

Meeting report of the BCA 25th Annual Meeting held at the University of Kent in Canterbury, UK, 16–19 April 2007

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'Looking back, leaping forward' was the title of the BCA Conference ('Hodgkin') Lecture by Professor Judith Howard CBE FRS. It has been 25 years since the inaugural BCA Spring Meeting in 1982 at the University of Durham, Judith reflected, noting that Dorothy Hodgkin was there as the BCA's first vice-president. Judith's lecture, and the conference programme as a whole, oral and posters, showed excitement in looking forward as well as pride in our past. Today it seems normal that we should meet as a unified body of British crystallographers. A basic, vital, benefit is that it is simple to jump between the various sessions organized by the various interest groups, namely the Biological Structures Group, the Chemical Crystallography Group, the Industrial Crystallography Group and the Physical Crystallography Group. Of especial significance today, though, is that the BCA has a Young Crystallographers Group, formed two years ago, and which held its own meeting on April 16, with talks from 19 young crystallographers on a wide variety of topics. 'Young Keynotes' were presented by Roy Copley on day one on 'Insights into pharmaceutical small molecule crystallography', and Andrea Hadfield on day two on 'Chasing lactate dehydrogenase in circles: making crystal movies'. My personal commendation on chosen title goes to Alexander Pohl of Reading University: 'Why couldn't Bragg solve the structure of nickel cyanide?'.

The Bragg Lecture, established under a legacy held at the Royal Institution, is held approximately every two years and has its own distinguished history. This lecture is given twice and, within the spirit of the RI and the public understanding of science aspect, one rendition is given, usually at the RI, with that in mind. At the BCA, or in the past at an academic venue, often where one of the two Braggs worked, a more academic rendition is given. Thus Sir Roger Penrose OM FRS was our Bragg Lecturer 2007 with his talk entitled 'Quasi-crystals and non-local assembly: a quantum-theory foundations issue?'. Sir Roger is a distinguished mathematician, a recipient with Stephen Hawking of a Wolf Prize in Physics (1988) for their cosmological discoveries. OM means 'Order of Merit', and only 24 people at any one time are so honoured in the UK. His lecture to the BCA was on his famous discovery of 'Penrose tiling'. The audience was held spellbound, and, as Chairman, I can confess to my usual feeling of being somewhat queasy facing fivefold symmetry on a plane surface. To this was added, however, the concluding section of Sir Roger's talk on the implications of quantum theory and the possible role of quantum entanglement for quasi-crystal growth.

Plenary Lecturers had been nominated from each of the BCA Groups and along with these the whole programme was defined under the energetic and enthusiastic Chairmanship of Professor Lindsay Sawyer (Edinburgh University). Two of these were Plenaries given by guests from 'across the pond', namely Professor John Moulton from Maryland, USA (Biological Structures Group nominee), who spoke on 'SNPs, protein structure and disease', and Professor Bob Snyder of the Georgia Institute of Technology (Industrial Group nominee), who spoke on nanomaterials. The Industrial Group Young Crystallographer Prize Talk was given by Dr Gordon Cressey of the

Natural History Museum, entitled 'Random diffraction patterns (without even trying)'. Professor Chick Wilson (Chemical Group nominee) had the tough call of the 'morning after the conference dinner' slot and declared his teaching emphasis title of 'Beans, sausages and pancakes: a recipe for understanding thermal motion in crystals' perhaps not so well chosen after all (but we will all now remember these analogies whenever explaining the topic!). Carrying on the theme of order towards disorder was 'Disorder, similarity and probability: improving our understanding of hydrogen bonding in the solid state', which was the CCDC Prize Presentation Talk by Dr Andy Parkin. The Physical Crystallography Plenary was by Professor Richard Catlow on 'Modelling and predicting structures of complex solids and nanoclusters'. Last but not least in this report, the Lonsdale Lecture, the opener of the whole event, was given by Professor Bill David on 'Combinatorial studies of hydrogen storage materials – playing the odds'.

International contributors of talks, in addition to those mentioned above, were spread through the meeting. Professor Simone Techert (Gottingen, Germany) spoke on 'Time-resolved X-ray diffraction: possibilities and limitations for studying light activated matter', including a look forward to the XFEL in Hamburg and the LCLS in Stanford, stressing the need to specify experiments in terms of the photons per pulse to define feasibilities. Dr Simon Brown from ESRF, Grenoble, spoke on science and instrumentation on the ESRF XMaS beamline. Dr Dmitri Svergun (EMBL Hamburg) spoke on the 'Analysis of biomacromolecular solutions with small-angle scattering'. Dr Tom Ryan travelled from Oregon, USA, and presented on 'Thin films and coatings by XRF and XRD; an overview'. Professor Peter Laggner from Graz in Austria not only spoke on 'SAXS and GI applications using a novel modular lab system' but enthusiastically answered questions on the HECUS products in the coffee times. Dr Tassos Perrakis of the Netherlands Cancer Institute spoke on 'Algorithms and ideas for automated model completion'. Dr Mark Johnson of the Institut Laue Langevin in Grenoble spoke on 'The role of total energy calculations in structure determination and related problems'.

The Exhibitors' Forum where each exhibitor can present for five minutes has become one of those 'must attend' events. Either one is looking to buy something or one is just curious to see the latest progress, e.g. via 'leapfrog ones competitors' or the 'new company on the block'. To see that X-ray fluxes from conventional X-ray sources (non-synchrotron radiation) had reached more than 10^{11} , I found an amazing achievement of the companies. There were over 30 exhibitors this year, a record number. This session also gives a chance to champion the IUCr's exhibit. This year the IUCr's launch of *International Tables Online*, an all-open-access *Acta Crystallographica Section E* and the *pubCIF* author tool for helping authors with the writing of chemical crystallography papers provided a full burst of promotional energy!

The remainder of the meeting was the 'Sam Motherwell Symposium', a special satellite meeting in honour of Sam's contributions to

crystallography in general and the CCDC in particular. Sam first gained international recognition in the 1970s for his *PLUTO* molecular visualizer computer program. Professor Carol Brock (Section Editor of *Acta Crystallographica Section B*) from the University of Kentucky lectured on the 'Phase sequences in some crystals containing $M(\text{NO}_3)_2$, water and 15-crown-5'. Professor Jack Dunitz from the Swiss Federal Institute of Technology Zurich described the crystal structures of fluorinated organic compounds, which still present unexpected changes in properties. Sam concluded the symposium with a talk entitled 'The CSD – 400 000 answers... but what are the questions?', presenting thoughts on as yet unanswered questions such as 'What will be the crystal structure of compound X under given conditions?', 'How many polymorphs of X are there?' and so on.

The poster sessions at the BCA follow the subject group splits, with 18 biological, 44 chemical, 18 industrial and 20 physical. There were poster prizes in each category. The Biological Structures Group 'David Blow Trophy' poster prize winner was Ivan Laponogov with colleagues from Kings College and St George's, both University of London, NASA MSFC, and Rigaku, USA, entitled 'Breakage-reunion domain of *Streptococcus pneumoniae* topoisomerase IV; crystal structure of a Gram-positive quinolone target'. The winners of the poster prizes for the Chemical Crystallography Group (CCG) were Pete Wood (Edinburgh University) for his poster entitled 'A study of the compression of small molecule crystal structures using Hirshfeld surfaces', and Andrew Bond (University of Southern Denmark) for his poster 'The remarkable polymorphism of aspirin'. The IG awarded a prize of £100 and a bottle of bubbly for the best young crystallographer presentation with industrial relevance. This was given to Markus Fries and colleagues of Queen Mary College: 'Crystallographic insights into the mechanism and specificity of pectin methylesterase'. The team assessing the presentations was also very impressed by Helen Maynard's 'The high pressure crystallography of methane' work with her colleagues in Edinburgh. The Physical Crystallography Group poster prize winner was Alistar Davidson and colleagues from Edinburgh, SRS at Daresbury and ISIS RAL, for 'Pressure behaviour of energetic materials'. The PANalytical PhD thesis Prize was awarded to Lynne Thomas. The time allocated for posters included the usual coffee, buffet and tea breaks, but also the Tuesday evening as the main session. The layout brought the commercial exhibition and the posters into close proximity. Logistics at Kent of the placement of the lectures in a different college prevented rapid transfer between the sessions, the posters and the exhibition, but did then allow for some nice open-air walks with fine views of the Cathedral.

The oral sessions were based on the following themes: 'Protein expression to data collection'; 'New science from big facilities'; 'Cocrystals of pharmaceutical materials'; 'Complementary and emerging developments in synchrotron radiation'; 'Solving difficult problems at central facilities'; 'X-ray fluorescence and X-ray diffraction joint session on thin films'; 'Disordered materials and glasses I and II'; 'Computational automation in protein crystallography'; 'Transport and reactivity in crystals' [within which the BCA president Professor Paul Raithby (Bath University) spoke on 'Bright ideas for exciting crystallography']; 'Diffraction from surfaces and 2-D crystallography'; 'Post-phasing and beyond in protein crystallography'; 'One hundred and one ways to prepare an XRPD sample'; 'Computational methods in crystallography'; 'Dynamics in crystals'; and 'A standardless future for quantitative XRPD?'. In addition, the X-ray Fluorescence community held their meeting alongside the BCA meeting.

The BCA Annual General Meeting was well attended. Written reports were received from the secretary Professor Christine Cardin and the Treasurer Dr Sheila Gould. The Treasurer showed that the BCA resources totalled £217 766 and that the BCA 24th conference held the previous year at Lancaster University involved an expenditure of £87 860, yielding a small meeting surplus of £3091 (a typical amount I would say, from memory, for the annual BCA conference, although occasionally reaching a surplus of up to £7000). Thus the sum total of obligations and risks makes these total resources a reasonable match for this stage of development of the BCA, in my view. Gill Houston of Northern Networking presented the meeting organization report, which drew applause. The AGM saw the election of a new secretary, Dr Georgina Rosair, and, in a contested election, a new vice president, Professor Sandy Blake, the latter in succession to Professor John Finney. The AGM was, of course, chaired by the president, Professor Paul Raithby.

The BCA Groups (Biological Structures Group, Chemical Crystallography Group, Industrial Group, Physical Crystallography Group and the newest group, Young Crystallographers) held their own AGMs through the meeting.

Overall, 370 crystallographers attended. In terms of logistics, the whole organization was splendidly done by Northern Networking, specifically Gill Houston and Elaine Fulton, the BCA's professional organizers who are based in Glasgow. The weather was sunny with mornings 'chilly'. At lunchtimes the temperature allowed very pleasant sitting out on the courtyard benches or on the grass. From my college study bedroom I had views of open countryside, including grazing bunny rabbits (Easter bunnies?); for others a neat courtyard bordering on a small lake. Food was full English breakfast on offer, sandwich lunch bags at midday and evening dinner. The wireless internet access did not work but word quickly got around that the network cable sockets allowed internet access happily enough.

The venue provided magnificent views of the cathedral from the campus. With an hour to spare before my train departure there was a chance to visit the cathedral and admire the awesome nature of the building as well as the history that lay within; Canterbury has been a place of Christian worship for ~1700 years. In 1072, the then Archbishop of Canterbury was the first confirmed as Primate (chief bishop) of All England. Thus it is the Archbishop of Canterbury that officiates at, for example, royal weddings. In the cathedral I found that the tomb of the Black Prince was a highlight. The Black Prince was known as such owing to 'the terror of his bravery and ferocity inspired', not because of any black armour; as well as the tomb, the Black Prince's funeral achievements, including surcoat, helmet and gauntlets, are displayed. Canterbury is linked inextricably with the martyrdom of Thomas Becket who was murdered in 1170 by four knights of King Henry II as a result of Becket's outspoken efforts towards the Church's independence from state control. At the far end of the cathedral, beyond the quire, in the corona, built to house part of St Thomas Becket's skull, are the records of the modern day martyrs, among which I found Martin Luther King's entry. The service of all of them to mankind, involving the loss of their own lives in a variety of tragic circumstances, including in the concentration camps, I found deeply moving.

Canterbury itself and the BCA 25th Conference left a broad mixture of happy, significant and profound memories, and lots to inspire all of us, I am sure, for the future.

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