with the Synchrotron Radiation Source (SRS) at Daresbury Laboratory, being in charge of the SRS in 2002. He played a major role in the establishment of the Diamond Light Source (DLS) and chaired the Research Councils Advisory Group input to the DLS Council. Many of us remember John's excellent Lonsdale Lecture, given at the BCA Spring Meeting in 2011, and he has once again demonstrated his commitment to the BCA by chairing the Programme Committee for our forthcoming Spring Meeting in 2015. John served as President of the European Crystallographic Association from 2006 to 2009. A loyal member of the ACA, he has worked closely on collaborative research with several American colleagues.

I have personal reasons to be grateful to John. In recent years I have become increasingly interested in the history of crystallography. One might expect that a forward-thinking scientist like John, so much involved in the development of new methods and the establishment of new facilities, would scorn such efforts. On the contrary, as Joint Main Editor of *Crystallography Reviews*, he has given me much encouragement and advice to develop my studies into properly peer-reviewed Historical Reviews.

Carl Schwalbe



We are very pleased to reproduce a letter from John Helliwell to David Keen

Dear David,

I write to you in your capacity as BCA President to offer my heartfelt thanks for everything the BCA has done for all my PhD students over the decades, two of whom were awarded the David Blow BSG Trophy for best BSG posters, as well as myself. They could not have gone onto their successes without the BCA conferences; a cohort of my students were explicitly mentioned in the recent ACA Summer Newsletter announcement summary of the ACA Patterson Award to me for 2014, those that have become SR instrument scientists. Several have gone onto careers in the USA ie at Stanford Synchrotron Radiation Lab, Yale University and the Hauptman Woodward Medical Research Institute in Buffalo. My own continual professional development absolutely required the BCA; the keeping up to date and the frequent meeting with other crystallographers is in effect a collegiate fellowship for us each to share our research initiatives and results. On a very specific memory, I vividly recall the Cardiff BCA where I gave the BCA Conference Lecture in the Cardiff opera house rotunda, mid 1990s I think, ie before it was called the BCA Lecture. Being applauded onto that stage was an unforgettable experience for me. That honour was one of those important milestones that served to reward but also inspired one further; I think my research group had about 10 posters at the Cardiff BCA.

Thankyou the BCA!

Best regards,

John

Prof John R Helliwell DSc

Obituary

Jerome Karle, Nobel Prize Laureate and Navy Scientist, Dies at 94

DR. Jerome Karle, former Naval Research Laboratory (NRL) scientist and Nobel Prize laureate, died on June 6, 2013, at the age of 94. Dr. Karle shared the 1985 Nobel Prize in Chemistry for developing the "Direct Method" in X-ray crystallography.

Dr. Jerome Karle, NRL scientist and Nobel Prize laureate. (Photo: U.S. Naval Research Laboratory)

Dr. Karle shared both his work and his life with his wife Dr. **Isabella Karle**, who worked alongside him at the Naval Research Laboratory. At NRL, Dr. Karle held the Chair of Science as Chief Scientist of the Laboratory for the Structure of Matter. Dr. Karle came to NRL in 1944; his wife joined him in 1946. At their retirement in 2009, they held a combined 127 years of federal service.

Jerome Karle, along with **Herbert Hauptman**, was awarded the Nobel Prize for Chemistry in 1985 for devising direct methods of determining complex crystal structures. Isabella Karle, building on this work, developed methods that led to the analysis and publication of the molecular structures of many thousands of complicated molecules annually. For years the technique developed by Karle and Hauptman was overlooked by scientists, who were not quite sure it worked. It was Isabella's work that drew attention to its usefulness.

At the time the Karles retired, Dr. **Bhakta Rath**, Associate Director of Research for Materials Science and Component Technology, spoke about the significance of the Karles' careers, saying, "The departure of Jerry and Isabella from our midst at the Naval Research Laboratory marked the end of an era. Through their persistent and dedicated research they opened the doors to our understanding of the complexities of atomic arrangements in large biological and organic molecules. Their theoretical and experimental research, which is now commonly known as the direct method for solving the multi-variable complex functions extracted from x-ray diffraction data has made immeasurable contribution to our understanding of the structure and function of biomolecules and consequently to the development of various pharmaceutical products. Through their continued research they created new areas known as quantum crystallography and kernel method. Researchers the world over can solve structures of molecules containing tens of thousands of atoms in a matter of hours, which otherwise would have taken careers to solve."

Jerome Karle attended New York City schools and graduated from the City College of New York in 1937, the first recipient of the Caduceus Award for excellence in the Natural Sciences. He obtained an M.A. degree in Biology in 1938 at Harvard University. After working at the New York State Health Department, he attended the University of Michigan and received M.S. and Ph.D. degrees in Physical Chemistry in 1942 and 1944, respectively. Jerome Karle met his wife Isabella while a student at University of Michigan. In the physical chemistry laboratory, seating was arranged alphabetically and so it was that Jerome Karle sat beside Isabella Lugoski. After they both completed their doctorates, they worked on the Manhattan Project in Chicago, focusing on the extraction and purification of plutonium. Dr. Karle joined NRL in 1944 and then from 1968 until his retirement in 2009, he was the Chief Scientist of the Laboratory for the Structure of Matter (LSM).

Jerome Karle's research was concerned with diffraction theory and its application to the determination of atomic arrangements in various states of aggregation, gases, liquids, amorphous solids, fibers, and macromolecules. This research resulted in new techniques for structure determination and a broad variety of applications.

A most recent interest was in a developing field that he and his research colleagues call quantum crystallography. It concerned a method for combining X-ray diffraction data for crystals with quantum mechanics in order to obtain wave functions that are consistent with the X-ray data. The objective is to extend the use of X-ray diffraction beyond the determination of atomic arrangements, to the determination of additional features such as charges on atoms and energies.

Jerome Karle was a Fellow of the American Physical Society, a member of the National Academy of Sciences and the American Philosophical Society, served as president of the International Union of Crystallography, and a member of a number of other professional societies. He was chairman of the Chemistry Section of the National Academy of Sciences. In addition to the 1985 Nobel Prize for Chemistry, he received 9 awards from the U.S. government, 8 honorary degrees or other distinctions from American universities, 7 distinguished honorary memberships from scientific societies and 4 awards from foreign governments and universities.

Jerome Karle is survived by his wife, three daughters (two chemists and a geologist), and four grandchildren.

Eulogy for Dr. Jerome Karle

Editor's Note: Dr. Lou Massa delivered the eulogy at Dr. Jerome Karle's funeral on June 22. Dr. Massa is Professor of Chemistry & Physics at Hunter College and the Graduate School, City University of New York. In addition, he spends his summers working at NRL and had the privilege of working alongside Dr. Karle.

I'm Lou Massa from City University of New York. I'm lucky enough to be a friend of Jerome Karle. I express condolences to Isabella, and to their daughters Louise, Jean, and Madeline, and all their larger family and friends. When a person dies it is fitting to reflect upon their life and the importance of it and its meaning for us.

Jerome Karle lived near to 95 years. He was a great man, living in a great country, supported by a great Laboratory, viz., the U.S. Naval Research Lab. He lived through much of our country's history, including the Great Depression, World War II, the Cold War, and collapse of the Soviet Union.

Over those years his own personal history included City College of New York, three hours a day on the subway, back and forth from his home on Coney Island. From there to Harvard for an MS in biology. Then onto University of Michigan, where he gets a PhD in chemistry, becomes an expert in electron diffraction, and meets and marries his equally expert classmate Isabella Lugoski. Next stop, the Manhattan project of WWII, where they both work on different aspects of plutonium chemistry. After that, they both settle into productive science careers at the NRL. Jerome Karle worked at NRL for some 60 years, becoming the U.S. Navy's highest ranking scientist, founding the Laboratory for the Structure of Matter, making fundamental discoveries, winning too many important awards to mention now, but by the way, one of them was the Nobel Prize in Chemistry. He became an advisor to Popes and Presidents. To remember, him riding three hours a day on that rattling subway, to get an education at City College, in contrast say to answering a phone call from President Reagan, at home, or discussing birth control with Pope John Paul, in the Vatican, that is a contrast to amaze.

The Nobel Prize – That of course crystallized his fame as one of the greatest scientists of his generation. Why? Because of his contribution to solving, X-ray crystal structures, not just a difficult problem, but one that was for decades thought to be mathematically impossible to solve. Karle and Hauptman realized, as no one before them had done, how to solve the problem and wrote the mathematics for how to solve for the unknown atomic positions. Isabella took that mathematics and applied it to actual X-ray measurements, which she herself made, in that way solving structures no one else could do. And thus the problem of crystal structures was truly solved. Theoretically and Experimentally. That was the Nobel prize, in a nut shell.

Louise was quoted in the New York Times a few days ago, saying her father's science was misunderstood for a long time. In that of course she was correct. But to put it slightly more strongly, one might say, people in the field of this crystallography were mostly downright hostile. Jerome, in his official autobiography on the Nobel website said, "The scientists in our field did not believe a single word we said"!

At a time when the world was saying the Karles could not be solving the crystallography problem, NRL never wavered. They believed in basic research. They believed in Jerome.

Even though it was not immediately evident if the work would be applicable to Naval interests, they maintained their support. That faith served both Jerome and the Navy well. There is now almost no field of science and technology wherein crystal structures are not important. Jerome told me many times he was grateful to the NRL for their support, in the face of so many "experts" saying "no way".

It's not just science that makes a great man, it also requires great traits of personality. No matter how important were his scientific contributions, he lived simply, and was extraordinarily humble. Always modest in behavior, attitude, and spirit. Never arrogant or prideful. Anyone that spoke to him, was made to feel as important as was he. I will give you an example, which I find to be both illustrative and slightly humorous. I spent a week with Jerome once at a conference in Florida. The chair of Physics from Brooklyn College was there too, but he did not know Jerome before the conference. After spending a few days with us at the seminars, meals, and so on, after one of these days we are in a cluster having drinks and talking. He says to Jerome, I notice from your name tag you are from NRL. Did you ever meet that Nobel Prize winner from NRL? A slight pause, and Jerome said "You may be speaking of me". He had that kind of humility.

He loved talking about science to young people. He went to their schools. He had them in his lab to work with him. Youngsters wrote to him from faraway places. He not only wrote back, he wrote to their parents too, with his best advice for supporting curiosity and freedom of thought in their children.

The people around him at the lab including, Lulu, Peggy, Steve, John, Richard, Maryann, Sid, and so many others, appreciated him enormously. I do not think it is too much exaggeration to say they were better scientists, and better people in imitation of him. I have always felt the kindness to those around him was simply a natural extension of the love of his own family.

Something I admired was his work ethic. He was a brilliant, steady, hard worker all his scientific life. He was not one to while away afternoons in the vast lobbies of grand hotels. The Karles drove to the Lab every day, worked all day, enjoyed what they were doing, understood its importance, shared with those around them, and did that every working day. The Nobel Prize did not change that one bit.

So the summary is simply, that Jerome Karle is to be remembered as a great person, who thrived in a great country, supported steadfastly by one of the country's greatest labs, NRL, and beyond that his humanity is something to wonder over, and emulate.

(An edited form of an obituary from the U.S. Naval Research Laboratory website, reprinted by permission)

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.

1-6 September 2013
EHPRG 51. European High Pressure Research Group International Meeting, London.
http://ehprg51.iope-confs.co.uk/home

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

2-6 September 2013
ICXOM22: 22nd International Congress on X-ray Optics and Microanalysis, Hamburg, Germany.
http://www.icxom22.de/

2-13 September 2013
13th Oxford School of Neutron Scattering, Oxford.
http://www.oxfordneutronschool.org/

2-13 September 2013
17th JCNS Laboratory Course – Neutron Scattering, Jülich/Garching, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/LabCourse/_node.html

3-6 September 2013
Challenges in Chemical Renewable Energy (ISACS12), Cambridge.
http://www.rsc.org/ConferencesAndEvents/ISACS/ISACS12/index.asp

3-6 September 2013
ALBA User Meeting 2013 and VI AUSE Conference, Cerdanyola del Vallegraves, Spain.
http://albausermeeting2013.cells.es/

4-8 September 2013
1st SIMP-AIC International Summer School on "Crystallography Beyond Diffraction, 2nd Edition", Camerino, Italy.
http://2013.aicschool.org

8-11 September 2013
11th International Conference on Biology and Synchrotron Radiation (BSR), Hamburg, Germany.
http://www.nature.com/natureevents/science/events/1728611th_International_Conference_on_Biology_and_Synchrotron_Radiation_BSR

8-11 September 2013
Workshop of the IUCr Commission on High Pressure – Advances in Static and Dynamic High-Pressure Crystallography, Hamburg, Germany.
https://indico.desy.de/conferenceDisplay.py?confId=7443

8-11 September 2013
Recent Advances in Macromolecular Crystallization, Le Bischenberg, France.
http://www.regonline.co.uk/builder/site/Default.aspx?EventID=1203686

9-11 September 2013
Physical Aspects of Polymer Science, Sheffield.
http://paps13.iopconfs.org/home

9-12 September 2013
NINMACH 2013 – Neutron Imaging and Neutron Methods in Archaeology and Cultural Heritage Research, FRM2, Garching, München, Germany.
http://www.frm2.tum.de/aktuelles/veranstaltungen/ninmach-2013/index.html

9-12 September 2013
First Meeting of the Italian, Spanish and Swiss Crystallographic Associations, Villa Olmo, Como, Italy.
http://missca.dsat.uninsubria.it/missca/home.html

12-13 September 2013
Structural and *in situ* materials science at beamline P02.1 @ PETRA III, Hamburg, Germany.
https://indico.desy.de/conferenceDisplay.py?confId=7900

15-20 September 2013
Free-electron X-ray Laser Physics. DPG Physics School, Bad Honnef, Germany.
http://www.dpg-physik.de/dpg/pbh/aktuelles/S213.html?lang=de&

16-18 September 2013
Self-Assembly of Biopolymers. Faraday Discussion 166, Bristol.
http://www.rsc.org/FD166

16-20 September 2013
X-ray Free Electron Laser School and Symposium, Dinard, France.
http://xfel2013.univ-rennes1.fr/

16-27 September 2013
XII School on Synchrotron Radiation: Fundamentals, Methods and Applications, Grado, Italy.
http://www.elettra.trieste.it/XIISILS/</inter-ref>).</further-info>

18-20 September 2013
71st Annual Pittsburgh Diffraction Conference, Buffalo, NY, USA.
http://www.pittdifsoc.org/PDC_2013/pittsburgh_diffraction_flyer.pdf

18-21 September 2013
Getting the best from your structural data: beyond black boxes.
Macromolecular crystallography practical workshop, Strasbourg, France.
http://structural-data.sciencesconf.org/

20 September 2013
X-ray Fundemantal Parameters for Reference-Free Analysis, Tsukuba, Japan.
http://www.exsa.hu/news/?page_id=430

22-27 September 2013
SISN Summer School 2013 on Inelastic Neutron Scattering, Valle Aurina, Italy.
http://www.sisn.it/link/scuola%20sisn%202013.htm

23-27 September 2013
15th International Conference on Total Reflection X-Ray Fluorescence Analysis and Related Methods, and the 49th Annual Conference on X-Ray Chemical Analysis (TXRF2013), Osaka, Japan.
http://www.a-chem.eng.osaka-cu.ac.jp/txrf2013/

25-27 September 2013
Absolute Structure and Twinning. ChemKrist-Workshop Aachen Mülheim 2013, Mülheim an der Ruhr, Germany.
http://www.gtecs.rwth-aachen.de/acmu/?page=home

25-27 September 2013
Euro Intelligent Materials 2013, Kiel, Germany.
www.intelligent-materials.de

27 September – 1 October 2013
III International Conference on Crystallogenesis and Mineralogy, Novosibirsk, Russia.
http://km.igm.nsc.ru/

30 September – 2 October 2013
Basic Rietveld Refinement & Indexing, ICDD, Newtown Square PA, USA.
http://www.icdd.com/education/rietveld-workshop.htm

30 September – 4 October 2013
Intermetallics 2013, Bad Staffelstein, Germany.
www.dgm-intermetallics.de

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

1-2 October 2013
Using X-rays to Analyze Cultural Heritage. AACS Workshop, Stanford, CA, USA.
http://ceramics.org/meetings/aacs-workshop<event

1-5 October 2013
Ubiquitin and ubiquitin-like proteins: from structure to function. EMBO Conference, Lucca, Italy.
http://events.embo.org/13-ubiquitin/

3-4 October 2013
Advanced Rietveld Refinement & Indexing, ICDD, Newtown Square PA, USA.
http://www.icdd.com/education/rietveld-workshop.htm

3-4 October 2013
On the frontier between cryo-EM and protein crystallography. International Symposium in honor of Jorge Navaza, Getxo, Spain.
http://www.fundacionbiofisicabizkaia.org/international-symposium/

6-10 October 2013
50th Anniversary of the Clay Minerals Society. Annual Meeting, Urbana-Champaign, IL, USA.
http://www.clays.org/annual%20meeting/50th_annual_meeting_website/

7-10 October 2013
JCNS Workshop 2013: Trends and Perspectives in Neutron Scattering: Magnetism and Correlated Electron Systems, Tutzing, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/JCNSWorkshops/2013Workshop/_node.html

7-11 October 2013
Science with advanced coherent light sources. Fall School, Hamburg, Germany.
https://indico.desy.de/conferenceDisplay.py?confId=7621

10-11 October 2013
Satellite Workshop: Single Crystal Spectroscopy: Multi-TAS or TOF? Tutzing, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/JCNSWorkshops/2013TAS-Workshop/_node.html

12-13 October 2013
Annual Meeting 2013 and General Assembly of Crystallography Society of Japan, Kumamoto, Japan.
http://crsj2013.main.jp/en/index.php

14-29 October 2013
X-ray Methods in Structural Biology, Cold Spring Harbor, NY, USA.
http://meetings.cshl.edu/courses/2013/c-crys13.shtml

14-16 October 2013
SoXRES-2013: International Workshop on Soft X-ray Resonant Elastic Scattering, Saint-Aubin, France.
http://www.synchrotron-soleil.fr/portal/page/portal/Soleil/ToutesActualites/Workshops/2013/SoXRES/Tab1

14-17 October 2013
Myofibrillar Z-disk Structure and Dynamics, Hamburg, Germany.
http://www.embl-hamburg.de/training/events/2013/SSS13-01/index.html

15-17 October 2013
Handheld XRF Workshop, ICDD, Newtown Square PA, USA.
http://www.icdd.com/education/handheld-xrf-workshop.htm

15-18 October 2013
Biophysics in Drug Discovery, Strasbourg, France.
www.ldorganisation.com/v2/page/novalix_conference_2013/products.html

16-17 October 2013
X-ray lasers in biology – techniques, Newport Pagnell.
http://royalsociety.org/events/2013/xray-lasers-satellite/

19-20 October 2013
ICNNN2013: 2nd International Conference on Nanostructures, Nanomaterials and Nanoengineering, Jeju, Korea.
http://www.icnnn.org/index.htm

27-31 October 2013
COM2013. Applied Neutron Scattering in Engineering and Materials Science Research, Montreal, Canada.
http://web.cim.org/COM2013/conference/AppliedNeutronScattering.cfm

28 October – 2 November 2013
Physics of Crystals 2013. International Symposium uniting the Fifth International Conference of Crystals in 21st Century and the Third Moscow Reading on the Strength of Materials. Dedicated to the 100th anniversary of the birth of Professor M. P. Shaskol'skaya, Moscow, Russian Federation.
http://www.misis.ru/ crystalxxi

3-6 November 2013
PSDI 2013: Protein Structure Determination in Industry, Lucerne, Switzerland.
http://indico.psi.ch/conferenceDisplay.py?confId=2235

4-5 November 2013
Hochtemperaturwerkstoffe für die Kristallzüchtung. Workshop of the DGKK-Arbeitskreis Industrielle Kristallzüchtung, Miltenberg, Germany.
http://www.iisb.fraunhofer.de/content/dam/iisb/de/documents/veranstaltungen_messen/veranstaltungen/2013/2013-02-11-Flyer_DGKK_AK_Industrielle Kristallzuechtung.pdf

4-6 November 2013
Modeling the Physical Properties of Clustering Crystal. Workshop, Lausanne, Switzerland.
http://www.cecam.org/workshop-928.html

11-22 November 2013
Synchrotron Radiation Techniques and Nanotechnology: a Synergic Approach to Life Sciences and Medicine, Cape Town, South Africa.
http://cdsagenda5.ictp.it/full_display.php?ida=a12238

12-13 November 2013
Together We Stand Divided We Fall, Crystallography Within Material Science, Diamond, Didcot.
https://sites.google.com/site/bcaindgrp/meetings/autumn-meeting-2013

14-15 November 2013
Italian Crystal Growth 2013: New Frontiers of Functional Materials, Parma, Italy.
http://icg2013.imem.cnr.it

18-22 November 2013
6th ILL Annual School on Advanced Neutron Diffraction Data Treatment using the FullProf Suite, ILL Grenoble, France.
http://www.ill.eu/FPSchool2013/

1-6 December 2013
2013 MRS Fall Meeting and Exhibit, Boston, MA, USA.
http://www.mrs.org/fall2013/

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

19-21 February 2014
NIBB 2014. Neutrons in Biology and Biotechnology, Grenoble, France.
http://www.ill.eu/html/news-events/events/nibb-2014-neutrons-in-biology-and-biotechnology/

17-20 March 2014
22nd Annual Conference of the German Crystallographic Society (DGK) 2014, Berlin, Germany.
http://www.dgk-conference.de

24-27 March 2014
Studying Kinetics with Neutrons (SKIN 2014). Third International Workshop, Grenoble, France.
http://www.ill.eu/html/news-events/events/skin-2014/

7-10 April 2014
BCA Annual Spring Meeting, University of Loughborough.
http://crystallography.org.uk/spring-meeting-2014/

7-11 April 2014
Computational Structural Biology – from data to structure to function. EMBL-EBI Training Course, Cambridge.
http://www.ebi.ac.uk/training/course/structural-biology-2014

14-16 April 2014
The Physics of Soft and Biological Matter, Cambridge.
http://softbio.iopconfs.org/home

24 April 2014
The Physics of Self-Assembling Biopolymers, London.
http://www.iop.org/events/scientific/conferences/calendar/index.html#/?i=1

7-9 May 2014
Molecular Simulations and Visualization. Faraday Discussion 169, Nottingham.
http://www.rsc.org/FD169

11-16 May 2014
QENS 2014/WINS 2014, Autrans, France.
http://www.ill.eu/news-events/events/qens-2014-wins-2014/

18-21 May 2014
Molecular Machines: lessons from integrating structure, biophysics and chemistry. EMBO EMBL Symposium, Heidelberg, Germany.
http://www.embo-embl-symposia.org/symposia/2014/EES14-03/index.html

30 May – 8 June 2014
Erice 2014 – Structural Basis of Pharmacology, Erice, Italy.
http://www.crystalerice.org/Erice2014/2014.htm

7-11 July 2014
International Conference on Highly Frustrated Magnetism 2014, Cambridge.
http://hfm2014.tcm.phy.cam.ac.uk/

21-25 July 2014
ICSOS'11: 11th International Conference on the Structure of Surfaces, Coventry.
http://icsos11.iopconfs.org

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

EMPYREAN

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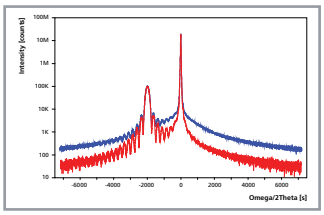

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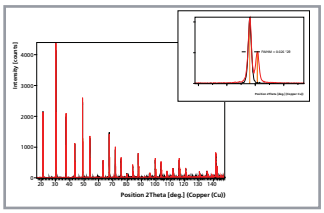

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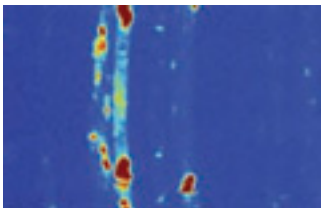

3D

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