Crystallography News

British Crystallographic Association

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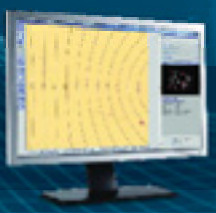

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Please ensure that items for inclusion in the September 2013 issue are sent to the Editor to arrive before 25 July 2013.

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This month's cover:

Exhibition at the Science Museum, London (photos by Jennie Hills); scenes from the Big Bang Fair

From the President

IN my last column I used the phrase 'no relation' when writing about Melvyn Bragg and his Radio 4 'In Our Time' programme on William and Lawrence Bragg. I had had it on good authority that although they came from the same part of the country, Melvyn and the crystallographic Braggs were indeed unrelated. Inevitably no sooner had *Crystallography News* been published than the same good authority (i.e. Mike Glazer) came back to me with a pair of family trees showing that William Henry Bragg's great, great, grandparents Henry (1724-1795) and Sarah (née Lightfoot, 1724-1779) were also Melvyn Bragg's ancestors. In the spirit of Leveson I apologise for my inaccurate journalism! I understand that this real, albeit somewhat distant, link between these Braggs has prompted Melvyn to collaborate on at least one other Bragg-related programme to be broadcast in due course.

The crystallography centenary story is indeed gathering momentum. As I got into my car to drive home this evening, the PM programme on Radio 4 (to think that I never used to listen to this station…) had a news article by BBC reporter **Louise Jackson** on the Bragg Centenary from Leeds University, with interviews with **Kersten Hall**, **Chris Hammond** and **Tom Edwards**. Chris Hammond suggested that "modesty" probably prevented the Braggs from being better known or being given their rightful place in history. It was excellent to hear that the message, "X-ray crystallography changed science" is reaching such a wide audience. If you are planning any Bragg Centenary related events this year or events for the International Year of Crystallography in 2014 then please do let us know so that we can advertise them. We are collating information on all events on our web site (crystallography.org.uk/bragg-centenary/). You can also use the Bragg Centenary Logo for your outreach events and can obtain free copies of the STFC-produced 'broadsheet' on crystallography from www.stfc.ac.uk/1889#PSG for giving out at your events. Four thousand of these were distributed at our stand at the Big Bang Fair so they are clearly popular.

The highlight of the past few months was undoubtedly our contribution to the Big Bang Science and Technology Fair at the ExCeL Centre in London. **Ross Harrington** writes more on this later in this issue of *Crystallography News*, but last March around 40 BCA members were yellow T-shirted demonstrators to around 75,000 visitors at the BCA-STFC-DLS stand "The Structure of Stuff is Sweet". It was a fantastic event and our stand attracted huge crowds of people of all ages. They were intrigued and enthralled by marshmallow unit cells, marble crystals, real time lysozyme crystal growth and even a lego diffractometer. I was only able to be there for one day, but this was enough to appreciate how rewarding the event was for everyone, volunteers and visitors alike. Half an hour of filling jugs with marbles and watching them being poured into a crystal shape every 30 seconds or so for wave upon wave of school pupils quickly took its toll on my stamina, so 'hats off' to those who were working on the stand for a whole day – let alone for four! **Robin Clegg**, the Head of Public Engagement at STFC wrote after he visited on the Friday, "The Crystallography stand was excellent and hugely popular. I understand that the BB management thought it one of the best." And **Laura Holland** from the Diamond Public Engagement team e-mailed me afterwards, "The event was fantastic, and I can't tell you how impressed I was by the enthusiasm and talent of the volunteers. You've got a really good group of communicators, which the association should be very proud of." I would like to single out Ross for particular thanks for his excellent coordination and hard work in making the event happen, and to thank STFC (and, in the background, RCUK) for their substantial funding, to Diamond for their many contributions and of course to all the BCA volunteers; keep – and wear – those yellow T-shirts with pride!

Preparations for the 28th European Crystallographic Meeting in Warwick are gathering pace and the scientific programme is looking really good. By the time that you read this I hope that you will have already registered for the meeting and have submitted abstracts for consideration as talks and/or posters. The meeting organisers, led by **Sandy Blake**, are adding content to the ECM28 web site (ecm28.ecanews.org/) almost daily. Please do check it regularly for up to date information about the meeting. I look forward to meeting a strong cohort of BCA members at this year's European Crystallographic Meeting on our home soil. We will also be holding our Annual General Meeting at ECM28 in Warwick. As part of this we will be electing members to BCA Council. Further details are given in this issue of *Crystallography News* and if you are interested in standing for one of the available positions then please either contact me or one of the other BCA Officers.

I hope 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

STARTING with the cover, readers will find numerous items about the many imaginative ways in which our community has been celebrating the Bragg centenary. Of paramount importance for the future of our discipline, and of UK science in general, the Big Bang Fair once again captivated the large number of school pupils who came. The Bragg connection gave our interactive displays of crystallography special relevance. Also highlighted on our cover is a "small but perfectly formed" Special Exhibition at the high-profile location that is the Science Museum. Taking a recommended 15 minutes to view and inwardly digest, it will be in place for the rest of 2013. Along with the Bragg centenary, this exhibit inspired a 2-page article in the Metro by Ben Gilliland which can be viewed at http://www.cosmonline.co.uk/blog/2013/04/14/conquering-realm-invisible . Of course, the Braggs' involvement with crystallography in the UK began with the appointment of W. H. Bragg to a professorship at Leeds. The University of Leeds duly celebrated with a day of special events. Along with imaginative hands-on displays they successfully pulled off the feat of providing a whole day of scholarly lectures which were appropriate for the general public. Importantly, these lectures, which are summarised in this issue, are now available online.

Furthermore, there is a crater on the moon named Bragg, after W. H. Bragg. Lest we be overcome with Braggmania, we should be aware that there also is a crater named Blagg. It is named for Mary Adela Blagg (1858-1944), who educated herself in mathematics and later learned about astronomy through a university extension course. She showed so much talent for astronomy that she became the first woman elected as a Fellow of the Royal Astronomical Society. She also proved to have tact and diplomacy, being tasked by the International Astronomical Union with reconciling the conflicting names that had been assigned to features on the moon. According to Wikipedia, "Bragg is an ancient lunar crater that is located on the far side of the Moon, just beyond the northwest limb. This formation has been heavily eroded and reshaped by subsequent impacts, leaving an irregular depression in the surface… It (Blagg) is a circular, breast-shaped crater with no appreciable erosion."

This particular June issue of *Crystallography News* seems to have something missing: first impressions of the Spring Meeting. Usually we could provide summaries of the Plenary Lectures and the overall theme of the meeting. Frequently we would also have a complete write-up of the Young Crystallographers' Satellite Meeting: many YCs seem to have a talent for speedy and accurate reporting. For the benefit of anyone who spent the last four winter months hibernating, there was no Spring Meeting this year so that we could concentrate our efforts on preparations for the European Crystallographic Meeting at the University of Warwick this August. A look at the ECM28 website shows that these efforts have been effectively deployed, and we have a treat in store.

Even a cursory look at the website http://iccoss2013.org/ shows that the forthcoming ICCOSS XXI has a starry list of speakers. Taking place conveniently in Oxford at the beginning of August, this meeting provides a fine opportunity for organic crystallographers to catch up on new developments in this field.

We feature reports from two Arnold Beevers bursary recipients who, even if they couldn't go to Warwick or Loughborough, still found exciting scientific conferences in interesting places. It also is a great pleasure to include a report on the first PANalytical Award, which is intended to furnish an outstanding researcher with support that is independent of (possibly dwindling) government funding. This year's recipient is **Dr Thomas Bennett** from Cambridge. We also have an announcement from our friends at the International Centre for Diffraction Data of the award of 13 Ludo Frevel Crystallography Scholarships in the round recently completed. This is a truly worldwide programme, with winners from as far afield as Frankfurt, Novosibirsk, New Delhi and Beijing, but none from the UK. It is evident that we crystallographers benefit from support by our generous sponsors, but we must grab it!

I presume that there are other BCA members who, like me, also belong to the Biochemical Society. I was delighted to examine my April 2013 issue of *The Biochemist* and find that it had the theme of "Symmetry". A sprightly introductory piece by the Science Editor is followed by four articles: "Symmetry in crystallography", "Learning from symmetry", "Pretty nasty: symmetry in virus architecture" and "Amplification of chirality in PNA:PNA duplexes is limited". Although these articles are currently available on the website www.biochemist.org/bio/ only to members, articles are made available to everyone starting in the year after publication. With their beautifully coloured illustrations they should make valuable teaching material in the future.

Finally, there is an article by me which started off to be about the crystal structure of solid argon, determined as early as 1924 by two German crystallographers. One of them, **Franz Simon**, subsequently emigrated to England and was awarded a British knighthood. The other, **Clara von Simson**, came from a German noble family. I was fascinated by the way each of them separately withstood the vicissitudes of life in the 1930s. Inevitably the Braggs enter into this story. Simon and Simson followed the Braggs' methodology to calculate the atomic radius of argon and compare it with the isoelectronic K^+ and Cl^- in the Braggs' KCl structure.

Carl Schwalbe

Puzzle Corner

IN his report in our last issue about the "Bragg's Law" meeting the eminently erudite Mike Glazer admitted that he had to look up the meaning of "ptychography" on the internet. I'm sure that this was just a lone lacuna in Mike's lore, and that readers will easily be able to define this word and a dozen other "pt" words:

1. ptarmigan
2. pteridine
3. pteridology
4. pteridosperm
5. pterigoid
6. pteropod
7. pterygium
8. pterylosis
9. ptisan
10. ptomaine
11. ptosis
12. ptyalin

As a tie-breaker, use as many of these words as you can in a single sentence. Can you read your sentence aloud?

Answer to March Puzzle Corner

The necessary clues can be found in this issue, relevant websites or general crystallographic knowledge.
Find the values of W, X, Y and Z, and hence derive the final answer.

1. Start with the seating capacity of the main lecture theatre at Warwick Arts Centre, the venue for ECM28. [1200]
2. Divide this number by the date in August on which ECM28 starts [25] to get number W. [48]
3. Multiply W by the cost in pounds to register for the European Young Crystallographers Meeting [15], yielding X. [720]
4. Multiply the date in May that is the last chance for Early Bird registration [6] by the highest number for a microsymposium [50] at ECM27 (in Bergen). Add X to this product to obtain Y. [1020]
5. Subtract the number of Sohncke space groups [65] from Y. Then add the number of Bravais lattices [14], producing Z. [969]
6. Take the first three digits of the ISBN [978] for the book "Drive and Curiosity..." Subtract Z from it. [9] Take the positive square root to get the number of Braggs featured on the "In Our Time" programme broadcast of November 29. [3; yes, 3: William Henry Bragg, William Lawrence Bragg and the presenter Melvyn Bragg]

Jim Trotter is the prize-winner.

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:

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2012 Annual General Meeting of the BCA

THE Annual General Meeting of the British Crystallographic Association was held on Wednesday 18 April 2012 at 6.40 pm at the University of Warwick. 87 members were present.

1. Approval of Agenda

A revised agenda was approved by **Bill Clegg** and **Colin Groom**.

2. Apologies for Absence

Alex Griffin and **John McGeehan**

3. Minutes of the last AGM (published in March 2012 Crystallography News)

These were approved by **Mike Glazer** and seconded by **Arwen Pearson**.

4. President's Report

The President spoke warmly of **Dr Andres Goeta** who passed away suddenly and unexpectedly last July. His death was a huge loss to his family, friends and colleagues at Durham and to the wider crystallography community.

The President thanked **Kirsten Christensen** and the rest of the Programme Committee for their hard work and for assembling an interesting and diverse scientific programme. She reported that the dance performers 'Stilled' enjoyed being part of the meeting. More than 50 visitors, including the President saw their performance (see http://youtu.be/uhlwOtfdTjY).

The Spring Meeting in 2014 will be held on 7-10 April at Loughborough University. The Programme Chair for SM 2014 will be **Professor Lee Brammer** (chemical crystallographer, University of Sheffield). The President thanked him for his willingness to undertake the scientific organisation of the meeting. There will be no BCA Spring meeting in 2013 as all the BCA efforts will be put into the ECM2013 at Warwick.

The International Union of Crystallography has postponed the International Year of Crystallography (IYCr) until 2014 but ideas on how to celebrate this are requested from the crystallographic community. IYCr will go ahead whether UN approval is granted or not. Currently the Moroccan UN delegation are presenting the case for the IYCr to the UN. The President strongly encouraged members to think now about how to capitalise on both IYCr and ECM2013 and extend our outreach to maximise their impact.

The Northern Networking Events contract with the BCA ended on 30/3/12 and **Dave Allan** (Vice President) put together Tenders in the summer 2011. The Officers met for a whole day to discuss the bids and HG3 were chosen as providers for 30/3/12 to 31/7/18 (The President and Council thanked NNE (**Gill Moore**, **Jennifer Kirkcaldy** and **David Massey**) for their 12 years of working with the BCA.

Members can now opt to receive *Crystallography News* electronically as a pdf by ticking a box on the Membership Form.

The President announced that our new Honorary Member is **Professor Jack Dunitz**, ETH, a founding member of the BCA. There will be a presentation on 16 May at the CCDC Student Symposium in Cambridge. The President explained that Honorary Members are elected for their contributions both to crystallography and to the BCA.

Two new BCA publicity posters went out with the December 2011 edition of *Crystallography News*. The President thanked **Andrea Mulholland** for all her work on these.

Since membership numbers were falling, the President initiated the "Members get a member" challenge. Embarrassingly, the President won the competition easily, having recruited 3 times more members than the next contender (**Amber Thompson**). She encouraged each member to recruit one other and so double the membership.

The President proposed free membership for students now for 2012 which would include a pdf of *CN* but not the right to apply for Arnold Beevers Bursaries until they became paid members. This option will be available on the web by 1 May. If any member has ideas for increasing membership they should contact **Alex Griffin**, who has offered to be our membership coordinator on Council. (Subsequent to the BCA AGM, **Alex Griffin** will not be taking on the BCA Membership Secretary role and will continue on BCA Council in another capacity)

The President thanked the current Officers: **Dave Allan**, **Georgina Rosair** and **Andrea Mulholland**, previous Officers, **Sandy Blake** and **Harry Powell**, the current and past members of Council for their enthusiasm, particularly **Richard Cooper** (BCA Webmaster) for his continuous updating, and **Carl Schwalbe** (*CN* Editor). She also thanked all the BCA members for their continued support for the Association.

5. Secretary's Annual Report

The Secretary announced that the European Crystallographic meeting (ECM27) will be held in Bergen Norway between the 6-11 August 2012 and she will be attending. The early bird registration rate finishes on 30 April and she encouraged others to register. The following ECM, ECM28, will be here in Warwick (25-29 August 2013) and **Sandy Blake** will report on this.

The ECA are proposing a European-wide crystallography school. UK stake holders are being consulted and the Secretary requires any comments to relay these to the ECA executive committee by the end of May 2012.

The Secretary has been nominated as ECA Secretary from August 2012 and comes to the end of her term as BCA secretary in 2013. Anyone interested in this position was asked to contact the Secretary for further information.

The Secretary thanked the Officers and Council members for their assistance over the past year and in particular the President **Elspeth Garman** for her enthusiasm and wisdom despite considerably challenging circumstances.

6. Northern Networking Events Report

The President read out the report provided by NNE. The number of full Registrations at this Spring meeting is 238, with 95 YC registrations (Monday): and 31 one Day Registrations.

The 120th edition of *Crystallography News* was published recently. The 6 advertisers were Agilent, ICDD, Oxford Cryosystems, PANalytical, Rigaku, Incoatec GmbH.

The BCA has 9 Corporate members: Agilent, Bruker, CCDC, ICDD, Incoatec GmbH Molecular Dimensions, Oxford Cryosystems, PANalytical and Rigaku and the BCA is very grateful for their support.

As of 30/3/12 BCA paid up Membership numbers are at 366 and these are by group: BSG: 146, CCG: 91, PCG: 43, ICG: 19, Not specified: 67 and by category: Ordinary: 179, Student/Retired/Unemployed: 93, Corporate: 46, Honorary: 23 and Life members: 26.

Northern Networking Events would like to wish the BCA the best of luck for the future of the Association.

7. Introduction of HG3

Nicola Peel of HG3 thanked those present for the invitation to speak and introduced herself and HG3 (the company chosen to administer the BCA membership and conferences). In her presentation she asked members to be aware that HG3 will shortly be sending an e-mail with a username and password to allow them to access their personal records and update contact details. HG3 are currently in the process of importing BCA membership details into a bespoke database created for the BCA. She asked members to add bca@hg3.co.uk to their email address books to prevent future emails being spam trapped.

In the membership area there will be a link to subscriptions whereby members will have the facility to renew their annual subscription via credit/debit card using a secure server. This area is fully automated and when payments are made, the member will receive an email confirmation with a receipt to acknowledge the payment. HG3 also receive a copy of this information so they know who has paid.

There is also the facility for a members' resource area which will allow relevant documents to be uploaded and accessible only to members within a password protected area. If members have any thoughts on what could be included here, they were asked to contact HG3 and the BCA Council. **Allan Pang** asked when the email would be sent out. The email will be sent out next week. **Pam Thomas** asked if HG3 would get the paper copies of membership forms where people joined at this Spring meeting. Nicola said that yes they will receive the paper forms but want to move to electronic communication and away from paper as that's when things get lost.

8. Treasurer's Report

Andrea Mulholland, the Treasurer presented the Accounts for 2011 and the Examining Accountant's Report. The Treasurer reported that the overall general fund had an increase of just under £5,000. Bank interest was only £102 this past year but was £5000 in 2008. Membership numbers are down. However, the net income from *Crystallography News* was £10,000 this year and she thanked Corporate members for their great support of the BCA. Major outgoings included the NNE administration costs of £35K which was not calculated according to number of members. Further outgoings include bursaries for younger members to attend meetings. The Keele meeting in 2011 made a 13K surplus but since payments of £12,000 to Warwick were made during the 2011 financial year the conference account was shown as being in deficit by £6,000. BCA Funds are stable and we are working to reduce overheads.

The IUCr Glasgow 1999 surplus is not required by Montreal or Hyderabad for their IUCr Congresses. Instead this fund has been allocated as seed corn funding for ECM28 and Council is grateful to **Chris Gilmore**, **Judith Howard** and others on the IUCr 1999 local organising committee for approving this.

The Treasurer mentioned that it would be extremely helpful if more members paid their subscriptions by Direct Debit. She thanked Council and Officers for their assistance.

David Taylor asked if the accounts handed out and those presented by the accountant should match. The Treasurer pointed out that she was intending to present the accounts where each conference was treated separately but the accountant treated conference funds according to year and since this report was received within the last couple of days there was not time to change it.

9. Acceptance of the Accounts

The accounts were accepted; nominated by **Simon Parsons** and seconded by **John Helliwell**.

10. Appointment of Examining Accountant for 2013

The Examining Accountant is Young Company of Huntingdon and the fee remains at £4,500. Proposed by **Mike Probert** and seconded by **Christine Cardin**.

11. Approval to hold the BCA AGM in 2013 at the ECM in 2013

Proposed by **Amber Thompson** and seconded by **Ann Chippendale**.

12. Report on ECM28 at Warwick (August 25-29 2013)

Sandy Blake said a charitable company has been set up to administer ECM28 and listed the Trustees which included himself. They had been in touch with the ECM27 organising committee and he asked for suggestions for events to be held during the 2013 ECM.

13. Arrangements for appointing the BCA Education Co-ordinator

The President said having the Education Co-ordinator as an electable post required a change to the BCA statutes and bylaws. The current President had decided that our new President should decide on how to appoint a new Education and Outreach Co-ordinator. **Mike Probert** is standing down. The Group educational representatives listed below are in place and will work with the new President.

Group Education representatives:

Airlie McCoy (BSG),
Liana Vella-Zarb (CCG),
Richard Morris (IG),
Mike Glazer (PCG),
Robert Young (YCG).

14. Elections to Council

The President thanked **Paul Fewster** for his wisdom and experience for his 12 years of service to Council in various roles as Vice-President, Ordinary and co-opted member.

Mike Probert (Education Co-ordinator) and **David Beveridge** (IG rep, Ordinary member) are also retiring.

An email went out asking for nominations for President and the request for nominations for President and Ordinary member was placed in *Crystallography News*. The President encouraged members to consider serving on Council.

Ordinary member

There was one Candidate nominated for Ordinary Member: **Simon Parsons**.

Proposed by **Claire Wilson** and seconded by **Stephen Moggach**.

Simon Parsons was Elected unopposed.

Council would like to co-opt **Alex Griffin** until April 2013 with a special responsibility for Membership and Recruitment (Note subsequent to the BCA AGM, Alex Griffin will not be taking on the BCA Membership Secretary role and will continue on BCA Council in another capacity).

Treasurer

Our Treasurer, **Andrea Mulholland** has asked to stand down if possible, due to unforeseen circumstances. **Pamela Williams** from Astex has kindly agreed to take over for the rest of Andrea's term, and AGM approval of this unexpected change is required. There were no objections to this change in personnel.

Proposed by **Pierre Rizkallah** and seconded by **Paul Fewster**.

Andrea will be co-opted to Council for 2012-2013 to smooth the handover.

President

Candidate: **David Keen**, ISIS, Visiting Professor, Oxford University.

Proposed by: **Ivana Radosavljevic Evans** and seconded by **Elizabeth Shotton**.

Elected unopposed.

David Keen introduced himself, describing his background and current work in crystallography. He is based at ISIS. He trained as a physicist but works closely with chemists and has even worked in protein crystallography; his PhD was in disordered crystalline materials. He would like to build on and consolidate what has been carried out by his predecessors to best place the BCA for successful implementation of ECM28 in 2013 and IYCr 2014, maintaining an even keel so the BCA can look outwards to Europe and beyond. He encouraged members to support each other and the association.

15. Any other business

Paul Fewster asked that the outgoing President be thanked and those present applauded

Meeting closed at 7.30pm.

2013 Annual General Meeting

The 2013 Annual General Meeting of the British Crystallographic Association will be held at lunchtime on August 27 at the University of Warwick, during ECM28. At this meeting we will elect a new Vice President, the Secretary and one Ordinary member of Council. Further details of the AGM will be provided by email to all members nearer the time.

Centenary Events

The Big Bang Fair 2013!

IT is all in the numbers really. Six months in the planning, 75,000 visitors, 62 bags of marshmallows and jelly babies, 500 cocktail sticks, countless molecules built and taken apart, millions (yes millions) of lysozyme crystals grown, 1 lego beamline measuring over 250 diffraction patterns, 300 marbles and 45 intrepid volunteers holding everything together over 4 incredibly long days in London.

The Fair is a celebration of science and engineering, with national and international companies and interest groups coming together with interactive stands to promote their respective subjects, from mechanical to electrical engineering, from particle physics to… crystallography! At the same time, pupils from all over the UK compete to be named young scientist and young engineer of the year.

The BCA/STFC/DLS stand celebrating the Bragg Centenary, 'The structure of stuff is sweet', wowed pretty much everyone who came to see us, child and adult alike. We did stand out a wee bit as one of very few stands who were not encouraging teenagers to take up a particular career, a fact that even flummoxed one or two people... It would be nice to say that all of the 75,000 visitors to the Big Bang Fair came to our stand, but to be fair there is no way we would have coped, and we did speak to a pretty hefty number of people of all ages, many of whom now 'know' that crystals are made out of marshmallows and cocktail sticks! By far the most popular demo on the stand, and possibly the simplest, was the fantastic replication by **Mike Glazer** of Bragg's experiment using marbles to demonstrate crystal growth.

If nothing else, the big bang showed that it is possible for all breeds of crystallographer (PCG, BSG, IG and CCG) to get along!

What next? Well, we may visit the regional big bang in Newcastle in July, will hopefully make it to the ECM in August, will definitely be at the British Science Festival in September, and have been invited to a science festival in Aberdeen, also in September, but we are postponing that until the International year of crystallography. If anyone would like to volunteer for any of these events, please get in touch. The structure of stuff is sweet won't be the only Bragg centenary activity, though! We are also planning a series of Cafe Scientifique events around the UK, so if you would like to get involved in that, do get in touch. Details of all events can be found on the dedicated pages on the BCA website.

Many thanks to **Neville Hollingworth** for getting us the space at the big bang, **Mark Wells** and his team from STFC for designing, transporting, building and taking down the stand, **Laura Holland** at Diamond Light Source for taking delivery of masses of kit, and buying us the lovely T-shirts, STFC for funding the stand, ISIS for more funding and the BCA for even more funding. Thanks too to Keele Chemistry department for the loan of the 'make it molecular' kit.

Special thanks to **Anna Warren** and **Claire Murray** at Diamond Light Source (and the YCG) for taking on more and more delegation and coming up with most of the activity ideas, and last but not least, to all the amazing volunteers who gave up their time and did all the hard work on the stands, particularly **Lynne Thomas**, **Nick Funnell** and **Mark Basham** (of lego beamline fame), who did all four days!, but not forgetting **Alice Taylor**, **Alun Biffin**, **Amber Thompson**, **Andrew Cairns**, **Anna Polyakova**, **Anna Warren**, **Arwen Pearson**, **Claire Jones**, **Claire Murray**, **Clare Stevenson**, **David Keen** (el presidente), **David Price**, **Diana Monteiro**, **Elna Pidcock**, **Emily MacCready**, **Emma McCabe**, **Gary Nichol**, **George Pidgeon**, **Gurdeep Minhas**, **Harry Powell**, **Isabelle Kirby**, **Ivo Tews**, **Jack Wright**, **Josh Hill**, **Karim Sutton**, **Katie Renouf**, **Kovilen Sawmynaden**, **Laura Holland**, **Lisa Blair**, **Louise Hamdy**, **Mairi Haddow**, **Matthew Rodrigues**, **Mike Glazer**, **Paula Selgado**, **Philip Bradfield**, **Sam Callear**, **Sam Morris**, **Simon Coles**, **Tristan MacLean** and **Wilfred Wu**.

Ross Harrington

Hidden Structures – 100 Years of X-ray Crystallography

THIS Special Exhibition will be displayed on the second floor of the Science Museum in London until Wednesday 1 January 2014. It celebrates the centenary of X-ray crystallography and its development by father-and-son team William H. Bragg and W. Lawrence Bragg in 1913.

X-ray crystallography was central to molecular biology, the science of proteins, viruses and other bio-molecules that developed in the years after World War II. Hidden Structures explores the stories behind some of the most striking molecular models from this golden age of X-ray crystallography, including DNA, insulin and haemoglobin.

Opening in time for International Women's Day, Hidden Structures also discusses the complex role of women in molecular biology and displays key models by **Kathleen Lonsdale** and **Dorothy Hodgkin**.

Bragg Centenary

'IT was a glorious time when we worked far into every night with new worlds unfolding before us in the silent laboratory': this was how Lawrence Bragg, recalled the feeling of excitement as he and his father William began to pioneer the science of X-ray crystallography in 1913. The origins of their work had begun during the summer of 1912 when, whilst on holiday on the East Yorkshire coast, Sir William had received a letter from a former PhD student informing him of work done in Germany showing that X-rays could be diffracted by crystals of zinc sulphide and copper sulphate. The letter could not have come at a more opportune time. Having enjoyed a successful career in Adelaide, Australia, Bragg had arrived in Leeds in 1909 to take up the post of Cavendish Professor of Physics, but administrative and bureacratic burdens at Leeds allowed little time for research and left him feeling rather deflated. Excited by the letter however, Bragg eagerly returned to Leeds where he built the first X-ray spectrometer, a device which enabled the quantitative analysis of scattered X-ray spectra. On his return to Cambridge where he was then an undergraduate, Lawrence meanwhile developed a mathematical account of X-ray diffraction that enabled the spatial position of atoms in the crystal to be deduced from the pattern of scattered X-rays. By working with his father's X-ray spectrometer at Leeds during University vacations, Lawrence was able to test his mathematical ideas and in the following year, the father and son team laid the foundations for X-ray crystallography by publishing a number of key papers on the crystal structure of substances such as diamond and sodium chloride. The impact of their work was quickly recognised by the scientific community and in 1915, whilst serving on the Western Front, Lawrence received a telegram informing him that he and his father had jointly been awarded the Nobel Prize in Physics. This was the first and only time that a father and son have both won this most coveted accolade in science and the Braggs' achievement is today commemorated with a blue plaque on the Parkinson Building at the University of Leeds, close to the original site of William Bragg's laboratory.

As 2013 marks the centenary of the birth of X-ray crystallography, the University of Leeds is hosting events throughout the year to commemorate the pioneering work of Sir William and Lawrence Bragg. In the first of these events, a day of public lectures was chaired by **Dr. Claire Jones** and **Dr. Emily Winterburn** of the Museum of the History of Science, Technology and Medicine at Leeds (for more details, see http://arts.leeds.ac.uk/museum-of-hstm/) and began with a welcome by **Prof. Tony North**, Emeritus Astbury Professor of Biophysics and a former colleague of Lawrence Bragg. A series of lively and engaging talks then explored both the historical aspects of the Braggs' story and also how their work is being used today. **Prof. Denis Greig**, Emeritus Professor of Physics and former head of the School of Physics and Astronomy, discussed the story of X-rays from 1890 to 1990, exploring their discovery by **Wilhelm Röntgen** and the sometimes heated debate over their nature which preoccupied William Bragg and his contemporary at Liverpool, **Charles Barkla**. **Dr. Chris Hammond**, former Senior Lecturer in the Institute for Materials and recent contributor to an edition of the Radio 4 programme '*In Our Time*' on crystallography, gave a lively talk on how the Braggs' collaboration first began and which involved the participation of an enthusiastic audience in demonstrating the principles of diffraction. In '*From Dark Satanic Mills to DNA*', **Dr. K. Hall**, Visiting Fellow in History of Science, explained how the Braggs' scientific legacy at Leeds was carried on after their departure through the work of William Bragg's protege, the physicist **William T. Astbury**. Having initially used X-ray diffraction for the analysis of textile fibres, Astbury went on to pioneer the study of biological fibres using X-rays and in the course of this work, made the very first X-ray analysis of the structure of DNA. Later in the day, Professor **Monty Losowsky** reflected on his personal contact with Astbury, whose laboratory at Leeds achieved such international renown that it was hailed by **Max Perutz** as 'the X-ray Vatican'. Astbury also popularised the term 'molecular biology', a theme which was developed by Professor North with a talk discussing how the solution of the 'phase problem' by Max Perutz and the introduction of electronic computers were two vital advances in the solution of biological macromolecules.

As well as exploring the historical aspects of the Braggs' story, the talks also looked at how their work is now currently applied across a broad range of scientific disciplines including geology, chemistry, materials science, biology and medicine. **Prof. Kevin Roberts**, Brotherton Professor of Chemical Engineering showed how the Braggs' work continues not only to have practical importance in imaging atomic-scale crystal lattice defects, but also an aesthetic beauty in allowing us to observe the growth and formation of crystals. **William Vickers** of the Dental Institute explained how the application of X-ray diffraction to materials science is being used to develop devices of the future ranging from carbon capture to the regeneration of bone in the human body whilst **Dr. Annie Jamieson**, School of Philosophy, Religion and History of Science, explored the wider public reception of X-rays and their rapid uptake by medical, photographic and commercial interests.

The lectures concluded with a showing of the film '*Hidden Glory*' by the science writer **Georgina Ferry** which told the story of the X-ray crystallographer, **Dorothy Hodgkin** who solved the structure of penicillin, Vitamin B12 and insulin. Also running in parallel with the lectures throughout the day were a series of related practical activities such as 'From the Microscope to the Magnified: the Science of Art', a workshop in which art was used to explore the importance of scale in science. Other activities included demonstrations of how a simple net curtain can give impressive diffraction effects and an exploration of the mathematical ideas underlying symmetry in crystal structure by making three-dimensional solids from 2D patterns. As well as being able to see William Bragg's X-ray spectrometer, induction coil and vacuum tube, visitors could also learn about a modern X-ray diffractometer and electron microscope and see how this equipment is used today.

Also on display was the home-made X-ray camera with which **William Astbury** later used the Braggs' methods to pioneer the study of biological fibres and which his PhD student **Florence Bell** used to take the very first X-ray photographs of DNA in 1938. In this way, the Braggs' work has a direct link with **Rosalind Franklin**'s X-ray studies of nucleic acids which was to give **James Watson** and

Francis Crick a vital clue in solving the structure of DNA. A practical demonstration showed how, using only washing up liquid, table salt and ice-cold rum, DNA can be precipitated in the kitchen from strawberries as a white, stringy fibre. Visitors then learned how the first studies on the molecular structure of nucleic acids had their origins in Astbury's work on another, seemingly unrelated, white, stringy fibre – wool!

These first events in what will be a year of centenary celebrations, ran over two days and were attended by parties from local schools and members of the public, as well as attracting interest from local media. By the end of the final day, members of the public who had braved the unseasonal arctic conditions had been given a fascinating insight into the Braggs' work, the importance of which was famously expressed by **Max Perutz** when he said that the molecular structure revealed by X-ray crystallography explained why blood is red, why grass is green and why water boils at 100°C. Echoing Perutz's words, a recent online poll to celebrate the theme of invention and discovery in National Science and Engineering Week (www.topbritishinnovations.org), voted X-ray crystallography as the third most important British scientific innovation of the past 100 years, beaten only by **Alan Turing**'s Universal Machine and, perhaps more surprisingly, the BMC mini!

Other forthcoming events to mark the Bragg centenary at Leeds include an exhibition at local museums in July and a guest public lecture scheduled for later this year. For more information and regular updates on these events, please visit http://www.leeds.ac.uk/info/125160/bragg_centenary_2013/1951/bragg_centenary_events .

Dr. Kersten Hall
Visiting Fellow,
School of Philosophy, Religion and History of Science,
University of Leeds

Announcing the 2013 Ludo Frevel Crystallography Scholarship Recipients

THE ICDD Ludo Frevel Crystallography Scholarship Committee has selected thirteen recipients for the 2013 Scholarship Program. These recipients were selected, on a competitive basis, from sixty-nine commendable applications received by the ICDD Scholarship Committee. The recipients are:

Ercan Cakmak
The University of Tennessee, Knoxville, Tennessee, USA

Investigation into the Effect of Martensitic Phase Transformations and Texture Evolution on the Deformation Micromechanics in TRIP Alloys as a Function of Stress-State using Synchrotron X-ray and Neutron Diffraction Techniques

Martin Donakowski
Northwestern University, Evanston, Illinois, USA

Toward Molecular Control of Early-Transition Metal Oxide Fluoride Materials

Rebecca Fischer
University of Chicago, Chicago, Illinois, USA

Phase diagram of SiO_2 at high pressures and temperatures

Marco Jost
Massachusetts Institute of Technology, Cambridge, Massachusetts, USA

X-ray crystallographic investigation of the light-responsive transcription factor CarH

Wang Hay Kan
University of Calgary, Alberta, Canada

Formation, characterization and application of non-templated mixed conductive nano-tubular CeO_2/$BaCeO_3$ composites for Solid Oxide Fuel Cell (SOFC)

Christopher Kane
Georgetown University, Washington, DC, USA

Low Packing Fraction Crystalline Cavitands Exhibiting Molecule-Sized Cavities

Yu Liu
Institute of Physics, Chinese Academy of Sciences, Beijing, China

Defects and deformation-induced new properties in SiC & related materials

Evgeniy Losev
Institute of Solid State Chemistry & Mechanochemistry SB RAS, Novosibirsk, Russian Federation

The formation of solid phases in the system «amino acid + dicarboxylic acid»

Nadine Rademacher
Goethe University Frankfurt am Main, Frankfurt, Germany

High pressure pair distribution function measurements in diamond anvil cells for the analysis of the local structure of compounds consisting of small molecules and their reaction products under extreme conditions

Yezhou Shi
Stanford University, Stanford, California, USA

Understanding the Surface Structure-Activity Relationship in Ceria-based Electro-catalysts Using In-Operando Surface X-ray Diffraction

Sarah Spisak
University of Albany, State University of New York, Albany, New York, USA

Multi-Electron Reduction of Fullerene Fragments: Structural Studies

Jennifer Urban
University of Rochester, Rochester, New York, USA

Studying Self-Assembled Small Molecule Hydrogels Using X-ray Crystallography

Shavait Yamini
All India Institute of Medical Sciences, Ansari Nagar, New Delhi, India

An impediment towards the advent of Breast Cancer: Structural analysis of LPO with various ligands

The ICDD will present each of these students with a check in the amount of $2,500 to assist in the continuation of studies in their selected fields of crystallographic research.

PCG Thesis Prize

Supported by long-term sponsorship from PANalytical, the PCG thesis Prize is noteworthy both for the amount of work done by the winner and for the amount of reading done by the prize-giving jury. This year's prize has been awarded to **Mark Senn** from Edinburgh. The title of Mark's thesis was *"Charge, orbital and magnetic ordering in transition metal oxides".*

PANalytical

Winner of the first PANalytical Award: Thomas Bennett

The inaugural PANalytical Award of 2012 has been won by Dr. Thomas Bennett, affiliated to the Department of Materials Science at the University of Cambridge, UK. The prize was based on a research article published in Physical Review Letters (104, 115503, (2010)), entitled: "Structure and Properties of an Amorphous Metal-Organic Framework". As entrant and first author on the publication Dr. Bennett is to receive the PANalytical Award trophy, a certificate and € 5,000.

The PANalytical Award initiative was launched to reward and encourage exceptional young researchers who are most affected by the reduced government research spending in many regions. PANalytical has sought to provide a substantial, but more importantly a meaningful injection to the career of such an outstanding scientist.

Researchers that have never held a professorship and who use laboratory-scale X-ray equipment as their primary analytical technique were eligible to apply for the award. Entries for the award could be submitted during the course of 2012 and had to have been published in the period between 1 January 2010 and 30 September 2012. The winning article was chosen by a committee composed primarily of independent researchers, unaffiliated to PANalytical and was selected from a strong field of entries submitted from across the globe.

A key feature of Dr. Bennett's work is the interpretation of X-ray total scattering data (PDF). In conjunction with a variety of other techniques such as neutron scattering, electron diffraction, optical microscopy and computer modelling the authors provide a cohesive picture of the metal-organic framework under investigation.

The selection committee was impressed by the level of understanding that Dr. Bennett and his co-workers were able to extract from combination of analytical techniques.

The study represents a significant step towards understanding this kind of amorphous materials, a realm that workers in the field of X-ray diffraction have found discouraging since the technique was established a century ago.

Dr. Bennett comments on his research: *"The real promise here is that we can introduce chemical functionality into the crystalline material, before amorphization into a glass-like one. This is most likely the route to functional amorphous materials such as electroluminescent and optically active glasses. Part of the battle however will be getting people to look past the traditional boundaries of needing a crystalline material to work with."*

Thomas Bennett studied Natural Sciences (Chemistry) at Trinity Hall, University of Cambridge, graduating with MSci (Hons) in 2008. He continued his studies at the Department of Materials Science and Metallurgy in the University, researching the thermo-mechanical properties of porous framework materials.

The characterization, properties and applications of amorphous metal-organic frameworks featured prominently in his PhD, awarded in 2012.

Bursary Recipients' Reports

Third International Conference on Multifunctional, Hybrid and Nanomaterials, 3-7 March 2013, Sorrento, Italy

HELD at the impressive Hilton Sorrento Palace overlooking the Bay of Naples, Italy, Hybrid Materials 2013 was a truly international conference which brought together nine hundred delegates from all over the world, representing six continents. The programme featured eight plenary and tutorial lectures and three parallel symposia in order to accommodate presentations on a wide range of research areas from Biohybrids and Biomaterials, Functional Hybrid Nanomaterials, Nanocomposites and their Applications and Functional Porous Materials. At the first of three large poster sessions accompanied by drinks in the congress centre foyer, I presented a poster on my PhD work concerning the synthesis and structural study of metal-organic complexes with a view to possibly developing porous materials. Due to my research interests, I spent the majority of my time attending the last of the three symposia while venturing to the other symposia for presentations which particularly captured my curiosity.

The conference began with a presentation by **J. Frazer Stoddart** entitled 'From molecular switches to molecular machines' in which he discussed artificial molecular switches (AMSs) and the challenges in developing these into artificial molecular machines (AMMs). In symposium C, **Salvador Eslava** gave a talk on zeolite monoliths prepared by freeze-casting, a technique that is new to me. **Markus Antonietti** delighted the audience with a video showing Pharaoh's Serpent, the combustion of mercury (II) thiocyanate, during his talk on electrocatalysis of N-doped carbon and carbon nitride metal hybrids. In day two, **Clément Sanchez** gave a good overview on hierarchically structured solids and highlighted the unlimited variety of nanostructured materials and the diversity of their applications. Much anticipated was a talk by **Gérard Férey** intriguingly titled 'Open the blackbox: The mechanisms of formation of some MOFs' in which he described in situ studies to follow the process of organisation of inorganic bricks in the framework. This day also featured **Dongyuan Zhao** who presented some absolutely stunning TEM images of core-shell nanostructures of mesoporous silica and uniform porous titania shells on various substrates including magnetite microspheres prepared by the Stöber coating method. Finishing the day, **Samuel I. Stupp** gave a talk with the admittedly general title of 'Supramolecular materials' reflecting the diverse nature of his research on functional networks and polymers. This included the development of supramolecular peptide amphiphile nanofibers which significantly enhance bone regeneration by mimicking properties of the extracellular environment.
Tuesday featured **Molly M. Stevens** who presented, at a very full symposium, her group's research on ultrasensitive biosensors through triggered changes in the aggregation states of biomolecule-functionalised nanoparticles for the diagnosis of diseases including HIV.
On Wednesday, **Jeffrey R. Long** delivered a fantastically informative presentation on CO_2 capture in MOFs, including an overview on the current technologies for CO_2 adsorption. The final plenary lecture was given on Thursday by a very enthusiastic **Takuzo Aida** on his work developing functional soft materials and who revelled in revealing to us 'aqua material,' a transparent hydrogel which is 98% water and composed of a macroscopic 3D network of naturally derived clay, sodium polyacrylate and dendritic macromolecules.

This talk brought to mind a sentiment that **Stoddart** had stressed during the first plenary talk of the conference, in that materials science is in its infancy and there are many fascinating discoveries ahead.

The conference was a very social meeting allowing time to talk to others and to enjoy the setting. At lunchtimes, typical Italian food was served by the beautiful indoor swimming pool at the host venue, where some lucky delegates (not including myself) resided for that week. On the Wednesday night the conference dinner was served at Ristorante o'Parrucchiano in Sorrento where delegates enjoyed a seafood banquet. These occasions, as well as the poster sessions, were great opportunities to meet people from other countries, especially other students, and to discuss our experiences during our careers so far. Talking to others specialising in analytical methods with which I am not familiar increased my awareness of our different approaches to research and the importance of using a variety of techniques for reliable results and thorough investigation. I also found it particularly helpful to talk to other female researchers about their various careers in academic and industrial institutions and how they manage and perceive their work/life balance.

Congratulations to **Rumen Duhlev** and colleagues at Elsevier and the student helpers for organising a successful conference and thanks to all the staff at the Hilton and the local Italians for humouring me with a corrective 'buongiorno' when I said 'buona sera' each morning.

I would like to express my thanks to the BCA for financial assistance to attend this conference which has been a very rewarding part of my postgraduate degree.

Louise Hamdy
University of Bath

38th Lorne Conference on Protein Structure and Function

I arrived in the small seaside town of Lorne, two hours drive southwest of Melbourne Australia, for the annual Protein Structure Function conference. I could already anticipate this conference was going to be one to remember, not only for the glorious sunshine and picture postcard beach, but the programme and list of speakers looked fantastic.

The conference kicked off on the afternoon of Sunday 10 February with a session on developing drugs and membrane receptors in which **Professor William Catterall** gave an amazing talk on his recent work of the structure of voltage-gated sodium channels. The session was then followed by a true Aussie social of a barbeque and beer in the fabulous grounds of the Mantra Lorne, a stone's throw from the beach. The evening ensued with the Leach Lecture, awarded to **Professor Stephen Kent**, who described his inspirational work of chemical protein synthesis and racemic crystallography.

The next three days covered divergent topics from protein folding to immunity and enzymes. A particular highlight for me was a session discussing emerging techniques, particularly **Dr Toshio Ando**'s talk on atomic force microscopy to film protein molecules in action.

The programme also incorporated techniques workshops such as the MALS dinner adding another dimension to the conference. Additionally the trade exhibition was great to talk to companies about their emerging technologies, as well as to pick up a few of the freebies on offer!

There was plenty of time for networking with scheduled networking events such as the students' lunch with speakers and the young investigator dinner for postdocs as well as poster sessions held in the evenings allowing for more relaxed, social discussions aided with a drink!

The conference came to a close with the awards granted to young investigators and poster prizes for students, followed by the conference dinner and party to finish a fabulous event. The breadth of biological topics covered alongside the focus on structural, biochemical and biophysical techniques meant all in all it was a stimulating conference and a great event to attend to aid my decisions for what I would like to research for my postdoc now that I am in my final year of PhD.

Charlotte Hodson
Cancer Research UK

The Worldwide Protein Data Bank: Safeguarding an indispensable archive

JULY 1 2013 marks the 10-year anniversary of the founding of the Worldwide Protein Data Bank (wwPDB; http://wwpdb.org), the international collaboration that manages the PDB archive (1).

From modest beginnings

Starting from just 7 protein crystal structures in 1971, the PDB archive has grown rapidly over the past 42 years. Last year alone, 9,972 new structures were deposited, more than in the first 25 years of the PDB combined. Today, the archive contains over 90,000 structures and at its current rate of growth will reach the 100,000 structure mark in 2014, the International Year of Crystallography.

On July 1 2003, the way in which the PDB archive was managed was transformed by the founding of the Worldwide Protein Data Bank organisation. From its inception, the PDB has been an international archive and the establishment of the wwPDB ensured that these valuable data will continue to be stored, managed and kept freely available for the benefit of scientists worldwide.

The wwPDB organisation nowadays consists of four partners: the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB; http://rcsb.org) and BioMagResBank (BMRB; http://bmrb.wisc.edu) in the USA, the Protein Data Bank in Europe (PDBe; http://pdbe.org) and the Protein Data Bank Japan (PDBj; http://pdbj.org).

wwPDB activities

The wwPDB partner sites each act as deposition, processing and distribution centres for PDB data. They work together and in consultation with the wider community to define deposition and annotation policies, file formats and validation standards for structural data. This close collaboration between the member organisations is vital to guarantee that the global community of PDB users is provided with reliable and consistent data.

While working jointly on all aspects of data representation and processing, each partner site also offers independent tools and services that help make the wealth of data about biomacromolecular structure and function easily accessible to the user community.

wwPDB activities are overseen by an international advisory committee comprising of experts in X-ray crystallography, 3DEM, NMR, and bioinformatics.

Future challenges

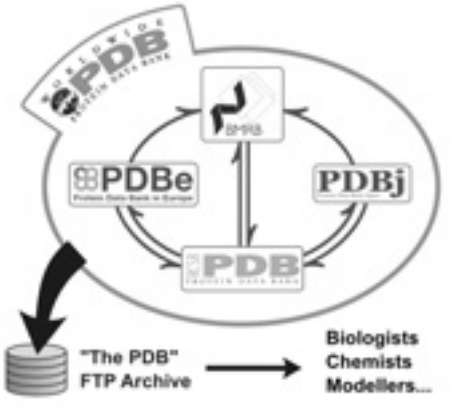
The increasing volume, diversity and complexity of biological data being deposited in the PDB and the emergence of hybrid techniques to obtain structural insights into biologically relevant molecules, complexes and molecular machines all present major challenges for the management and presentation of structural data.

To address these challenges, the wwPDB partners are jointly developing a software system that will allow deposition, validation and annotation of complex and diverse macromolecular structures along with the underlying experimental data using a single interface. This new system will go into full production at all the wwPDB deposition sites early in 2014 and will then be able to handle depositions of structures of any size, determined using diffraction, NMR and/or EM methods.

Validation will be an integral part of the new deposition and annotation system. Assessment of coordinates, experimental data and associated meta data at the time of deposition is vital for improving the quality of the archive. In addition, it will help users with no or limited structural biology background to select the most appropriate structural models for their purposes.

Whatever new challenges the next 10 years will bring, the wwPDB will remain committed to maintain high standards of quality, integrity and consistency of the macromolecular structure archive and to make it freely available to an increasingly large, diverse and demanding global community of users.

1. Announcing the worldwide Protein Data Bank. Berman H, Henrick K, Nakamura H. *Nat. Struct. Biol.* **10**, 980 (2003) doi:10.1038/nsb1203-980



The wwPDB partner sites collaborate on annotating, archiving, managing and distributing the PDB data, ensuring a single global, freely accessible archive.

Members of the PDB, past and present, in attendance at the PDB40 symposium http://www.wwpdb.org/PDB40.html (Photo by Constance Brukin)

wwPDB Milestones Through the Years

Year	*wwPDB Milestone*
2003	The wwPDB is established by the RCSB PDB, PDBe (called MSD at the time) and PDBj with the aim to maintain a single, freely available PDB archive of macromolecular structure data
2004	First X-ray crystal structure from Africa is released in the PDB (1ydk)
2005	PDB data available in PDBML/XML format
2006	BMRB joins the wwPDB
2007	First archive-wide remediation includes updated sequence information and primary citations, improved representation of virus assemblies, and standardized chemistry and nomenclature for monomers and ligands
2008	50,000 entries in the PDB archive Experimental data are mandatory for deposition (structure factors or intensities for crystallography, restraints for NMR) The wwPDB X-ray Validation Task Force (VTF) is convened and meets at the EMBL-EBI
2009	Further improvements are made to the archive, to include details about the chemistry of polymers and the ligands bound to it, biological assemblies, and binding sites of ligands and metal ions The wwPDB NMR VTF is convened Deposition of chemical shifts becomes mandatory for NMR structures
2010	Provision of wwPDB validation reports becomes a requirement for manuscript submission, starting with the IUCr journals 3DEM VTF is convened
2011	PDB40 symposium commemorating 4 decades of the archive held at Cold Spring Harbor Laboratory; the PDB is now the oldest electronic archive of biomolecular data At a seminal wwPDB workshop at EMBL-EBI, the major developers of X-ray structure-determination software agree to adopt PDBx/mmCIF as the principal format for structure deposition
2012	PDB data and EMDB maps become part of the same ftp tree, simplifying distribution of these two important structural archives SAS Task Force is convened
2013	10,000th NMR structure is released PDBx/mmCIF becomes the standard format for deposition and distribution of PDB data Updated wwPDB Charter goes into effect on July 1, starting the second decade of the wwPDB

Argon: a Noble Gas and Two Noble Crystallographers

RECENTLY I found that the crystal structure of argon had been published in 1924 by Franz Simon and Clara von Simson [*Z. Phys.,* 25, 160 (1924)]. They fed liquid hydrogen as refrigerant through a capillary along the axis of an evacuated Debye-Scherrer camera to which argon had been admitted at a low pressure. The polycrystalline argon that formed on the external surface of the capillary at a temperature estimated at 40 K was irradiated. From 12 indexed reflections they found a close-packed face-centred cubic arrangement with cell edge 5.42 ± 0.02 Å. Based on this geometry and using Bragg's methodology, they calculated an atomic radius of 1.92 Å for argon. Comparing this value with the average of 1.56 Å for the isoelectronic K^+ and Cl^- in solid KCl, they could evaluate the effect of nonbonded interaction without interference from ionic attraction. The early date and the participation of a woman with a German title of nobility prompted me to investigate further. It turns out that these two crystallographers were fascinating characters.

Franz Eugen Simon (1893-1956) was born in Berlin, the son of a wealthy Jewish merchant family. During World War I he served with distinction in the German army, earning the Iron Cross First Class. Educated as a physicist, he earned his doctorate for his research on specific heats at low temperatures at the University of Berlin under the supervision of **Walther Nernst**. Rapidly building a successful career there, he became Associate Professor in 1927 and then moved to Breslau in 1931 to take up the Chair of Physical Chemistry. By this time he was a world-renowned low-temperature physicist. Immediately after the Nazis took over, he was spared because of his distinguished war record; but he wisely took up a position in Oxford at the invitation of Winston Churchill's friend **Frederick Lindemann**, who had much earlier earned his PhD in Berlin under the supervision of Nernst. Anglicising his name to Francis Simon, he progressed rapidly at Oxford. He became Reader in Thermodynamics in 1936 and both Professor and FRS in 1941. His pioneering low-temperature research included the solidification of helium. He did important work on the British "Tube Alloys" nuclear weapons project, in particular writing an evaluation that the separation of uranium isotopes by gaseous diffusion would be feasible and calculating the size and cost of the industrial facilities needed. During the 1950s he was knighted and succeeded Lindemann as Head of the Clarendon Laboratory, the latter honour occurring shortly before his death in 1956.

Clara von Simson (1897-1983) had an ancestor who achieved great distinction in law and politics. Her great-grandfather Martin Sigismund **Eduard Simson** (1810-1899) came from a Jewish family (Simson being a German variant of Samson) that converted to Christianity in 1823. Educated in law, he became a professor in Königsberg with Roman law as his special field. He was elected to the National

Assembly in Frankfurt in 1846 and soon became its president. In 1849 he led the delegation that unsuccessfully offered the King of Prussia election as German Emperor. In 1870, at the head of another delegation, he made the same offer to another King of Prussia. Since in the meantime Prussia had defeated both Austria and France, William I had no fears of foreign repercussions and gladly accepted. Simson served as president of the Reichstag until 1874. Although as a liberal he had disagreements with Bismarck, nevertheless with Bismarck's encouragement he became president of the German supreme court. He was inducted into the Order of the Black Eagle and raised to the hereditary nobility.

Clara grew up in a liberal family. She wrote that her parents inculcated a strong sense of social responsibility and encouraged her to learn whatever interested her. From 1903 to 1907 she received private tuition. Her subsequent schooling concentrated on languages, which proved to be a vital asset in her later life. However, at university, first in Heidelberg and then in Berlin, she did something very unusual for a girl and studied chemistry and physics. In 1923, supervised by Franz Simon, she produced her doctoral thesis with the title "Investigations on Amalgams". Evidently Simon must have had great confidence in his young protégée, for the external examiners were **Max von Laue** and **Max Bodenstein**. Laue must have been impressed too. While she continued working with Simon until 1927 and then was appointed to the faculty, she co-authored a volume of stereoscopic pictures of crystal lattices with **Laue**, **Elisabeth Verständig Rehbock** and **Georg Menzer**. After the Nazi takeover, even though her family had renounced its Jewish faith over a century previously, under the Nazis' racial theory her background was "tainted" and she was dismissed from her academic post. With Laue's support she continued to attend physics colloquia, but even that privilege was subsequently denied her. Possibly because of the remoteness of her Jewish background and the noble "von" in her name, she was not sent to the death camps; and thanks to her proficiency with languages she could support herself by working as a translator in a patent attorney's office. After the end of the war she was appointed to a commission planning the reform of German schools.

Since I am writing scientific biography rather than an airport paperback, I shall refrain from speculating on the personal chemistry that may have developed between the war hero and the free-spirited young woman as they toiled over the inert gas. However, it is clear that they had a great professional regard for each other. In 1947 Clara von Simson was appointed to the Faculty of Engineering of the Technical University of Berlin. She admitted that her knowledge of engineering was limited; but, because she had a record unblemished by Nazism, she was "a good advertisement". Fortunately she obtained one of the fellowships that had been established by the Allies for non-Nazi researchers to re-connect with their subject. She used it to spend 1949-1950 at Oxford with... Francis Simon! This research provided the basis for her Habilitation at the TU Berlin in 1951, albeit on the thermal conductivity of ammonium chloride rather than structure determination. Having made her point with the "men's university", she resigned the next year to become head of the Lette-Verein, which promotes the education of women; and she was elected to the Berlin assembly as a Free Democrat. For almost 20 years she served on the board of the Friedrich-Naumann-Stiftung, a foundation promoting liberal political thought. She was awarded honours by Berlin and by the German Federal Republic. The TU Berlin now awards the Clara von Simson Prize annually for the best undergraduate or Master's thesis in science or engineering submitted by a woman.

In the following year, 1925, an independent determination of the argon structure emerged from a more expected source: the world-leading cryogenics laboratory established in Leiden by Nobel laureate **Heike Kamerlingh Onnes**. **J. De Smedt** and **W. H. Keesom** published their structure in *Commun. Phys. Lab. Univ. Leiden,* 178B, 17 (1925). Keesom, who succeeded Kamerlingh Onnes as co-director of the laboratory, was a leading authority on intermolecular forces, and the attractions between rotating dipoles are still known as Keesom interactions.

Carl Schwalbe

News from the Groups

FOR the European Crystallographic Meeting in Warwick, the Young Crystallographers' Group of the British Crystallographic Association and the European General Interest Group for Young Crystallographers (GIG-YC) are joining forces to establish the European Young Crystallographers satellite meeting, in order to promote interaction between up-and-coming and more established crystallographers.

The European Young Crystallographers satellite meeting will take place at ECM28, Warwick, UK in the Warwick Arts Centre on Sunday 25 August 2013, prior to the ECM opening ceremony. This satellite meeting will be the first of its kind at a European level and will run from 9.00 am to 5.00 pm. The opening lecture will be a plenary by **Dr Birger Dittrich**, followed by three sessions for oral presentations and a poster session dedicated to young crystallographers (anyone under the age of 35) presenting their work. The meeting will cost £15 to attend, and this includes registration, coffee and lunch. This fee has been subsidized by the European Crystallographic Association and the International Union of Crystallography, and we are very grateful for their financial support.

We feel that this satellite meeting is an extremely valuable event for young researchers and believe that it will help create a network for young crystallographers, enabling them to communicate their research in an informal environment and to establish connections with other young crystallographers. Given the significance of 2013 to many crystallographers around the world with the centenary of the Braggs, we want to ensure that we celebrate the contributions of younger members and to continue promoting the fantastic work of these up-and-coming scientists. We strongly urge all young crystallographers to support this meeting and present their work via a poster or an oral presentation.

Register **NOW** and don't miss out! We look forward to welcoming you to Warwick!

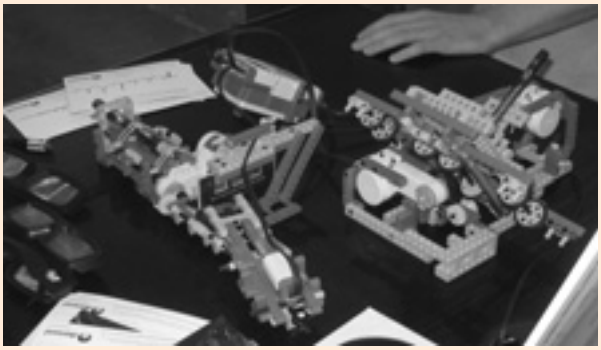
Images from the Big Bang Fair 2013

Day 1: Getting busy

Getting busier…

The yellow shirts stick together for safety

So a crystal is made from marshmallows and cocktail sticks?



The legend that is the 'Lego Beamline'

Smelly molecules!

More converts to Protein crystallography!

Yum, sweets!

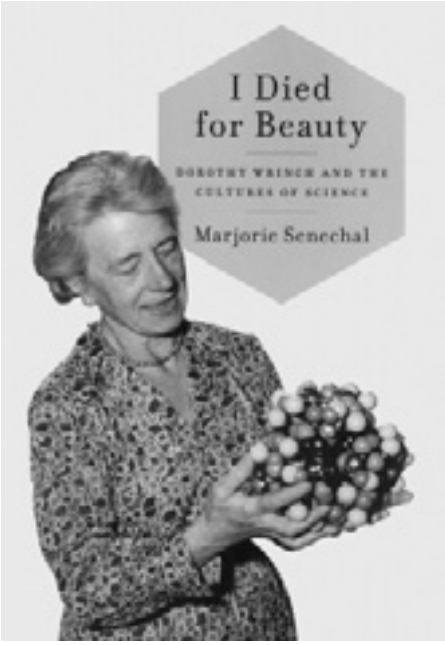
It has been a long few days….

Wrinch: mathematics, models and molecular biology

I Died for Beauty: Dorothy Wrinch and the Cultures of Science

By Marjorie Senechal

Smith College, Massachusetts: Oxford University Press USA
Price £22.50 (hardback)
ISBN 978-0-19-973259-3 ix + 300pp



CAMBRIDGE-educated Dorothy Wrinch (1894-1976) was a brilliant mathematician who in the 1920s and 1930s studied and worked with the pacifist philosopher Bertrand Russell and knew crystallographers Desmond Bernal and Dorothy Crowfoot (later Hodgkin). She collaborated with geophysicist Harold Jeffreys and published with Nobel prizewinning chemist Irving Langmuir but is best known for her long-running feud with Linus Pauling over her cyclol theory of proteins.

There is no Preface in this fine biography of **Dorothy Wrinch** (DW) by **Marjorie Senechal**, Professor Emerita in Mathematics and History of Science at the College in New England where DW ended her career. However, as the Prologue shows, the young maths tutor was a part-time assistant to DW, then in her 70s. Senechal has served on an IUCr Commission and is much travelled; she spent Sabbatical years at Groningen (with crystallographer **W Perdok**) and in the USSR. At the Shubnikov Institute for Crystallography, Moscow, **Nikolai Belov** told her 'We consider Wrinch the greatest American crystallographer'. The book's title may be poetic (and the chapter on the 1938 feud is in a pseudo-operatic style) but the 24 chapters in six parts deal with DW's story authoritatively, from English and North American archives, and largely chronologically. Explanations of the Oxbridge system and accounts of early X-ray crystallographic history, unnecessary for BCA members, will broaden the non-crystallographic American readership.

Dorothy Wrinch was born in Argentina to parents from Suffolk, England: a railway and water engineer Hugh and a former headmistress. They returned to England in 1897 to live at Surbiton, where Hugh was employed by the Chelsea Water Co and DW's sister Muriel Louise was born in 1899. Both girls were educated at the then small struggling Surbiton High School under its long-time Head, Miss **Alice Procter**. Although Girton 'graduate' (women were not granted full degrees) Procter abolished marks, emphasized **Matthew Arnold**'s moral and academic integrity, and told DW she would come to a bad end, DW entered Girton with a maths scholarship in 1913. Here, her contemporary and closest friend was **Dora Black**, who in 1921 married the much older Russell, 1950 Literature Nobel prizewinner, and bore some of his children. DW had some correspondence with Russell as a student and, in 1913, a year of notable crystallographic events, became Girton's only Wrangler (one of the top 30 in Part II of the Mathematical Tripos).The arrangement for DW to now read Moral Sciences Tripos under Russell, financed by a Girton scholarship, collapsed when Trinity cancelled Russell's mathematics lectureship on account of his militant pacifism (in 1918 he served six months in Brixton). In London, Russell tutored DW and four other students privately in philosophy and type theory; ultimately GH Hardy and Russell jointly supervised DW in research training with the Girton scholarship. Her first paper in *Mind* in 1917 defended Russell (two later ones covered Judgement and Memory) and in 1918 her paper/thesis on Transfinite Types won Girton's prestigious triennial Gamble prize.

DW's professional career falls into three phases: Mathematics and the scientific method, and first marriage, in the 1920s; and then Theoretical biology, evolving and defending the cyclol theory, first in England and, from 1939, in the USA. Between 1918 and 1932, she published 20 mathematics papers and 16 on the scientific method (with probability as its cornerstone), some in *Phil Mag* with Jeffreys (a Wrangler). From 1918 to 1920 she taught mathematics at UCL and began research in applied maths

for a London D Sc with another Wrangler, **Prof John Nicholson**, then at King's College. Jeffreys and DW were close but in 1922 she married Nicholson, who by now had left London for Balliol. Their only child Pamela arrived in 1927 but in 1929 DW was the first woman to receive an Oxford D Sc; in 1930 she published under the name Jean Ayling a largely sociological book (calling for a national Child Rearing Service) *The Retreat from Parenthood*. By this time Nicholson's nervous condition had deteriorated so that they were legally separated (alleviated by advice and close friendship from yet another Wrangler, **Prof Eric Neville** of Reading); with Nicholson confined to a sanatorium, they divorced in 1938.

Financed by Girton and LMH (following fruitless attempts elsewhere), and with encouragement from her friend the naturalist **D'arcy Thompson**, DW spent 1931-32 in Vienna. Here she learned cell topology from and loved **Karl Menger** and metamorphosed into a mathematical biologist. Back in the UK, the Theoretical Biology Club, founded by the Cambridge biologist **Joseph Woodger** and biochemist **Joseph Needham**, with DW and Bernal, aimed to explain the form of living things. The concept of a Morphology Institute of Embryology, with Bernal heading crystallography, funded by the Rockefeller Foundation, was the inspiration for the Institute in CP Snow's X-ray crystallography novel *The Search*. In the event, in 1935, the Rockefeller, favouring brains over buildings, awarded Wrinch a five-year grant on protein aggregates. She had already suggested that proteins were cyclic structures forming two-dimensional patterns or lace-like fabrics. There was support from FC Frank and even at first from Pauling but soon his criticism became harsh; DW was equally egocentric and caustic. **Harold Urey** (who thought DW a genius) and **Irving Langmuir** remained loyal to the cyclol but Bernal was critical; some critics cried plagiarism. Crystallographer Wyckoff pleaded for compromise between the approaches of chemists and biologists plus DW's concept of fabrics and cages for globular proteins. DW's publication of an insulin structure in the *Faraday* in1937 was soon undermined by Crowfoot (Hodgkin) in *Proc Roy Soc*. At the 1938 month-long Cold Spring Harbor Conference on molecular biology, DW was the only mathematician, and one of only five women (and one of the two female lecturers) among 72 invited scientists. By 1939, DW's papers in *Phil Mag* had shifted to more general vector map methods of analyzing X-ray data.

When in 1939 there was no response to her offer of war work, DW sailed with her daughter to the USA to embark on the third phase of her career, initially with **David Harker** at Johns Hopkins and ultimately at Smith College, Mass. There she married **Prof Otto Glaser**, a biologist at nearby Amherst, in 1941 and became an American citizen in 1943. When her monograph *Fourier Transforms and Structure Factors* was published in 1946, **William Lipscomb** reviewed it as 'a short and excellent record of Fourier Transforms (FT) of [many] structural types', and **Andrew Booth** (*Cryst News* No **112** 31, Mar, 2010) praised it in his *Fourier Technique in X-ray Organic Structure Analysis* and wrote that Bragg and Lonsdale were impressed; even Kendrew and Perutz acknowledged it in 1952. Thinking it too formal for non-mathematicians, Lipson and **Charles Taylor** wrote the more student-friendly *Fourier Transforms and X-ray Diffraction*. At a 1947 meeting in Schenectady of DW, Booth, the mathematician von Neumann, Langmuir and Harker, a vast metal protein crystallographic computing project was judged too ambitious for a Rockefeller grant. There was some relief for DW in 1951 when cyclol rings (but not fabrics or cages) were discovered in ergot alkaloids. The 1960's saw two DW books on chemical aspects of peptides and the cyclol theory and, with ONR support, other FT papers.

Certainly DW sparked controversy and, as one of the pioneers in bringing other sciences into biology, she stimulated research in several fields, despite experiencing personal tragedies and professional prejudice. She was nominated for the Royal Society and the Nobel prize but was elected to neither. Many distinguished scientists get some things wrong (Pauling and quasicrystals) but are still revered whereas Wrinch is largely forgotten. Senechal's perceptive and entertaining account with its shared memories of this flawed genius will appeal to crystallographers and non-scientists. It also helps explain why this exacting, enthusiastic and intriguing polymath did not have 'a finish worthy of the start' (WB Yeats).

Derry W Jones
University of Bradford

DWJ asks us to say that his review of Hargittai's book headed **Perception**... on p 20 of No **124** (March 2013) had appeared in RSC History Group Newsletter No **63** p 43 (winter 2013).

Professor John Alec Sidney Smith

1927-2013

JOHN Smith interrupted his NMR in the 1950s to determine, with Gordon Cox and Durward Cruickshank, the detailed structure of benzene using Dennis Beard's cold room at Leeds University.

Professor John Smith devoted most of his career to NMR (called unclear magnetic resonance by **Eric Truter**) and, especially, to Nuclear Quadrupole Resonance (NQR). However, as a young lecturer at Leeds, he was the experimental participant in an important crystal structure analysis, that of benzene at -3 deg C. The work was ultimately published in full, with EG (later Sir Gordon) Cox and DWJ Cruickshank, in *Proc Roy Soc* **247**, 1 (1958), confirming Cox's approximate structure of 1932. In the early 1950s, Smith, clad in flying suit, spent many hours collecting data for several hundred structure factors from an oscillation camera in the cold room of which the construction was supervised by Dennis Beard of the Leeds Weissenberg (see page 20 of the December 2012 issue of *Crystallography News*). Although the data led to a beautiful electron density map in the plane of the molecule, the C-C bond length appeared to be 0.02 Å shorter than had been found from gas-phase Raman spectra of benzene. Peaks outside each C-C bond on the F(obs)-F(calc) difference map led to the detection of a new type of systematic error [*Nature* **175**, 766 (1955)] and the introduction of angular libration corrections.

Smith was the last surviving member of the crystallographic academic staff assembled by Cox in Chemistry at Leeds after the war: Cruickshank, **NH Hartshorn** (optical microscopy), **GA Jeffrey** (Pittsburgh), **GE Pringle**, **JH Robertson**, Smith, **MR Truter** (later **Lady Cox**, UCL), and **PJ Wheatley** (Zurich and Oxford). After school in Nottingham, Smith was a student of **RE** (later **Sir Rex**) **Richards** at Oxford. From Leeds, JASS went to research in NMR at Warwick and then spent much of his later academic career on NQR at Queen Elizabeth College and in its merger with King's College, London. JASS died suddenly while on holiday in Portugal with his Portugese wife **Selma**. I heard the sad news from their daughter **Isabel** when trying to arrange to see John (who had been my best man in 1957).

Derry W Jones
University of Bradford

Dr. Beryl Rimmer

MARTIN Packer has informed us that Dr. (Mrs.) Beryl Rimmer, nee Oughton, an associate of Dorothy Hodgkin, died recently. She received her doctorate at the University of Leeds in 1950. From published sources: "Together with Sydney Brenner, Dorothy Hodgkin, Leslie Orgel, and Jack Dunitz, Beryl M. Oughton was one of the first people in April 1953 to see the model of the structure of DNA, constructed by Francis Crick and James Watson; at the time she and the other scientists were working at Oxford University's Chemistry Department. All were impressed by the new DNA model, especially Brenner who subsequently worked with Crick. According to Beryl Oughton, later Rimmer, they all travelled together in two cars once Dorothy Hodgkin announced to them that they were off to Cambridge to see the model of the structure of DNA."

Important publications co-authored with Dorothy Hodgkin:

1. HODGKIN DC, OUGHTON BM (1957). Possible molecular models for gramicidin S and their relationship to present ideas of protein structure. Biochem J. 65(4):752-6.

2. SCHMIDT GM, HODGKIN DC, OUGHTON BM (1957). A crystallographic study of some derivatives of gramicidin S. Biochem J. 65(4):744-50.

International Workshop on Powder & Electron Crystallography

University of Patras (UPAT), Greece July 8-12, 2013

Conference and Cultural Centre

http://epdic.ing.unitn.it/2013_Workshops_at_the_University_of_Patras.pdf

Tutors

Detlef Beckers, PaNalytical, Almelo, The Netherlands

Corrado Cuocci, Institute of Crystallography, Bari, Italy

Partha Pratim Das, UPAT, Patras, Greece

Andrew N. Fitch, ESRF, Grenoble, France

Mauro Gemmi, IIT@NEST, Pisa, Italy

Carmelo Giacovazzo, Institute of Crystallography, Bari, Italy

Fabia Gozzo, Excelsus Structural Solutions S.P.R.L, Brussels. Belgium

Irene Margiolaki, UPAT, Patras, Greece

Stavros Nicolopoulos, NanoMEGAS, Brussels, Belgium

Rosanna Rizzi, Institute of Crystallography, Bari, Italy

Andrew Stewart, University of Mainz, Germany

Robert B. Von Dreele, APS, Argonne National Laboratory, Chicago, USA

Jonathan P. Wright, ESRF, Grenoble, France

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Registration Fee 200 Euros for Faculty members and post docs, 100 euros for students

Registration Deadline: 30th May 2013 (may be extended)

Student Bursaries Available from IUCr. For registration and/ or bursary application email: partha@upatras.gr

University of Patras

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Excelsus Structural Solutions

NanoMEGAS Advanced Tools for electron diffraction

IUCr Commission on Electron Crystallography

International Workshop on Powder & Electron Crystallography

University of Patras (UPAT), Greece July 8-12, 2013

Conference and Cultural Centre

PROGRAM

Time	July 7 Sunday	July 8 Monday	July 9 Tuesday	July 10 Wednesday	July 11 Thursday	July 12 Friday
8:30-9:20		**Direct Methods** Giacovazzo	**Recent Developments in Precession Electron Diffraction (PED)** Nicolopoulos	**Synchrotron X-ray Powder Diffraction** Fitch	**Model refinement in EXPO: wLSQ, RBM, COVMAP** Rizzi	**Introduction to Protein Powder Diffraction: Overview** Von Dreele
9:20-10:00		**Direct Methods** Giacovazzo	**Automated Diffraction Tomography (ADT)** Nicolopoulos/ Gemmi	**Synchrotron X-ray Powder Diffraction** Gozzo	**Model refinement in EXPO: wLSQ, RBM, COVMAP** Rizzi	**Protein Crystallization & Data collection** Margiolaki
10:00-10:30		Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
10:30-12:30		**VLD Phasing Method** Giacovazzo	Lab 1 Nicolopoulos/ Stewart/ Gemmi/ Das	**Sample preparation & Laboratory X-ray diffraction** Beckers	**Real Space Methods** Rizzi	**Structure solution using the MR and SIR/ MIR methods** Wright, Margiolaki
12:30-13:30		**Practicals** Giacovazzo	Lab 1 Nicolopoulos/ Stewart/ Gemmi/ Das	**Unit cell identification** Giacovazzo	Lab 2 Cuocci, Rizzi,	**Intensity extraction from multiple datasets & Accuracy of protein powder diffraction data** Wright
13:30-15:00		Lunch	Lunch	Lunch	Lunch	Lunch
15:00-16:00	Registration	**Introduction to Precession Electron Diffraction (PED)** Gemmi	Lab 1 Nicolopoulos/ Stewart/ Gemmi/ Das	**Full pattern decomposition in powders** Rizzi	Lab 2 Cuocci, Rizzi	Lab 3 Von Dreele
16:00-16:30	Registration	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
16:30-17:30	Registration	**Recent Developments in Precession Electron Diffraction (PED)** Nicolopoulos	Lab 1 Nicolopoulos/ Stewart/ Gemmi/ Das	**Space group identification from powder and electron diffraction data** Giacovazzo	Lab 2 Cuocci, Rizzi	Lab 3 Von Dreele
18:00-22:00	**Welcome Ceremony**					

Lab 1 : Hands on introduction to the programs ELD, Trice, ADT3D
Lab 2 : Hands on introduction to the programs EXPO
Lab 3 : Hands on introduction to the program GSAS-2

Meetings of interest

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

2-5 June 2013
Next-Generation Organic Photovoltaics, Groningen, The Netherlands.
http://conference.groningensolar.nl/welcome

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

3-6 June 2013
EMU School: Minerals at the Nanoscale, Granada, Spain.
http://www.ugr.es/~emuschool2013/index.html

3 June – 13 July 2013
Bachelor Summer Program, Grenoble, France.

6-7 June 2013
European Lab Automation, Hamburg, Germany.
http://selectbiosciences.com/conferences/index.aspx?conf=ELA2013

9-11 June 2013
Crystal Forms@Bologna – Multiple Crystal Forms: Sword of Damocles or Opportunity for the Pharma Industry? Bologna, Italy.
http://www.polycrystalline.it/sezioni.asp?cat=9

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

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

10-14 June 2013
Advanced Methods in X-ray Powder Diffraction, ICDD, Newtown Square, PA, USA.
http://www.icdd.com/education/xrd.htm

10-14 June 2013
Quantitative X-ray Microanalysis: Problem Solving Using EDS and WDS Techniques, Bethlehem, PA, USA.
http://www.lehigh.edu/microscopy/courses/quantitative_xray.html

12 June 2013
Plasmas, Surfaces and Thin Films, London.
https://www.eventsforce.net/iop/frontend/reg/thome.csp?pageID=160077&eventID=371&eventID=371

12-16 June 2013
22nd Croatian-Slovenian Crystallographic Meeting (CSCM22), Hotel Ilirija, Biograd, Adriatic Coast, Croatia.

13-15 June 2013
20th Anniversary Conference of the Serbian Crystallographic Society, Belgrade, Serbia.
http://www2.df.pmf.uns.ac.rs/skd/

16-20 June 2013
Workshop on Dynamic Photocrystallography for Chemistry and Materials Science, Buffalo, NY, USA.
http://www.amercrystalassn.org/photocrystallographyworkshop

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

16-21 June 2013
Proteins – Gordon Research Conference, Holderness, NH, USA.
http://www.grc.org/programs.aspx?year=2013&program=proteins

18-21 June 2013
Challenges in Organic Materials & Supramolecular Chemistry, Kyoto Japan.
http://www.rsc.org/ConferencesAndEvents/ISACS/ISACS10/index.asp

19-21 June 2013
The Future of Scientific Data: Strategies for Facilities, Berkeley, CA, USA.
http://www.nufo.org/events.aspx?id=64

23-29 June 2013
CRETE13: The 2013 International Conference on Applications of Nuclear Techniques, Crete, Greece.
http://www.crete13.org/

24-27 June 2013
15th International Workshop on Physical Characterization of Pharmaceutical Solids (IWPCPS-15), Philadelphia, PA, USA.

24-28 June 2013
4th Workshop on Neutron Scattering Applications in Structural Biology, Oak Ridge National Laboratory, Oak Ridge, TN, USA.
http://www.iucr.org/news/notices/meetings/meeting_2013_58

24-28 June 2013
Third Annual Niels Bohr International Academy Workshop on ESS Science: Crossing Space and Time Domains with SAS and QENS, Niels Bohr International Academy, Copenhagen, Denmark.
https://indico.nbi.ku.dk/conferenceDisplay.py?confId=545

30 June – 5 July 2013
ICMAT2013 – 7th International Conference on Materials for Advanced Technologies Symposium X: Crystal Engineering of New Materials, Singapore.
http://www.mrs.org.sg/icmat2013/public.asp?page=home.asp

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

30 June – 5 July 2013
REI-17: 17th International Conference on Radiation Effects in Insulators, Helsinki, Finland.
http://rei2013.org/

1-2 July 2013
South West Structural Biology Consortium meeting, University of Bristol.
http://www.bris.ac.uk/fmvs/research/swsbc-2013/.

1-2 July 2013
Emerging Themes in Analysis of Grazing Incidence Small Angle Scattering Data, Abingdon.
http://diamond.ac.uk/Home/Events/Emerging-Themes-in-Analysis-of-Grazing-Incidence-Small-Angle-Scattering-Data.html

1-5 July 2013
1st International Conference on Tomography of Materials and Structures, Ghent, Belgium.
http://www.ictms.ugent.be/

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

2-6 July 2013
International Workshop on Powder & Electron Crystallography, University of Patras, Patras, Greece.
http://www.iucr.org/news/notices/meetings/meeting_2012_406

5-6 July 2013
DMM-II Dynamics of Molecules and Materials II – Satellite Workshop of ICNS2013, Glasgow.
http://www.ill.eu/news-events/events/dmm-ii/

5-6 July 2013
International Zeolite Pre-Conference Intensive Summer School, Moscow, Russia.
http://izc17.com/

7-12 July 2013
17th International Zeolite Conference, Moscow, Russia.
http://izc17.com/

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

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

8 July 2013
3rd Science & Scientists at European Spallation Source, Edinburgh.
http://www.europeanspallationsource.se/3rd-science-scientists-ess

8-11 July 2013
11th International Conference on Materials Chemistry (MC11), Warwick.
http://www.rsc.org/ConferencesAndEvents/RSCConferences/MC11/index.asp

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

8-12 July 2013
Combined Analysis Using X-Ray and Neutron Scattering, Caen, France.
http://www.inel.fr/en/news-events/workshop-2013-rietveld

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

13-18 July 2013
VUVX2013: 38th International Conference on Vacuum Ultraviolet and X-ray Radiation Physics, Hefei, Anhui, China.
http://vuvx2013.ustc.edu.cn/dct/page/1

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

15-19 July 2013
REXS 2013 – Workshop on Resonant Elastic X-ray Scattering in Condensed Matter, Oxford.
http://www.rexs2013.org/

20-23 July 2013
The Protein Society 27th Annual Symposium, Boston, MA, USA.
http://www.proteinsociety.org/symposium/

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

22-26 July 2013
ICBIC16: 16th International Conference on Bioinorganic Chemistry, Grenoble, France.
http://icbic16.com/index.htm

23-26 July 2013
Challenges in Chemical Biology (ISACS11), Boston, MA, USA.
http://www.rsc.org/ConferencesAndEvents/ISACS/ISACS11/index.asp

28 July – 2 August 2013
Physical Metallurgy Gordon Research Conference, Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2013&program=physmet

29 July – 1 August 2013
International Conference on Structural Genomics 2013 "Structural Life Science", Sapporo, Japan.
http://www.c-linkage.co.jp/ICSG2013/

2-7 August 2013
SYMMETRY FESTIVAL 2013, Delft, The Netherlands.
http://symmetry.hu/festival2013.html

3-4 August 2013
X-Ray Science – Gordon Research Seminar, Easton, MA, USA.
http://www.grc.org/programs.aspx?year=2013&program=grs_xray

4-9 August 2013
X-Ray Science – Gordon Research Conference Easton, MA, USA.
http://www.grc.org/programs.aspx?year=2013&program=xray

3-4 August 2013
Clusters, Nanocrystals and Nanostructures – Gordon Research Seminar, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2013&program=grs_clust

4-9 August 2013
Clusters, Nanocrystals and Nanostructures – Gordon Research Conference, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2013&program=clusters

4-9 August 2013
Advanced Neutron and Synchrotron Studies of Materials, Waikoloa, HI, USA.
http://www.tms.org/meetings/specialty/pricm8/home.aspx

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

5-9 August 2013
62nd Annual Denver X-ray Conference (DXC2013), Westminster, CO, USA.
http://www.dxcicdd.com/13/index.htm

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

11-16 August 2013
Nanoporous Materials & Their Applications – Gordon Research Conference, Holderness, NH, USA.
http://www.grc.org/programs.aspx?year=2013&program=nanopor

11-16 August 2013
XXII International Materials Research Congress, Cancun, Mexico.
http://www.mrs.org/imrc2013/

17-23 August 2013
2013 PSI Summer School on Condensed Matter Research: Materials – structure and magnetism, PSI Villingen, Switzerland.
http://indico.psi.ch/conferenceDisplay.py?confId=1975

18-23 August 2013
ICANS25: The 25th International Conference on Amorphous and Nanocrystalline Semiconductors, Toronto, Ontario Canada.
http://www.icans25.org/index.shtml

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

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

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/17286-11th_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

9-12 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

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

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

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

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/

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

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

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

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

14-29 October 2013
X-ray Methods in Structural Biology, Cold Spring Harbor, NY, USA.

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

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

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

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/

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/

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

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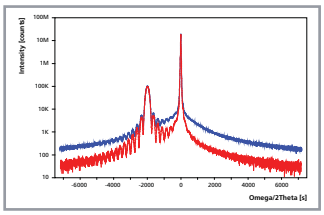

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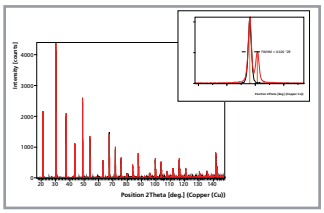
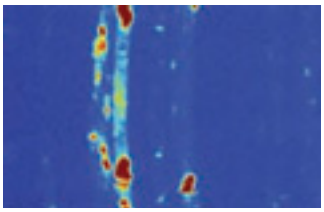


2D



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