

Crystallography News

British Crystallographic Association



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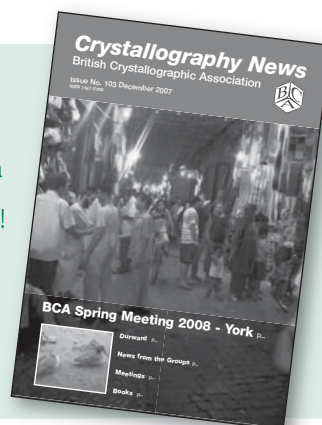
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This month's cover:

Last summer - "European" with a difference - a street in Marrakech!
The inset shows some of the natives waiting for us next spring in York.



From the President



THE Christmas vacation is almost upon us so let me start this column by wishing all our readers a very Happy Christmas and a peaceful and prosperous 2008.

The Christmas period is often a time when we have a chance to reflect on the past year and to plan for the coming one.

2007 has been a good year for the BCA. The membership numbers have strengthened and the Groups are continuing to go from strength to strength. It was a particular pleasure to see the "Young Crystallographers" fully establish their own Group and play a full role in the organisation of the BCA. As I have said previously, I know of no other society or organisation that has such an enthusiastic group of young members and, I am sure you will agree this bodes well for the future of the Association.

The conference website came into being this year which allowed on-line registrations for the Spring Meeting. This seemed to be a great success. At the BCA Council Meeting in September plans were put in place to transfer the main BCA website to a new server and redesign it incorporating the Education website.

Also this Autumn, **Elaine Fulton** left Northern Networking Events Ltd. Elaine had been looking after BCA matters on a day-to-day basis for the last couple of years and we are sad to see her go. I am sure that you would all wish to join with me in thanking her for the enormous amount of hard

work that she put in while with NN and wish her all the best for the future. I am pleased to say that NN have taken on a new member of staff, **David Massey**, who will be looking after BCA business from now on. We welcome David and look forward to seeing him at future meetings.

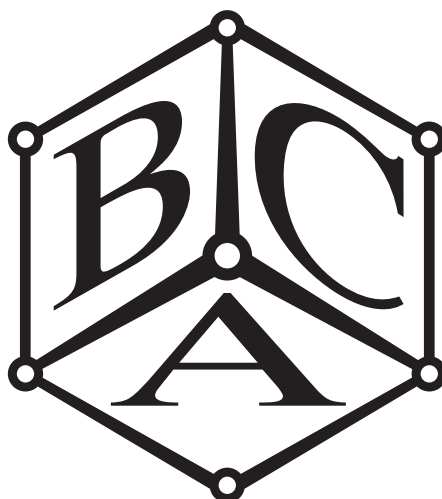
Very sadly, this year has seen the passing of three extremely eminent and respected crystallographers, **Durward Cruickshank, Keith Prout** and **Geoff King**. Their enthusiasm and dedication to crystallography will be greatly missed by all. Obituaries, highlighting their many contributions to the subject, can be found later in this issue of *Crystallography News*.

Looking to the future, as you will also see in this issue, the programme for the Spring Meeting at York, to be held between Tuesday 8 and Thursday 10 April, 2008, is almost complete. I would like to thank **John** and **Ivana Evans** and the Programme Committee for their sterling efforts. I think that it is undoubtedly true that the scientific programme has never been so far advanced at this stage of the year.

I know that a number of you will also be beginning to make plans to attend the IUCr XXI Congress to be held at Osaka from 23 - 31 August. The planning for this meeting is also well underway and the BCA is making a significant input to the programme through the various IUCr Commissions.

Finally, at the AGM at the Spring Meeting, we have to elect a new Treasurer as **Sheila Gould** is coming to the end of her term in office. So the Council officers and I look forward to receiving nominations for this key post.

Paul Raithby



BCA Council 2006-07

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From the Editor



WELCOME to issue 103! As **Garrison Keillor** would put it - "It's been a quiet three months at Lake BCA!" That's why we have a bumper issue with lots to read, preferably before the Christmas holidays!

First of all, it is sad that we have to report the deaths of **Keith Prout** and **Geoff King**, for whom we have recollections written by colleagues. In addition, we have the memories of **Durward Cruickshank**, submitted by several of his friends. As the President says, all of these people will be much missed.

We have a happier record, though in having five (5!) book reviews for you, on a wide range of topics in and around crystallography. I am very grateful to those who have reviewed the books - especially the quick ones! We are sent a range of books, and it is often difficult to find the right person to take them, particularly since many of them are on highly specialised topics. You do get a free copy of the book if you review it, so it's not all asking for favours on my part!

This summer saw the ECM once again in Africa - the ECA does take seriously the fact that crystallographic "Europe" includes Africa and the Near East! We have a review of the meeting in general by one of our bursars, **Simon Cairns**, and a "proper" report on one of the sessions. Reports from BCA bursars make one of the most readable parts of *Crystallography News* and we have another, from **Peter Byrne**, who was at September's Charge Density Workshop in Boston, USA.

You will notice a couple of new photographs on pages 1 and 2. Our **President** has decided to change his, and, while he'd get nowhere with the Passport Office trying on this one, your editor is more tolerant! We don't think he intends to bring the mountain with him to the Spring Meeting. The other new face is **David Massey**, who has now taken over from **Elaine Fulton** at Northern Networking. It has been a very smooth transition from our point of view, but I would like to take the opportunity for thanking Elaine for all that she did to expedite the production of *Crystallography News*.

David, meantime, is off to a good start with the practical details for the spring meeting in York, while **John** and **Ivana Evans** and their committee have been getting on most impressively with the scientific programme. A copy of a Registration form is enclosed, but we hope that few of you will use it. On-line registration is now very convenient for you and for the Office. If you haven't yet done so, have a look at the new website: www.crystallography-meetings.org.uk, which is interactive for everything to do with the

Spring Meeting and also for membership subscriptions. Our "traditional" website www.crystallography.org.uk continues to host archives, general information, and the activities of the groups.

Finally, we have several smaller gems - particularly the knowledge that **William Barlow** (1845-1934) has been awarded a plaque on his Haringey house. Thanks for **Alan Mackay** for sending this in. If you don't know who Barlow was, shame on you! A piece of advice to Googlers: there were many eminent men of that name, so try "William Barlow space groups".

Bob Gould

William Barlow

READERS will be glad to hear of this small honour done to one of the great men whose work made International Tables A possible! We are grateful to Alan Mackay for the following letter and picture - **Ed**



Dear Bob,

After some three years of discussions a plaque to William Barlow has been put up by Haringey Council on a shop in Muswell Hill Broadway where Barlow had a house. Fortunately I have not had to explain to the populace what the space groups are.

Peter Tandy at the Natural History Museum has a paper on the internet about Barlow and is the expert. There is a Royal Society obituary of course and other biographical material.

This is the first of six plaques to distinguished citizens of Haringey. (The next is Oliver Tambo).

Kind regards,

Alan Mackay

Puzzle Corner

THIS month's puzzle, in keeping with the season, is a caption competition! The cartoon below is the work of **Luke Yates**, a summer student with **Jon Cooper** at Southampton. A prize of a £20 Book Token for the best, in the editor's opinion, of course, speech bubble for the finger-tapping man at the desk in this macromolecular laboratory.



For extra points, you might like to try a caption for the new photograph of the President on page 2. Here's a try to get you going: "What is that thing standing next to the President of the BCA?" But some of you can do better, I'm sure!

Last month's puzzle got its first answer before my own copy of *Crystallography News* had arrived. Tim Weakley's answer is:

Whether in the monoclinic or Rhombic form, those of Sulfur, or, more traditionally Sulphur, are Yellow in colour. Viewed through Calcite, one of them may appear to be two. They are Apolar, and hence not pyroelectric. If the molecules in them are treated as rigid, they may translate and screw; they may also Librate and this motion may be represented by a symmetric Toroid.

which is fine, except that I would prefer Tensor for the final word. These first letters rearrange to *CRYSTALS*, and some entrants admitted that they worked backwards from this to get a few answers they weren't sure of!



BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
- A 10% discount on exhibition stands on the annual BCA Spring Meeting, OR - A promotional poster at the annual BCA Spring Meeting.
- Free insert in the annual Spring Meeting delegate bag.
- Two free full registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly BCA Newsletter.
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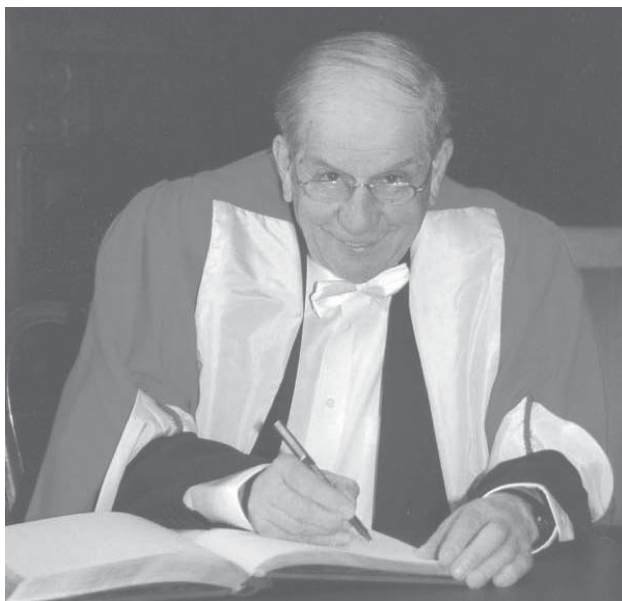
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Obituaries

Durward William John Cruickshank FRS (1924-2007)

IN DURWARD, we have lost a uniquely faithful and joyous attender of meetings of the BCA. We have gathered some memories of those who knew him well. I will make only one comment. His health did not permit him to attend last year's meeting in Canterbury, so he sent an apology to the Treasurer, asking her not to refund his registration fee, but to credit it to the Arnold Beavers Bursary Fund. "And don't forget," he added, "to Gift Aid it!" ED.



Durward receiving an honorary degree at the University of Glasgow. The clothing may be untypical, but the smile is not!

The clearest of my early recollections of Durward was our meeting at the fourth IUCr Congress in Montreal where he delivered three papers. One was on naphthalene, a structure I had toiled on as a graduate student of **Monteath Robertson** a decade earlier. Visually estimating intensity magnitudes for the evaluation of triple Fourier series on punched card machines, then manually evaluating the electron density in the central molecular plane, clearly revealed the location of each hydrogen atom, a triumph in 1949. We also detected systematic variations in the lengths of chemically distinct C-C bonds. Durward's major advance was to interpret the evident C atom vibrations in terms of their anisotropic translational and rotational oscillations. His analysis agreed well with the results inferred from Raman

spectra, giving C-C bond lengths that largely agreed with ours but of greater accuracy. It was thus memorable in 1957 to hear Durward's elegant approach to a problem, initially tackled by **William Bragg** in 1921 and Monteath in 1933, that so clearly personified the course of true scientific progress.

Sidney Abrahams
Bell Laboratories

IN 1983 at the Cornell High Energy Synchrotron Source, CHESS, we obtained the first X-ray Laue diffraction patterns from protein crystals (**Moffat, Szebenyi & Bilderback, Science 223, 1423-25 (1984)**) and began to explore the redevelopment of Laue diffraction as a complement to monochromatic techniques, eyeing time-resolved crystallography. With a sabbatical leave upcoming from Cornell in 1985-86, I decided to work at Daresbury Laboratory with **John Helliwell**, a like scientific spirit also embedded in a synchrotron environment. In the event, John was in the throes of moving to the Department of Physics at the University of York so after three months at Daresbury, I joined him at York in January 1986. There I met **Durward Cruickshank**, his frequent visitor who had recently retired from UMIST. The three of us began what proved to be the most stimulating and yes, fun, collaboration of my career as we explored together the fundamentals of the Laue X-ray diffraction technique, initially and most intensely at York and later at Cornell during visits by John and Durward.

Laue diffraction patterns are obtained by illuminating a stationary crystal with a polychromatic beam of X-rays. The patterns are subject to the overlapping orders problem (diffraction from all reciprocal lattice points along a ray - a central line in reciprocal space - falls on a single Laue spot), crowded (each pattern contains many Laue spots, for which spatial overlaps must be resolved), and obtained with very short exposures (diffraction from all reciprocal lattice points between the limiting Ewald spheres occurs throughout the total exposure). Although the Laue technique was successfully used for structure determination of numerous small inorganic and organic species by Pauling, Wyckoff and others in the 1920s, it was superseded in the 1930s by monochromatic oscillation, Weissenberg and precession techniques that did not suffer from the overlapping orders problem and yielded more accurate structure amplitudes, even with the primitive computational methods and hardware then available. But, is this problem fatal or merely inconvenient? What fraction of the diffraction data is affected? In which regions of reciprocal space? What Laue spots are

in close spatial proximity? What is the distribution of inter-spot distances? How should a Laue diffraction experiment be conducted, to obtain the most accurate, complete set of structure amplitudes? In short, was Laue diffraction merely a historical curiosity, or useful for particular classes of experiments using then-new synchrotron sources?



John and I were brash, young(er) men in a hurry to get the answers, no strangers to vigorous disputation and with an array of experimental facts and literature at our disposal. Not so fast, said Durward. Do we really understand the fundamental principles? The two of you spout authorities such as Pauling and Bragg but is it really so? Did they get it all right? Are your facts and literature really solid or are there holes? Like a true theoretician, he persuaded us to consider first the experimentally unrealistic but illuminating ‘infinite wavelength bandpass case’, then extend it to include appropriate experimental constraints. The three of us went at it hammer and tongs, in the physics department coffee room at York or in John’s office or mine. We’d begin at the morning coffee break, and (we confess) sometimes continue over lunch in the nearby Charles XII pub in Heslington, and always argue through the afternoon until the tea break. Tiring yes, but without a doubt, exhilarating. We’d retire to our offices, write out in longhand a draft of the day’s argument and fire it off to the other two, stimulating another round of discussion. Under frequent prodding from Durward we returned to first principles, in the process examined and dismantled some old prejudices, and laid a foundation that survives today. He insisted that we argue all points through to conclusions that were not merely correct but elegantly and concisely expressed, in a form that he believed readers could easily grasp. Our arguments became so intertwined that in the papers that finally emerged (Cruickshank, Helliwell and Moffat, *Acta Cryst.* **A43**, 656-74 (1987); *ibid.*, **A47**, 352-73 (1991)), Durward allowed that he couldn’t distinguish which ideas or lines of attack originated with which of the three of us; all were cooperative. Now that’s a real collaboration. I will not see its like again.

Keith Moffatt
University of Chicago

AS a research student in E.G.Cox’s Inorganic and Physical Chemistry Dept. at Leeds University, I must have encountered Durward first as he visited Leeds from Cambridge during Henry Viervoll’s period at Leeds in Autumn 1948. Collaboration between the two presumably sparked Durward’s interest in gas electron diffraction that developed at Glasgow and UMIST. (His pre-Cambridge period at Leeds 1946 -1947 made use of his engineering training and unconventional war research experience. These, when supplemented by the mathematical tripos 1947-1950, provided a broad preparation for his later scientific career).

Cox’s crystal-structure academic staff in 1948 was, for its time, remarkably interdisciplinary, with several physicists (including Cox), and embracing optical microscopy, U-V spectroscopy and solid surface studies, later supplemented by NMR. The main aim was to tackle theoretical chemistry problems of bond character and valency, in pursuit of which Cox regarded development of computing techniques and the critical examination of accuracy in X-ray refinement as fundamental. These were areas that Durward was to develop further as he returned to a lectureship in mathematical chemistry at Leeds in 1950. Despite his experience and central role on refinement processes in a major school of X-ray analysis, Durward remained retiring and relaxed and sometimes had an almost shambling approach.

At one of the earliest conferences I attended of the X-ray Analysis Group, a forerunner of the BCA, at Leamington Spa in 1949, “Mr Cruickshank” gave the opening paper on theoretical developments on precision. He described corrections for systematic thermal-motion and termination-of-series errors as well as estimates of random errors. Most Fourier syntheses were computed with Beevers-Lipson sine and cosine strips, but for three-dimensional syntheses B.T.M. Hollerith punched-card methods were already employed at Leeds, first at the Electricity Board and then within the Department, in part with Mr. D.M.S. Greenhalgh’s assistance.

Durward established sufficient rapport with research student **John Rollett**, fresh out of the Navy and then with a rather direct analytical but enthusiastic and informed approach to conversation, to join in a mountain walking holiday in Norway after the 1950 IUCr Congress and remained a lifelong friend. In 1951, Durward was the first Chairman of the Pippin Club of Cox’s workers, which had a tie and newsletter.

In the 1950s Durward’s Leeds refinement programs exploited the power of the Ferranti Mk I digital computer at Manchester, in cooperation with **Peter Wheatley**. Paper tape was input twice to help spot punching errors. Soon after my return to Leeds in 1957, the Ferranti Pegasus was installed at Leeds under **Sandy Douglas** in a converted chapel opposite the Chemistry Dept. and refinements continued, again with Durward’s programs (with collaboration from **Diana Pilling**).

Our only publishing collaborations were around 1960 but Durward and I were in frequent touch in recent years over refereeing, the 2003 RSC Bragg Chemical Landmark event at Leeds, Durward’s travels to Utah and to cold climates,

and obituaries of crystallographers. His family genealogical surveys led both to Wordsworth and also to **John Hymers**, the founder of my school in Hull. Only in our last telephone conversation, shortly before his death, did he spend time discussing the technicalities, treatment and prognosis of his illness.

Durward was clearly brighter than many of us but there was never a hint that one's own view was not as valid as his. Whether he would like the term or not, Durward was a gentleman scientist who gave full value to both words: one remembers him with regard and affection.

Derry Jones (another DWJ!)



I don't think I can remember when DWJC wasn't part of my crystallographic life. I have notes right from the start as an undergraduate project student on all sorts of topics where references are made to the papers of 'DWJC' of the 50's & 60's and I well recall when I first met Durward at AERE, Harwell while studying at Oxford for my DPhil with **Dorothy Hodgkin**. Durward had come to Harwell to work with **Terry Willis** and me and to discuss my hexamethylenetetramine (HMT) neutron data. I was in the DIDO Reactor Hall on the experiment and suddenly Terry was there with another 'young man' leaping up onto the experimental platform and looking at the old Ferranti Mark II diffractometers. I asked the others discretely who this was and was completely amazed to hear it was 'Professor Cruickshank from Manchester', as I had expected to see a really old man given the dates of the seminal publications from this great man and to which everyone referred for ideas and issues of thermal motion. Then of course I worked out how young he had been when he wrote these important papers and felt suitably humble. We had many good interactions from then on, concerning the HMT results in the first instance and the detailed thermal motion analyses Terry and I carried out on these. Later this work also included **Stuart Pawley** (Edinburgh) when we considered joint refinements of X-ray and Neutron data using HMT as a test case.

Subsequently Durward was my external examiner for my DPhil at Oxford and he was incredibly kind, or so it seemed from my side of the desk where I faced **David Philips** and Durward together that summer afternoon and there began my career in chemical crystallography.

I can hardly recall a crystallographic meeting where Durward didn't appear, either as a speaker, an organiser, a participant or with his IUCr hat on for many years. He would always take the time to talk to the students and postdocs at meetings and when posters were introduced he was brilliant at walking around and finding a lonely young person and asking them to explain their work to him and very often giving helpful advice or gentle criticism if he knew they'd made a mistake somewhere and could improve before next time. Durward was interested in all aspects of the subject or so it seemed and impressively knowledgeable in most as well. It was a pleasure to spend time with him on these occasions and to gain so much insight and detail in so many ways about crystallography and science in general. He acted as external examiner for my PhD students as the years went by and we always kept in touch over papers and ideas. He would pick up on ideas and write to me. I recall one time visiting Manchester after he'd retired; we were having lunch in the staff dining room before my seminar with **John Helliwell** and we got into a discussion on the use of R_{free} by the protein community. Thereafter followed many long letters and re/pre-prints from him which I still keep in my office.

Durward had a splendid sense of humour which he combined well with his love of life, nature and people in general.

It was absolutely delightful to drive across to Alderley Edge, near Manchester, 2 summers ago to collect his complete (from day 1) Acta Crystallographic Collection which Durward had advertised at the preceding spring BCA meeting on an 'all or nothing' basis. So one of my group and I collected these in many boxes over two visits and they now adorn the research room here in Durham. While I was at his home, I spent some considerable time looking at the reasons for Durward needing the archive space in his house and this was his new research into the family tree and his exploits to the Antarctic. Time had moved on. We pored over many old photos of past meetings where there were a few faces he couldn't name - and nor could I?! - and we looked through many other historical notes and reprints, as well as his recent photos from his long trips into the icy regions. I wish I had a better memory or that I had had a tape recorder with me, it was absolutely fascinating to listen to and watch. We sat in his lovely garden over tea and looked at the various excellent borders of flowers he had growing there, until it was time for me to leave, the car groaning under Actas!

Durward was a tremendous friend to the crystallographic community and did so much more for it than the brilliant papers he published for our education and benefit. He was an inspiration to me and I shall never forget, but rather hope to emulate, his open friendship towards others.

Judith A. K Howard

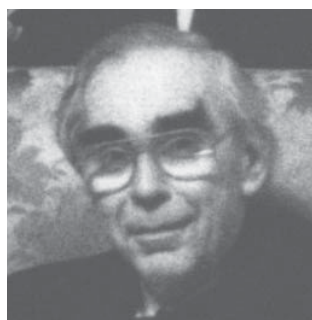


THE photograph from 1998 shows **Durward Cruickshank** along with **Michael Woolfson** and **Margaret Woolfson** at the conference dinner of the University of Manchester celebration of its role in the history of computing. Durward was a pioneer in applying the use of computers in crystallography, particularly crystal structure refinement. Michael and his team at York University led the way in computing and direct methods of phasing and were incredibly successful with 'MULTAN'. The 'first stored program computer' was built by Kilburn and Williams at the University of Manchester in 1948; a key innovative feature was the storage tube for recording zeros or ones *i.e.* binary code. This machine, the 'Manchester Baby' was commercialised by Ferranti and was the computer that attracted Durward to come from the University of Leeds to use it when he was based in **Gordon Cox's** crystallography research group. My association with Durward both as a collaborator and friend, began in 1982 when I was introduced to him by **David Blow**; he was soon to be 'retiring', and wished to form a collaboration with me. Of course I knew of the Cruickshank weighting scheme, another of Durward's many achievements in crystallography! We began, along with Prof. Keith Moffat, working on the Laue method, but continued to work together right up to his death, when his knowledge about the protonation of oxalic acid dihydrate proved important, and which he and his first student **Farid Ahmed** had studied both in the crystal and in the gas phase. This provided us with important insights into our study into the protonation states of proteins in general and the effect of microenvironment on side chain protonation in particular. Our joint paper in *Acta Cryst Section D* appeared in August 2007. He used to say he was my 'irreverent Postdoc' but it became clear to me, as I wrote in my obituary piece for Durward in *The Independent*, that Durward and his abilities were like having 'a Ferrari in the garage'! Also very recently, The University of Leeds sent a TV crew to interview Durward in the month before he died and the result is an hour long Q&A session, which is both fascinating early history of scientific computing but also insights into many aspects of science from Durward. As his 80th birthday celebration notes showed (in March 2004) Durward's view of the history of modern science was that it was still rather little time since Newton, the first person to understand the mathematics of space flight. As well as his huge impact in crystallography, Durward had many outside interests, including golf, and his expeditions to the Arctic and

Antarctic. Recently he gave me a book about the Colossus computer project of the Second World War since Durward had mistakenly ordered two copies. This book is a superb account from the leading players in the top secret project for code breaking of German war messages. Colossus I and Colossus II obviously predated the civil developments in computers. Thus Durward was active both in crystallography and his other interests right to the end. I deeply miss a close colleague and a friend over some 25 years.

John Helliwell

C Keith Prout 1934-2007



I worked with Keith for 40 years.

When I came to Oxford in 1967 as a fresh post doc, Keith was already the Lecturer in Chemical Crystallography, running a successful research group alongside those of **Tiny Powell** and

Dorothy Hodgkin. Although he was not my supervisor, I quickly learned that it was he who held all the practical knowledge that kept the laboratory running. He had already accumulated a wide circle of colleagues throughout crystallography, so that when he could not answer a question himself, he was always on first-name terms with someone who could.

Within a few years of my arrival, Tiny retired and Keith became Head of the Chemical Crystallography Laboratory. Under Keith's stewardship the laboratory blossomed, building on the foundations laid down by Tiny and Dorothy. The laboratory attracted academic visitors from all over the world, with most of these people remaining life-long friends of Keith and Lesley.

Keith was born in Barnsley in 1934 and was a pupil at Barnsley Holgate Grammar School before coming up to Wadham College at Oxford. It was during his Part II (research project) year with **Bob Williams** that his interest in transition metal chemistry and in crystallography began to develop (*An Investigation into Some Transition Metal Complexes with Hydrazine*, Wadham, 1957). The Part II thesis also shows an interest in twinning and polymorphism, interests which were to develop during his D.Phil studies. He presented his D.Phil thesis in 1959, after only two years of very productive research. The thesis shows very clearly both Keith's curiosity about the solid state, and his determination to work at problems until they were solved.

The thesis is also a window onto the almost unbelievable world in which Science moved ahead without computers,

but which was also being revolutionised as he worked. His first crystallographic computations were carried out using punched (Hollerith) cards on mechanical tabulators, but by the end of his project he was writing programs for the Ferranti Mercury computers. In spite of the fact that the programs were written in Autocode (a semi-machine language) Keith realised the importance of the user interface, and produced a program with a surprisingly modern keyword-based input. This early brush with computers convinced him that he did not really like writing programs, but, paradoxically, this later enabled him to father a number of important software projects. Because he was not interested in encoding the answer to a problem, his imagination was liberated to push crystallographic and chemical computing to new frontiers.

In the early 1970's he raised a grant with **John Rollett** to employ **Bob Carruthers** to create a program for the refinement of twinned data - a program that eventually grew into CRYSTALS. It was their misfortune that the program emerged at just the time that photographic methods (which provide copious information about twinning) were being replaced by serial diffractometers (which made the handling of twins rather difficult) so that the significance of their creation was not appreciated. Keith was also instrumental in the formation of the Molecular Graphics Group, leading to the launch of the Journal of Molecular Graphics. He was consultant to **James Crabbe** and **John Appleyard** as they created the Desktop Molecular Modeller, and worked with **Bob Diamond**, **Tom Koetzle** and **Jane Richardson** on an enormously ambitious project with IBM and Oxford Electronic Publishing- the CD-ROM based Molecular Structures in Biology. This was a project at the very cutting edge of technology. ChemX, from Chemical Design, and Cobra, from Oxford Molecular, were developments of academic projects he started.

Keith was much more than a software innovator. It was as a chemical crystallographer that he worked in laboratories in Sweden (with Sixten Abrahamsson), in Rome with Sandro Vaciago, in Yugoslavia with Boris Kamenar, and many times in North America with **Jenny Glusker** and **Abe Clearfield**. In addition to his fascination with the chemistry of copper and molybdenum, Keith was drawn to studying charge transfer complexes, cyclopentadienyl complexes, pharmaceutical materials and liquid crystals. He had a long collaboration with **Andy Vinter** and **Anthony Roe** at Smith, Kline & French, during which he was instrumental in the milestone solution of the structure of cimetidine from powder data. In the years leading to his retirement he reprised his old interest in the organic solid state, and was a strong advocate for the complimentary use of X-ray crystallography and solid-state nmr.

Although he rarely appeared on stage at BCA meetings, Keith was an accomplished speaker, with the knack of appearing to talk *with* the audience rather than at them.

In the laboratory, however, he was much more than just a talker - he was a doer. It was not unusual to find him with his sleeves rolled up, half way inside an X-ray generator or re-building a vacuum line. He was a hands-on scientist, and loved practical work of every kind. This led him into doing research in all the difficult corners of crystallography, so that his experience was both deep and wide.

His other real love was teaching, and it is perhaps through this that he will be most fondly remembered. He had the knowledge and insight to debate problems with the best students, and the patience and understanding to help the weaker ones. Even after his retirement he continued to come into the laboratory, and clearly took great satisfaction from sharing his expertise with young research workers and visitors.

Keith was what one might call an old-fashioned scientist, coming from a culture that has now slipped away. For his generation it was not necessary, or even seemly, to promote oneself at every opportunity. He was not interested in joining the *International Lecture Circus*. Because of this, he was able to devote much of his time and energy to the well-being of his colleagues, staff and students, and to providing the environment and encouragement needed for first class research. The measure of his success is both the scope of his published work, and the large number of crystallographers in both the UK and the rest of the world whose training started or developed in the Chemical Crystallography Laboratory, Oxford.

In spite of his BBC accent, Keith remained a Yorkshire man all his life - bluff on the outside but gentle within. He could not abide evasiveness or deceit. He told things as they were. I was once summoned to see the Head of Inorganic Chemistry. The day before the interview Keith took me aside and suggested that I might look neater than usual for the occasion. Almost certainly good advice, but its effect was not lasting. He had the same attitude to science. If he saw a flaw in a project or results he would say so, usually coming directly to the point. This directness did upset some people, but most of the crystallographic community valued his judgments.

His astute assessment of situations was not restricted to science. Keith was always active in the affairs of Oriel College, being a fellow from 1966 until 2001, and then an Emeritus Fellow until his early death. He took on the roles of Vice Provost, Acting Provost, Senior Tutor and finally Tutor for Graduates. He was always willing to listen to other people's problems, and if appropriate, offer advice or help.

Underneath the brooding eyebrows there lived a shy and kindly man. He will be remembered as a remarkable scientist and a loyal friend.

David Watkin

Geoffrey Stephen Douglas King 1924-2007



GEOFFREY KING (Geoff) was born on 7 December 1924 in Ealing. He studied at the Royal College of Science (now Imperial College, London) and obtained a B.Sc. in Chemistry and Physics in 1944. From 1944 to 1953, he was employed by J. Lyons & Co. He began as an analytical chemist, and shortly specialised in crystallographic work, developing software for the

LEO computer. While there, he obtained the M.Sc. in Crystallography from Birkbeck College, and determined several crystal structures, including those of nicotinic acid and nicotinamide. Between 1953 and 1956, he held a research fellowship at Birkbeck, where he moved into protein crystallography; among the structures on which he worked were lysozyme nitrate and iodide.

In 1957, Geoff joined the Union Carbide European Research Association in Brussels, where he returned to the field of organic and organometallic structures. Alongside his structural work, he wrote a set of programs for the IBM 1620 computer. He started an international IBM 1620 users' group with more than 70 members, who developed these programs.

In 1971, Geoff was appointed Professor of Crystallography in the Department of Geology and Geography at the University of Leuven. His research dealt with the structures of minerals, and of organic and organometallic compounds. Along with that, he assisted with the development of important software packages, including XRAY-76 and XTAL, in particular their implementation on IBM systems. For a considerable time, he was responsible for the implementation and use of the Cambridge Structural Database in Belgium. In 1976, he was made a foreign member of the Royal Flemish Academy of Science and Arts. In that year, he joined the Belgian National Committee for Crystallography, of which he was secretary from 1980-82 and chair from 1985-88. In 1997, he was made an honorary member. Geoff was for many years a member of the European Crystallographic Committee, the forerunner of the ECA, and was its chair from 1987-89. Colleagues in Belgium and abroad valued his unselfish concern for the crystallographic community, his good critical spirit and his warm humanity.

After his retirement with emeritus status in 1990, he remained very active in crystallographic research; many people benefited from his expertise. Geoff died suddenly in Leuven on 11 September, 2007.

Luc van Meervelt, Leuven
(from Dutch version in the journal of the Koninklijke Vlaamse Academie van België voor Wetenschappen en Kunsten - ED.)

Roy Thesis Prize in Condensed Matter Physics

FOLLOWING a generous donation by Professor **Bimalendu Narayan Roy**, the Condensed Matter and Materials Physics Division has established a Ph.D. Thesis prize. The prize will be awarded annually and will be worth a cash sum of £500, plus a certificate.

Nominations for the award should be sent to the Division secretary at the following address to arrive no later than 14 December 2007:

Professor John Inglesfield
School of Physics and Astronomy,
Cardiff University,
The Parade,
Cardiff,
CF24 3AA

InglesfieldJ@cardiff.ac.uk

There is no application form but the nomination should comprise:

- The name and affiliation of the student
- The name of the supervisor(s)
- The title of the thesis
- A maximum one page A4, point size 11, summary of the thesis from the supervisor, indicating the contribution made by the student
- A maximum one page A4, point size 11, statement from the external examiner

All students registered in universities in the UK and Ireland are eligible provided that their viva voce examination took place between 1st October 2006 and 30th September 2007. Candidates who have already won a thesis prize awarded by a group of the Institute of Physics will not be eligible for the award.



York 2008

BCA 2008 Spring Meeting: University of York, 8-10 April 2008: Practical Information

THE BCA meeting starts at 11.30 on Tuesday 8 April, and concludes at 13.30 on Thursday 10 April 2008.

The Young Crystallographers session will commence on Monday 7 April. All scientific lectures including the Young Crystallographers will take place within the Exhibition centre.

We will have our traditional Commercial Exhibition, located within the Exhibition Centre. Because of the popularity of the Young Crystallographers session at the Spring Meeting in Kent, the Commercial Exhibition will be open from 19.00 on Monday 7 April and will close after the morning refreshment on Thursday 10 April. Delegates will have the opportunity to visit all stands during the poster and exhibition buffet dinner on Tuesday 8 April as well as during all refreshment breaks.

Registration and refreshment breaks during the main scientific programme will take place within the Exhibition Centre. The Young Crystallographers session on Monday 7 April will take place within the Exhibition Centre lecture theatre and evening buffet will be held in the exhibition hall.

For more information on the Exhibition and Sponsorship opportunities, or for any other enquiries about registration or accommodation, please contact **David Massey** at the BCA Administrative Office, **01355 244966** or email bca@glasconf.demon.co.uk

The best way to register is on-line at the meetings website: www.crystallography-meetings.org.uk where forms will be available from 10 December 2007. If this is inconvenient, please phone or e-mail David Massey.

Registration

Early Registration Costs (*before 3 March 2008*)

Full Registration	£200.00
Student/Unemployed/Retired	£100.00
Non-Member Surcharge	£30.00
One-Day Registration (no concessions)	£100.00

Late Registration Costs (*after 3 March 2008*)

Full Registration	£250.00
Student/Unemployed/Retired	£100.00
Non-Member Surcharge	£30.00
One-Day Registration (no concessions)	£125.00

Accommodation

There are two types of accommodation available at the University of York.

Standard B&B	£36.00 per night
En-suite B&B	£48.00 per night

Accommodation is divided across two locations within the University campus. Standard accommodation is in the Vanbrugh Building and en-suite accommodation is in the James building. Breakfast and dinner will be served in the Galleria restaurant.

Check- In time is from 14.00 and keys must be returned on departure no later than 09.30.

Collection of Accommodation Keys

Delegates staying in Vanbrugh collect their keys from Vanbrugh porters' lodge reception 24 hours.

Delegates staying in James collect their keys from Goodrick porters' lodge reception 24 hours.

Catering

Morning and afternoon refreshments from Tuesday 8 April - Thursday 10 April will be served in the Exhibition Centre. Refreshments and Lunch for the Young Crystallographers will also be served in the Exhibition Centre.

Breakfast and Dinner (including the Conference Dinner on Wednesday 9 April) will be served in the Galleria restaurant.

The Young Crystallographers Buffet Dinner on Monday 7 April and the Poster and Exhibition Buffet Dinner on Tuesday 8 April will be served in the Exhibition Centre.

All lunches and evening meals must be booked in advance and will be ticketed.

Packed Lunch	£7.50
Dinner on campus (Monday 16 April)	£15.00
Conference Dinner	£35.00/ for concessions £20.00

Please be aware that if packed lunches and evening meals are not selected on the registration form and paid for prior to attending the meeting it is the individual's responsibility to make alternative arrangements.

Social Events

On Tuesday 8 April, the poster and exhibition reception will be held in the early evening. A buffet meal with wine will be served in the Exhibition Centre. Delegates will have the opportunity to meet with the exhibitors and poster presenters in a relaxed and informal setting. There will not be an additional charge for attending this evening reception; sponsorship is welcome.

The Conference dinner will be held on Wednesday 9 April in the Galleria restaurant at a cost of £35.00 (£20.00 for concessions).

Car Parking

Those wishing to park within the University Campus must request a car parking permit on the registration form. Permits, along with joining instructions will be sent along with registration confirmations. Parking is charged at £3/day if pre-booked, and £5/day if requested at the meeting.

Email Facilities

Computer access will be available in the library at the University of York and wireless is also available in certain designated areas on campus. Logins must be purchased in advance on the registration form and are charged at £12.00 for the meeting. More details regarding the wireless network at York University can be found on the Spring Meeting website www.crystallography-meetings.org.uk

Poster Abstract Deadlines - 4th February 2008

Abstracts for poster presentations should be submitted via the website using the Word template. The deadline for submissions is Monday the 4th of February 2008.

In 2008 we will be also be introducing "graphical posters" which will be projected on screens in the exhibition area during the meeting. These should contain the title of your poster, a striking graphic and a few words which advertise the main highlights of the work. Don't try and cram in all the information on the poster itself; keep

font sizes at >20 point! If you'd like your poster highlighted in this way please send a single PowerPoint slide to ivana.radosavljevic@durham.ac.uk at the time of registration. Please adjust picture resolution so that the file size is less than 0.5 Mb.

For printing reasons the abstract length is limited to 500 words and must be prepared using the conference template. In single space Arial 10 point this is around half an A4 page. If you wish to include black and white figures they should be inserted into the document and the text length reduced accordingly.

The abstract template and the submission form and the template are available at:

www.crystallography-meetings.org.uk/abstracts.htm

BCA Bursaries

A limited number of bursaries are available from the Arnold Beevers bursary Fund to cover the cost of registration, two nights **standard** accommodation, lunches from Tuesday 8 - Thursday 10 April, evening buffet on Tuesday 8 and the Conference dinner on Wednesday 9 April. The bursary will not cover travel expenses and recipients will be expected to present a poster and produce a report on part of the meeting.

Council is again seeking commercial sponsors of Spring Meeting Bursaries at £250.00 per student and it is hoped that some Named Bursaries will be awarded at this meeting.

Individual BCA members may also wish to give a living legacy by sponsoring their own named student bursary. All sponsors will receive a certificate of appreciation and be acknowledged in the annual bursary report.

The closing date for all applications is Friday 4th February 2008. Only on-line applications via the BCA website: www.crystallography.org.uk will be accepted.

Insight into York

York is a historic walled city in North Yorkshire, England. The city was founded in AD 71 and became in turn the capital of a Roman province and of the kingdoms of Northumbria and Jorvik. After the establishment of the Kingdom of England, York was regarded as the capital of the North, and housed the Council of the North. York is also the traditional county town of Yorkshire, to which it lends its name.

Traditionally the term *City of York* was used for the area within the city walls but the modern City of York, created on April 1, 1996, is a much larger unitary authority that includes several neighbouring parishes which formerly belonged to surrounding districts. The York urban area has a population of 137,505 while the entire unitary authority has a population of 184,900.



The historic core of the city is a major tourist destination in itself, attracting visitors from both the United Kingdom and overseas. York is also the site of several major tourist attractions, including York Minster, York Castle Museum, and the National Railway Museum

By Road

You can get to York quickly from the UK motorway network. Travelling north on the M1 or A1 you'll come to the A64 intersection. The city is 15 minutes away via dual carriageway. Travelling south on the A1, you'll also leave the motorway at the A64. From the west on the M62, join the M1 northbound until you reach the intersection with the A64. York is also served by the A19, A1079 and A166 routes into the city. Frequent Park & Ride bus services operate into the city centre from sites adjacent to the A64, A19, A1079 and A166.

By coach and rail

You can travel to York from destinations all around the UK. Fares and timetables are available on the National Express

and National Rail websites www.nationalexpress.com and www.nationalrail.co.uk

Web-Link for directions:

York: www.york.gov.uk/visiting

York University: www.york.ac.uk/

Travel to York: www.york.ac.uk/np/maps/

Spring Meeting Exhibitors Forum

Because of the continuing success of the Exhibitors Forum, presentation slots will be allocated on a strictly first come first served basis. However, those companies that select a 5 x 3 exhibition stand will automatically receive a dedicated slot on Tuesday 8 April prior to the exhibition and poster buffet. The forum will provide each exhibitor with the opportunity to present their latest developments and encourage participants along to their stands in the Commercial Exhibition.

To register your interest in presenting, please contact **David Massey** at the BCA Administrative Office, **01355 244966** or email bca@glasconf.demon.co.uk

Scientific Programme - “Structure, Property & Function”

Plenary Lectures

BSG Plenary and BCA Prize Lecture:

Tony Crowther (MRC LMB Cambridge) *From Molecular Replacement to the Structure of Viruses: a Tale of Two Careers*

PCG Plenary: Paul Attfield (Edinburgh) *Charge Order in Oxides - Putting the Fun into Functional Materials*

IG Plenary: Rob Delhez (Delft) *X-ray Diffraction on Mars?*

CCG Teaching Plenary - Controlling Difficult

Refinements: Peter Muller (MIT) *Dead End Highway 13 - the Carriage of No Return*



Description of Sessions and Confirmed Speakers

Local Structure and Disorder in Crystalline Materials

This session will focus on total scattering methods which aim to obtain information on both long and short range order. For many functional materials structural knowledge on a range of length scales is vital for understanding their properties.

Thomas Proffen (Los Alamos Neutron Science Center) *Total Scattering: the Key to Understanding the Local- and Medium-Range Structure of Materials*

Sharon Ashbrook (St Andrews) *Investigating Local Structure and Disorder by MAS NMR*

Simon Hibble (Reading) *Not So Simple: The Structures and Dynamics of Simple Transition-Metal Cyanides from Total Diffraction*

Alex Hannon (ISIS) *Polyhedral Distortion in Glasses and Crystals*

Crystal Chemistry of Functional Extended Solids

Properties of solid state materials and their functionalities are inherently related to their crystal structures. This session

Symposium Title	Chairperson	Contact
<i>Local Structure and Disorder in Crystalline Materials</i>	Matt Tucker	m.g.tucker@rl.ac.uk
<i>Crystal Chemistry of Functional Extended Solids</i>	Ivana Evans	ivana.radosavljevic@dur.ac.uk
<i>Functional Molecular Materials I</i>	Andrew Bond	adb@ifk.sdu.dk
<i>Functional Molecular Materials II</i>	Serena Margadonna	serena.margadonna@ed.ac.uk
<i>Strongly Correlated Electron Systems I</i>	Paolo Radaelli	p.g.radaelli@rl.ac.uk
<i>Strongly Correlated Electron Systems II</i>	Peter Hatton	p.d.hatton@durham.ac.uk
<i>Calculating Properties from Structure</i>	Simon Coles	s.j.coles@soton.ac.uk
<i>Design of Functional Materials</i>	Neil Champness	neil.champness@nottingham.ac.uk
<i>Structures from Pharmaceutical Powders</i>	Kenneth Shankland	k.shankland@rl.ac.uk
<i>Jekyll and Hydrate</i>	Roy Copley	royston.c.copley@gsk.com
<i>Applied Crystallography Showcase</i>	Chris Staddon	chris.staddon@nottingham.ac.uk
<i>Small Is Smart</i>	Judith Shackleton	judith.shackleton@manchester.ac.uk
<i>Big Is Beautiful</i>	Judith Shackleton	judith.shackleton@manchester.ac.uk
<i>Membrane Proteins I</i>	Neil Isaacs	n.isaacs@chem.gla.ac.uk
<i>Membrane Proteins II</i>	Neil Isaacs	n.isaacs@chem.gla.ac.uk
<i>Neutrons in Biology</i>	Garry McIntyre	mcintyre@ill.fr
<i>Probing Fast Biological Reactions</i>	David Leys	david.leys@manchester.ac.uk
<i>Complementary Methods in Structural Biology</i>	Helen Saibil	h.saibil@mail.cryst.bbk.ac.uk
<i>Ligand Binding and Drug Design I</i>	Rod Hubbard	rod@ysbl.york.ac.uk
<i>Ligand Binding and Drug Design II</i>	Rod Hubbard	rod@ysbl.york.ac.uk

will highlight examples of structure-property relationship studies in extended solids, such as inorganic oxides and chalcogenides.

Peter Slater (Surrey) *Relationship between Structure and Conductivity in New Ionic Conductors*

Edmund Cussen (Strathclyde) *Switching on Fast Lithium Ion Conductivity: Structure and Transport Properties of the Garnet Structure*

Ian Reaney (Sheffield) *Crystal Chemistry of Dielectric Ceramics*

Functional Molecular Materials I & II

The field of molecule-based materials has seen a very rapid progress since the discovery of compounds with a variety of technologically important properties such as conductivity, superconductivity and ferromagnetism. One of the major opportunities offered by this area is the possibility of designing building blocks which combine properties allowing the preparation of multifunctional materials. This session will focus on the new discoveries and achievements in the field.

Kosmas Prassides (Durham) *Fullerene Superconductivity: Are There Any Surprises Left?*

Darren Bradshaw (Liverpool) *Pressure-Dependent Hysteretic Sorption Behaviour in a Flexible Metal-Organic Framework*

Alessandro Prescimone (Edinburgh) *High Pressure And Magneto-Structural Correlations in Single Molecule Magnets*

Jeremy Rawson (Cambridge) *Sulfur-Nitrogen Radicals: Systematic Design of Spin-Transition Materials*

Peter Skabara (Strathclyde) *Controlling the Conformation of Conjugated Molecules through Non-Covalent Interactions*

Guillermo Mínguez Espallargas (Sheffield) *Non-Porous Materials Can Also Take Up Gases*

Strongly Correlated Electron Systems I & II

Strongly correlated systems where changes in structural properties are intimately linked with changes in electronic and/or magnetic properties remain an extremely topical area in condensed matter physics. These sessions will cover various aspects of this field such as multiferroics, materials displaying charge ordering, materials with electronic and/or magnetic phase transitions and GMR materials.

Radu Coldea (Bristol) *Charge Order to Remove Orbital Degeneracy in Triangular Antiferromagnet AgNiO_2*

Claudio Mazzoli (ESRF) *New Magnetic Spin State Evidenced by RXS in a Frustrated Spin System*

Alan Tennant (Hahn-Meitner Institut) *Title TBA*

Jon Goff (Royal Holloway) *Title TBA*

Neil Mathur (Cambridge) *Limited Local Electron-Lattice Coupling in Manganites*

Calculating Properties from Structure

This session will demonstrate the wide diversity in current approaches to the derivation of physical properties from crystal structure. Talks will be presented from the areas of computational drug delivery, chemoinformatics, charge density determination and solid state quantum chemistry.

John Mitchell (Cambridge) *Informed by Informatics?*

Amshed Anwar (Bradford) *Phase Transition Phenomena from Molecular Simulation*

Chick Wilson (Glasgow) *Computing the Solid State: Complementing Experiment with Plane-Wave DFT Approaches to Understanding Hydrogen Bonding and Associated Physical Effects*

Michael Probert (Durham) *Electrostatic Molecular Properties of Non Steroidal Anti-Inflammatory Drugs from Studies of Their Charge Density Distributions*

Design of Functional Materials

In keeping with the structure, property, function theme of the meeting, this session will contain talks on the topic of material design (crystal engineering) and its application to obtain materials with desired properties.

Martin Schroder (Nottingham) *Metal-Organic Framework Materials: Porosity and Storage*

Stuart James (Belfast) *Solvent-Free Synthesis and Some 'Design' Aspects of Metal-Organic Frameworks*

Structures from Pharmaceutical Powders

This session will present some applied examples of structure determination of molecular materials by powder diffraction. Practical methods, common problems and software tools will be exemplified in talks by users of this technique.

Matthew Johnson (GSK) *Pharmaceutical Crystal Structures from Powder Diffraction Data*

Alastair Florence (Strathclyde) *Title TBA*

Vincent Favre-Nicolin (CEA) *FOX: Structure Determination from Powder Diffraction*

Jekyll and Hydrate

Hydrated solid-state forms are commonly found in the pharmaceutical industry and their discovery can be both a benefit and a hindrance. This session will concentrate on the characterisation, properties and behaviour of hydrates.

G rard Coquerel (Rouen) *The Different Roles of Water Molecules in Chiral Discrimination in the Solid State*

Alan Kennedy (Strathclyde) *Mony a Meickel Maks a Muckel: Systematic Investigations of Crystal Structures of Organic Salt Hydrates*

Applied Crystallography Showcase

A range of talks will be presented from all areas of the BCA describing how X-rays are used in commercial/industrial applications. The speakers will be asked to give a tutorial like overview of their work for a non specialized audience.

Alison Burke (Huntsman Pigments) *Application of XRD within the Pigments Industry*

Judit Debreczeni (AstraZeneca) *Protein Structures in Drug Discovery*

Ashley Hulme (Pharmorphix Limited) *Application of XRD and other Analytical Techniques to Pharmaceuticals*

Mark Farnworth (Pilkington Group Ltd) *Application of XRD within the Glass Industry Including 2D Mapping*

Small Is Smart

Sub-micron crystallites can present peculiar challenges to X-ray powder diffraction, as the crystallite size decreases the reflections broaden and can become difficult to detect. However, nanotechnology is an area of great interest to both industry and academia. X-ray diffraction can give a useful insight into the structure and subsequent behaviour of these novel materials. In this session we will look at these challenges, how they can be overcome and what type of information can be obtained.

Steve Norval (Intertek MSG) *Powder Diffraction of Nanomaterials*

Big Is Beautiful

Large objects can be just as much of a challenge to diffractionists as very small crystallites. Do you take the sample to the diffractometer, or the diffractometer to the sample? In either case, how do you get an accurate diffraction pattern? There may also be problems with the microstructure, for example large grains or preferred orientation. This session will focus on samples which are inconvenient to handle, usually through their size, shape or micro structure.

Membrane Proteins I & II

Karen McLuskey (Glasgow) *High Throughput Methods*

Liz Carpenter (Imperial & Diamond) *The Membrane Protein Laboratory at Diamond*

Kaspar Locher (Zurich) *Structure and Mechanism of ATP-Binding Cassette (ABC) Transporter Proteins*

Thomas Sorenson (Diamond) *Ca-ATPase and Na,K-ATP Structures*

Neutrons in Biology

The recent upgrade at the ILL of LADI-I to LADI-III gave a three- to five-fold gain in detection efficiency, to extend the range of biological problems that can be tackled by neutron diffraction. There is also the promise of a dedicated biological diffractometer, LMX, at target station II at ISIS. This session will outline the new instrumental capabilities and limitations for biological neutron diffraction, present some recent highlights, and explore the problems that we might consider with the new instruments.

John Helliwell (Manchester) *The Determination of Protonation States in Proteins*

Matthew Blakeley (ILL) *TBA*

Probing Fast Biological Reactions

This session will focus on time resolved crystallography, reaction intermediate trapping and other emergent techniques as a means of probing fast biological reactions.

Dominique Bourgeois (ESRF/IBS) *Title TBA*

Arwen Pearson (Leeds) *Title TBA*

Ylva Lindqvist (Karolinska Institut) *Title TBA*

BCA 2008 Spring Meeting -

	Monday, 7th April		Tuesday, 8th April						
9:00			YC 4	PDF workshop					
9:15									
9:30									
9:45									
10:00									
10:15									
10:30			Registration/exhibition 10.30-11.30						
10:45									
11:00			BSG Plenary 11.30-12.30 From Molecular Replacement to the Structure of Viruses: a Tale of Two Careers						
11:15									
11:30									
11:45									
12:00									
12:15									
12:30			Lunch/Exhibition/Registration 12.30-13.30						
12:45									
13:00	YC 1	PDF workshop	Sessions 13.30-15.00						
13:15									
13:30				Local structure	Membrane proteins	Pharmaceutical powder diffraction			
13:45									
14:00									
14:15									
14:30									
14:45									
15:00	Coffee 15.00-15.30		Coffee 15.00-15.30						
15:15									
15:30	YC 2	PDF workshop	Sessions 15.30-17.00						
15:45				CCG Prize	Membrane proteins	Hydration of pharmaceutical materials			
16:00				PCG Prize					
16:15									
16:30									
16:45									
17:00	Break	Break	Break 15 minutes						
17:15									
17:30	YC 3	PDF workshop	Exhibitors Forum 17.15-18.45		DASH workshop				
17:45									
18:00									
18:15									
18:30									
18:45	Break	Break							
19:00	YC dinner	Dinner	Dinner, exhibition and posters						
19:15									
19:30									
19:45									
20:00									
20:15									
20:30									
20:45									
21:00									

Timetable

Wednesday, 9th April			Thursday, 10th April		
PCG Plenary 9.00-9.45 Charge Order in Oxides: Putting the Fun into Functional Materials			Teaching Plenary 9.00-9.45 Controlling Difficult Refinements		
Coffee 9.45-10.15			Coffee 9.45-10.15		
Parallel sessions 10.15-11.45			Sessions 10.15-11.45		
Functional extended solids	Neutrons in biology	Applied crystallography	Strongly correlated systems	Ligand binding and drug design	Design of functional materials
PCG AGM 11.45-12.30	BSG AGM 11.45-12.30	IG AGM 11.45-12.30	Break 15 minutes		
Lunch, Exhibition 11.45-13.30			Sessions 12.00-13.30		
		CCG AGM 12.45-13.30	Strongly correlated systems	Ligand binding and drug design	Calculating properties from structure
Sessions 13.30-15.00			Close 13.30		
Functional molecular materials	Probing fast biological reactions	Small is smart			
Coffee 15.00-15.30					
Sessions 15.30-17.00					
Functional molecular materials	Complementary methods in structural biology	Big is beautiful			
Break 15 minutes					
IG Plenary 17.15-18.00 IG: X-Ray Diffraction on Mars					
BCA AGM 18.00-19.00					
Comfort time					
Conference dinner 19.30 for 20.00					

Complementary Methods in Structural Biology

Justin Benesch (Cambridge) *Mass Spectrometry for Functional Genomics? Structure and Dynamics of the Small Heat Shock Proteins*

John Christodoulou (Cambridge) *Structure and Dynamics of Ribosome-Bound Nascent Chains by NMR Spectroscopy*

Helen Saibil (Birkbeck) *Understanding Molecular Machines by Combining Cryo EM and Crystallography*

Ligand Binding and Drug Design I & II

There has been much excitement in recent years in using high throughput crystallography in drug discovery, both in identifying new hit compounds (virtual screening and fragment-based discovery) and in structure-guided drug design. However, even with such large datasets of structures, we are still fairly poor at predicting the strength of protein-ligand interactions. As well as helping predictive drug discovery, an improved understanding of the thermodynamics and kinetics of these interactions would enrich our appreciation of molecular recognition events. These sessions will explore how the recent explosion in the use of high throughput crystal structures has been linked to various biophysical and modelling approaches and how these have informed our views on ligand binding.

Nicolas Foloppe (Vernalis R&D Ltd) *Exploiting Crystal Structures for Ligand Discovery and Design*

Tom Davies (Astex Therapeutics) *Fragments, Structures and Drug Discovery*

Chris Phillips (Pfizer) *HIV-1 Reverse Transcriptase: Crystals to Clinic*

Matthew Higgins (Cambridge) *The Structure of a Chondroitin Sulphate: A Binding Domain in Placental Malaria*

Stephen Curry (Imperial) *Crystallographic Analysis of Metabolite and Drug Binding to Human Serum Albumin*

Workshops

PDF Workshop: Shedding Light on the Local Structure and Disorder in Crystalline Materials

Organisers: **Matt Tucker** (ISIS) & **Ivana Evans** (Durham)

Matt Tucker (ISIS) and **Thomas Proffen** (LANSCE) will run a full day hands-on PDF workshop. The importance of local structure and disorder in crystalline materials is increasingly

being recognised as a key property of many functional materials. From negative thermal expansion to solid state amorphisation and the 'nanoscale' problem to improved fuel cell technology, a clear picture of the local atomic structure is essential to understanding these phenomena and solving the associated problems. A powerful technique for exploring the local structure of materials is total scattering, also known as the PDF method. Synchrotron X-ray and/or neutron powder diffraction data can be used to obtain information on the local, medium and long range atomic structure simultaneously. To gain the maximum information from the data, specialised refinement methods are required. Two of the most powerful methods currently available for refining this type of data are RMCProfile and PDFFIT. The aim of this workshop is to provide an overview of the methods and the opportunity to gain some hands-on experience of applying them to total scattering data. No previous experience is required. For more information about the PDF workshop please email Matt Tucker (m.g.tucker@rl.ac.uk) or Ivana Evans (ivana.radosavljevic@durham.ac.uk).

DASH Workshop

Organisers: **Richard Cooper** (Oxray) & **Kenneth Shankland** (ISIS)

Kenneth Shankland will be running a hands-on workshop in the computing lab, using the DASH software. DASH is a program for crystal structure determination from powder diffraction data. This workshop is aimed at students and researchers who have no previous experience using DASH and who are interested in structure determination from powders. For more information please email **Richard Cooper** (richard.cooper@oxray.com) or contact **Kenneth Shankland**.

Olex2 Workshop

Organisers: **Horst Puschmann** and **Oleg Dolomanov** (Durham)

Immediately following the main BCA Spring Meeting, an Olex2 Workshop will be held on the afternoon of Thursday 10th April, 2008. Olex2 is free software which is developed in collaboration between Oxford and Durham Universities. It is aimed at making working with molecular crystal structures easy and intuitive while giving experienced crystallographers access to powerful new modelling and refinement tools (www.olex2.org).

The workshop is suitable for crystallographers of all levels of experience. For further information and registration, please contact us at horst.puschmann@durham.ac.uk.

Young Crystallographers at York: 7-8 April 2007

FOLLOWING the great successes of the last two years, the YC2008 meeting in York will be the place for Young Crystallographers to meet each other and discuss research in a relaxed and friendly environment. Please take a look at the general information section for details on how to apply for a Bursary (the main thing to remember is that the deadline is 4 February 2008, and that you must present a poster or a talk to be eligible!). Remember, right up until 11th January 2008, you can still contribute an abstract to be considered for giving a short presentation at the Young Crystallographers meeting by visiting the YCG website at www.chem.gla.ac.uk/yc/

The programme at the time of going to press is as follows - more information will be available on the website as soon as the session speakers are confirmed. There will be four sessions; sessions 1-3 are in the afternoon of 7 April and session 4 on the morning of 8 April.

YC1 Plenary (Biological)

Ehmke Pohl (Durham) *Why is Macromolecular Crystallization so Difficult*, and why do we still obtain Suitable Crystals?

YC2 Plenary (Chemical / Physical)

David Allan (Diamond) *Beamline I19: A Facility for Small-Molecule Single-Crystal Diffraction at Diamond*

YC3

2 minute poster adverts

YC4 Plenary (Industrial)

David Beveridge (HARMAN technology Ltd.) *Crystals, Grots and X-rays'*

See you there!

Simon Coles

(on behalf of the YCG committee)

Membership Subscriptions Introducing On-Line Payments

I am delighted to announce that we can now pay membership subscriptions by card on-line via the secure membership subscription page on:

www.crystallography-meetings.org.uk/membership.php

The office will continue to accept forms and card details by post for those who do not wish to pay on-line, but we hope that many of you will find this new facility useful.

Sheila Gould
Hon. Treasurer



THE BRITISH CRYSTALLOGRAPHIC ASSOCIATION
BCA Membership Form 2008

Personal Details

First Name: _____ Surname: _____
Address 1: _____
Address 2: _____
City: _____ Post code: _____
Email: _____

Membership Fee

Category	1st Year	2nd Year	3rd Year	4th Year
Student (BCA Member)	£ 20.00	£ 20.00	£ 20.00	£ 20.00
Young (BCA Member)	£ 10.00	£ 10.00	£ 10.00	£ 10.00
New (BCA Member)	£ 20.00	£ 20.00	£ 20.00	£ 20.00
Life (BCA Member)	£ 1000.00	£ 1000.00	£ 1000.00	£ 1000.00
Corporate Member of an industrial/Commercial/Service industry Group	£ 1000.00	£ 1000.00	£ 1000.00	£ 1000.00
Student (non-BCA)	£ 10.00	£ 10.00	£ 10.00	£ 10.00
Young (non-BCA)	£ 5.00	£ 5.00	£ 5.00	£ 5.00
Life (non-BCA)	£ 1000.00	£ 1000.00	£ 1000.00	£ 1000.00

CRYSTALS NEWS

www.xtl.ox.ac.uk/

THERE are no plans to carry out any further substantial developments to CRYSTALS in Oxford because our major research effort is now aimed at extending the smtbx (Small Molecule Tool Box) to sit alongside the cctbx as our contribution to the Age Concern project. This work involves taking the best ideas from CRYSTALS, other programs and the literature and re-casting them into a modern C++ based framework to provide the engine for a new generation of applications.

Maintenance work will however continue for several more years, and we continue to respond to comments, criticisms and advice. **Mark Light** (Southampton) reports that CRYSTALS runs satisfactorily under Microsoft Vista - I have not had the courage to migrate there yet. Since Richard Cooper left Oxford there has been little prospect of further development here of a LINUX version. However, Pascal Parois in Glasgow has made substantial progress and seems happy to share his experience with others.

The principal changes in the current version are:

adp principal axes

Compute some additional statistics in #AXES.

hydrogen atoms

New menu item in the Guide to refine hydrogen atoms at any time subject to slack restraints. After optimisation in this way, the hydrogens can just 'ride' on their parent atom. This method works well with modern CCD data. Automatic systematic re-numbering of hydrogen atoms. Useful if some hydrogens have been found in difference maps.

Further tune sp³ hydrogen detection.

Improved *cif* file and hydrogen bond generation. Support for multi-structure *cif* files.

restraints

Restraints similar to the SHELXL SAME, DELU, & SIMU added.

refinement

Adaptive shift reduction for the control of run-away refinements.

CAMERON

Automatic saving of archive file after writing a postscript image. This enables the image to be opened and edited at a later date.

external links

Arie van der Lee has provided the FORTRAN code needed to create input files for Superflip (Palatinus L., Chapuis G.) and EDML (Sander van Smaalen). The authors of these programs have kindly agreed to us including them in the CRYSTALS distribution kit. They provide a competitive alternative to Direct Methods, especially when there are uncertainties about the composition or space group. For more details visit <http://superspace.epfl.ch/superflip/>. CRYSTALS menu items have been added to assist in post-processing of the Superflip/EDML output, including piping the results into SIR for further development by tangent refinement and least squares. These applications are being developed at a number of sites, so that a special pre-release of CRYSTALS with the latest changes is also available from the website. Use with caution.

Also in the Beta test version: Help in interpreting the CRYSTALS Analyse features.

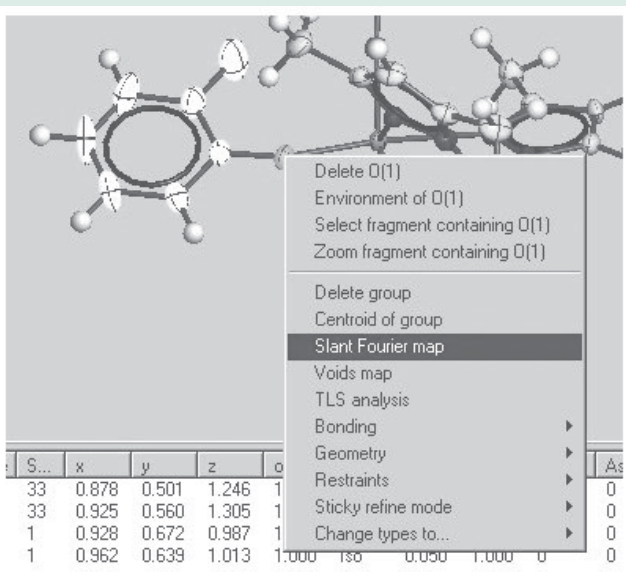
David Watkin

Graphics Window

Highlighted atoms + Slant Fourier

This computes the best plane through the selected atoms and then the electron density (or difference density) in sections parallel to the plane. You will probably need to raise the number of sections from the default (2) in order to obtain a thicker slab of the structure. Michael Husaks MCE viewer lets you examine the density.

This is a really useful utility for



News from the Groups



RSC Solid State Chemistry Group Christmas Meeting

THE 2007 RSC Solid State Group Christmas Meeting will be held in the Department of Chemistry and at Trevelyan College, Durham University on Monday 17th and Tuesday 18th December. The meeting will start after lunch on Monday afternoon and run until lunchtime on Tuesday.

There's a great line up of plenary speakers in place, including:

Gustaaf van Tendeloo, University of Antwerp

Dr Mark Wilson, UCL/Oxford

Prof Tony Cheetham, Santa Barbara/Cambridge

Prof John Irvine, University of St Andrews

Registration and abstract submission are now available on line via the conference website at:

www.dur.ac.uk/john.evans/webpages/ssg_xmas_2007

Contact john.evans@durham.ac.uk or ivana.radosavljevic@durham.ac.uk for more information.

We look forward to seeing you in Durham!

PCG Winter Meeting 2007

THE PCG Winter Meeting will take place on 17 January 2008, at the Cosener's House in Abingdon. The meeting will be held in conjunction with the PCG-SCMP Magnetic Rietveld workshop and will be entitled "*Novel Instrumentation and Methods for Magnetic Structure Determination*". If you will not be attending the Magnetic Rietveld workshop and would like to register for the day of the PCG winter meeting only, please contact the organisers:

Dr. Laurent C. Chapon (L.C.Chapon@rl.ac.uk)

Dr. A. Daoud-Aladine (A.Daoud-Aladine@rl.ac.uk)

Dr. Carlo Vecchini (C.Vecchini@rl.ac.uk)

The meeting will feature student presentations and four invited speakers.

9.00-10.30: *Clipboard session and student presentations*

10.30-11.00: *Coffee break*

11.00-11.45 *Jane Brown (ILL)*

11.45-12.30: *Alessandro Bombardi (Diamond)*

12.30-14.00: *Lunch*

14.00-14.45: *Oleg Petrenko (Warwick)*

14.45-15.30: *Tom Fennel (UCL)*

15.30-16.00: *Discussion and closing*

Full programme will be advertised nearer the time on the PCG-SCMP wiki at:

www.pcg-scmp.org

PCG-SCMP Powder Diffraction & Rietveld Refinement School 2008

THE PCG-SCMP (Physical Crystallography Group of the British Crystallographic Association/Structural Condensed Matter Physics group of the Institute of Physics) will be holding a 4 day powder diffraction and Rietveld refinement school at the University of Durham from 30th March - 3rd April 2008.

This EPSRC and IUCr sponsored teaching school will be run along similar lines to the January 2007 course, with a combination of lectures covering the theoretical aspects of powder diffraction and Rietveld refinement, supported by small group tutorials and extensive hands-on practical sessions using a variety of modern software packages. Examples and tutorials will cover both extended and molecular systems. Lectures will be given by Prof. **John Evans**, Dr. **Ivana Evans**, Dr. **Jeremy Cockroft** and Prof. **Andy Fitch**.

You'll have ample opportunity to interact with expert lecturers and tutors!



BSG Winter Meeting

DETAILS of the BCA BSG Winter Meeting 2007 are now available on www.bmsg.ulsop.ac.uk/BCA/index, or from the BSG website: <http://img.cryst.bbk.ac.uk/bca/bsg/welcome>

The one-day meeting will be held on the 18th December at The School of Pharmacy in London. General theme of the meeting is 'Structural Investigations of Gene Regulation' in the broadest sense. The programme is now nearly complete although we still have places for two short (10 min) talks. We strongly encourage students and post-docs to participate. Please visit the web site and register.

Registration fee of £50 includes BCA membership and it can be paid on the day of the meeting, However we need you to register ahead of the meeting so that we can provide adequate catering.

Looking forward to seeing you in December.

Snezana Djordjevic & Gary Parkinson

Topics to be covered will include:

- Basic introduction to space group symmetry and International Tables as required for powder diffraction work
- Fundamentals of powder diffraction
- Data collection strategies for X-ray and neutron diffraction
- Constant wavelength and time of flight diffraction
- Indexing powder patterns
- Le Bail and Pawley fitting methods
- Rietveld refinement method
- Important Rietveld packages and their distinct features and strengths
- Restrained refinements
- Rigid body refinements
- Combined X-ray and neutron combined Rietveld refinements
- Introduction to structure solution
- Peak shapes: analytical and fundamental parameters approaches

Online applications will be accepted from late 2007 at the School website:

www.dur.ac.uk/john.evans/webpages/pcg_rietveld_school_2008

John and Ivana Evans

XD2006 Workshop on Advanced Methods in X-ray Charge Density Analysis



IN September 2007, some sixty users of the XD2006 refinement package assembled in the picturesque town of Martina Franca in the south west of Italy to attend a 5 day

workshop. It covered advanced methods in evaluating X-ray Charge density with a view to extracting properties from a "Multipole" refinement and additional applications for the software.

Delegates comprised both senior and junior researchers from all around the world including the United States, China, India and Europe. Everyone had come to acquire and ultimately deliver to their respective institutions the most up to date information available about this growing and improving field of high-resolution X-ray diffraction techniques.

Topics covered in the morning lectures ranged from the basic use and applications of the program, led by **Piero Macchi**, to the description of the complex algorithms required for this type of modelling, which was led by **Tibor Koritsanszky** and **Philip Coppens**. The afternoon sessions offered a more hands-on approach

with live tutorials and demonstrations. This was a great opportunity for delegates to talk personally to the developers of the software and ascertain the correct way to use it in order to achieve the best possible model.

Wolfgang Scherer and his group delivered an insightful lecture on the topological studies of structures, which revealed interesting analogies between the chemical world and the real world. Comparisons were drawn between contour maps used to show areas of high electron density and those used by hill walkers.

The final day of the conference was equally as interesting as the first; with more questions from delegates as this was the last opportunity to seek advice from the experts. **Carlo Gatti** discussed the quantum theory of atoms in molecules and **Jacob Overgaard** from the University of Aarhus explained the importance of using neutron data in addition to X-ray data in order to get a comprehensive picture of the structure by showing precisely the location of Hydrogen atoms.

Networking and social opportunities were not overlooked and on the penultimate evening we were treated to a truly memorable dinner with wonderful traditional Italian food, fine wine and good music. I would like to take this opportunity to thank the BCA for providing the financial support that enabled me to participate in this very valuable and informative programme. I would also like to thank the XD group for all their organisation and arrangements that have made this event so relevant and helpful to my work.

Peter J Byrne
University of St. Andrews

ECM24 - A Student View

THIS years ECM was held at the Palais des Congres in the city of Marrakech in Morocco. In order to get to Marrakech I had to fly from Glasgow to London and then from London to Marrakech via Casablanca. While waiting to board the flight at Heathrow, I was looking about to see if I could spot any other crystallographers, and the abundance of poster tubes and sandals worn with socks made it easy to spot many of them!

The conference started with the usual opening speeches from **Abdelmalek Thalal** the Chairperson of the ECM24, **John Richard Helliwell** the president of the ECM and **Yoji Ohashi** the president of the IUCr. Normally the opening ceremonies can be quite dull affairs with one speech after another, but this year's ceremony was anything but boring. After each speech we were treated to an exhibition of traditional Moroccan music and dancing, and, much to my surprise, the music was excellent and the dancing was both energetic and skillful.

After the opening ceremony, we were all invited to the welcome reception that was held beside the pool of the Mansour Eddahbi Hotel, adjacent to the Congress Centre. This was the perfect setting for a reception, with palm trees surrounding the beautifully lit pool and plenty of free food and drink for all the delegates. The reception provided the perfect opportunity for delegates to catch up with old friends and make new ones. The fact that the temperature was still in the high 20's and the drink was free and plentiful certainly helped to make it a very enjoyable evening and ensured that there were a few sore heads on the first day of the conference.

The first lecture that I attended was the opening keynote given by **Vaclav Petricek**, entitled *Software for the refinement of aperiodic and incommensurate structures*. I was looking forward to this lecture but it was disappointing, because of its venue. The lecture was held in Fez 1, which is a long narrow room, which, because of the popularity of the lecture, was nearly full. This was hugely disappointing for the all of the people in the back third of the lecture theatre, who could neither see the slides nor hear the speaker.

The Thursday morning microsymposium that I attended was *Mineralogical Crystallography* and contained two 30-minute talks and three 20-minute talks. This same format was adopted by all of the other microsymposia at the conference. The opening talk, *Crystal structure of nanocrystalline manganese oxides*, was given by **Bruno Lanson** from the Joseph Fourier University. In this talk he discussed the importance of birnessite, a phyllosulfate, and its interactions with environmental pollutants such as

organics and heavy metals. He showed that in spite of the many structural defects present in these systems, the structure could be determined by calculating the XRD patterns using the mathematical formalisms derived by Drits & Tchoubar. He then went on to demonstrate the usefulness of this approach using various synthetic and natural birnessite examples.

At most conferences, you find that there is at least one session where none of the microsymposia appeal to you and you are left with the choice of going to a session that you are not particularly interested in or going to the pub. At this year's ECM, I had such a choice, and luckily chose to go *Empirical evaluation of bond strength in inorganic structures*, rather than to the pub. I know that this may not sound like the smartest thing I have ever done, but there were a couple of talks at the microsymposia that were well worth missing the pub for and which were a pleasant surprise in an otherwise long and boring afternoon. The first talk, *The basis of the bond valence Model, its strength and weaknesses* was by **I.D. Brown** of McMaster University. He started by introducing the "bond valence model", which was good, as I had never heard of it before. He described it as an exact representation of the ionic model, which gives a good empirical description of all types of polar bond, regardless of ionicity or covalency. Unlike "atoms in molecules" (Bader), where the property of the atom depends on its context, the atoms in the ionic model are invariant soft charged spheres bound together in a crystal by electrostatic forces. Each cation is linked (bonded) to its neighboring anions by electrostatic flux (lines of field) that sum around each atom to the atomic charge; the magnitude of the flux is known as the bond valence. The bond valence model appears to be in direct competition with the atoms in molecules model proposed by Bader for the description of atoms and bonds, so I was very surprised to learn that Brown works down the corridor from Bader at McMaster. The discussions after the talk were quite heated with a number of people obviously in favor of the atoms in molecules model, but Brown managed to defend the bond valence model with great vigour and his talk definitely left the audience with a lot to think about.

The next talk in the session, *Chemical bond in inorganic structures: the quantum view*, was by **Mauro Prencipe** from the University of Torino. In his talk he discussed using the Hellmann-Feynman theorem within the framework of Bader's Theory (AIM), which extends quantum mechanics to open systems, to obtain a physically consistent description of the forces acting on a nucleus. This was demonstrated by looking at simple ionic systems to determine a fully quantum mechanical view of the interactions, without the introduction of any fictitious forces. The discussions after this talk were also heated, with supporters of both models discussing their

pros and cons. While both debates were vigorous, they were at all times polite and certainly made for a very interesting session. I am afraid to say that after listening to both talks, I am none the wiser about which model is best suited for the description of atoms and bonds, but the talks have certainly encouraged me to become better informed about both models, which is hopefully the aim of these sessions.

There were many other fine talks given at the ECM conference but amongst those that stood out the most was the talk given by **Graeme Day** from the University of Cambridge, *The blind tests of crystal structure prediction, 15 years of development: where are we now?* This was a very lively and entertaining summary of the history of the blind tests and some of the drawbacks encountered with them. Graeme also gave us a sneak peak at the results of the latest blind test and while the results are encouraging, it appears that there is still a long way to go in crystal structure prediction.

Another of the stand out talks from the ECM was *From small molecules to extended structures* given by **Leonard Barbour** of the University of Stellenbosch. His talk focused on the facile assembly of complex synthetic systems, in both solution and the solid state, for the encapsulation of chemical space. He used various examples of solvents being encapsulated in these chemical spaces in single crystals, and demonstrated his group's attempts to model how the crystal structures moved to allow the passage of these solvents. He emphasized that crystal structures are dynamic systems, not rigid bodies, and can allow solvents to transfer through them. He finished by discussing some of the progress that has been made in influencing both the volume and composition of enclosed chemical space within the shells of non-covalent capsules that have been assembled by means of hydrogen bonding.

I must finish my report on the ECM conference by telling you about the excellent conference gala dinner. This was held on the final night of the conference at an old fort on the outskirts of the city of Marrakech. All of the delegates were bussed to the venue from the conference centre and were met by eight traditional Moroccan horsemen astride their horses and bearing rifles. After the horses there was a long row of women wearing traditional clothes and singing a song of welcome. From there we were guided into a massive tent, adjacent to the central court of the fort, where we were seated for our meal. The meal consisted of a traditional Moroccan salad, a roasted half lamb (which we were told must be eaten with our hands, messy but yummy), the biggest bowl of couscous I have ever seen and a large tray of traditional deserts. There was also lots of bread with each course and the drinks were free, so a good time was had by all. During the course of the meal we were treated to entertainment in the form of traditional singing and dancing next to our tables. This involved audience participation, and unfortunately that meant that I was dragged up onto the dance floor, made to lie on the floor, and had six women sit on top of me. I still do not know what this was for, or what it signified, all I know is that it was embarrassing and heavy, but fun. After the meal was finished we were invited to go outside and watch a display of horsemanship accompanied

by lots of shooting of guns. This was a spectacular display and a perfect way to finish what was a perfect evening and an excellent conference.

Stephen Cairns

Symposium Report: New Algorithms for Small Molecule Crystallography

A symposium on software development in small molecule crystallography was held on Saturday 25th August 2007 as part of the 24th ECM in Marrakech.

David Watkin started his lecture, entitled Small Molecule Computing - Where Next?, with a brief look at the history of crystallographic computing. Though low-level computing languages were used in early work, by the mid-1960s they had been displaced by higher-level languages such as ALGOL and FORTRAN. The latter has proved to be remarkably durable because of its maintainability and understandability. A number of modern software development projects have leant towards development of 'toolboxes', mostly based on C++ and scripting in PYTHON. While toolboxes enable experts to implement programming ideas rapidly, they are still as daunting for a beginner to learn as any other language. **Chris Gilmore** made the interesting point during the discussion that in some applications this trend is now being reversed, and software re-written in FORTRAN!

Programming activity in small molecule crystallography peaked in about 1985. At that time there were numerous programs available, but many of these had begun to fall out of use by the mid 1990s. This trend can be related to the problem of software maintenance, which is an on-going need, extending well beyond the life-time of a grant used to develop the software; it can account for 75% of the costs of a program. Large-scale programming projects benefit from integrated program design and a large development team, but the program systems produced are very costly to maintain. Long-lived programs, such as SHELX, have been written by a small group of programmers (in the case of SHELX, just one programmer), have a very simple input structure, and a large user-base.

The 1950s and 1960s were adventurous, heroic times in crystallographic computing. In 2007 there is a sense that if a feature is not on a GUI menu then it cannot be done. Well-designed user interfaces are essential in modern programs. The effort need to produce effective documentation rises exponentially with the size of a programming project, and discipline is needed in large projects to ensure that programmers adhere to a common data structure. What passes as 'creativity' can be a recipe for anarchy.

Lukas Palatinus discussed charge flipping, the name given to an algorithm by Oszlányi and Sütó which has been shown to be an alternative to direct and Patterson methods for the

solution of small molecule crystal structures. The procedure starts by first assigning random phases to observed structure factors, and then calculating a Fourier map. Any electron density below a threshold (δ) is inverted (charge flipping), and the phases recalculated and combined with the observed structure factor magnitudes. The procedure then iterates: a new electron density map is calculated, the charge flipped, new phases calculated, and then Fourier transformed to a new map. Cycling yields a solved crystal structure. A number of programs are available for charge flipping; these are SUPERFLIP (Palatinus), FLIPPER (Spek, incorporated into PLATON), TOPAS (Coelho) and RUBY (MDI-Products). Charge flipping has proved to be especially valuable for incommensurate structures, but this talk focussed on how charge flipping can solve problems of unknown composition, unknown symmetry and pseudosymmetry.

The basis of charge flipping, as applied to X-ray data, is that the electron density should be positive and contain extended plateaux of zero density. In most implementations it works with $|F|$ rather than $|E|$ and so no assumptions need to be made about chemical composition. Charge flipping also makes no assumptions about symmetry, and solutions are obtained in P1. In some implementations (e.g. FLIPPER) the space group symmetry is derived automatically from the electron density. In SUPERFLIP figures of merit for possible symmetry elements are calculated, and can be assessed by the user. The advantage of this method is that pseudosymmetry shows up clearly in the figures of merit.

Charge flipping has recently been applied to the solution of structures from neutron data, but since scattering density can be negative, the charge is only flipped in a band between $\pm\delta$. This is called band flipping and it can also be applied to the analysis of pseudosymmetric structures. In these cases the diffraction pattern consists of a set of strong reflections representing a symmetrical sub-structure, and weaker ones which contain the information about the way the symmetrical structure has distorted. After solution of the symmetrical substructure, band flipping on the differences $F_o - F_{\text{symm}}$ shows regions of positive and negative density which reveal the way in which the symmetrical structure distorts. This is particularly useful for symmetry-determination, as it shows clearly which symmetry elements are retained and which are lost on distortion.

Oleg Dolomanov described recent work on development of the GUI for the Olex2 project, which provides an interface for the solution, refinement, manipulation and visualization of crystal structures. The code is open-source. The GUI is based on a flexible infrastructure with a modular design; it is also independent of the structural model. PYTHON scripting based on cctbx tools enables complex tasks to be accomplished, and the cctbx toolbox has been augmented with facilities for small molecule crystallographers. The modular structure of the set of libraries used by Olex2 was described in this presentation. For example the XLIB library enables manipulation of crystallographic objects such as the asymmetric unit, defining the current state of the model and providing access to geometric calculations. The GILIB library handles graphical objects. The GUI is written in HTML and has a layered

architecture; and can be modified by the user if necessary.

New software for indexing single crystal diffraction patterns was described by **Jürgen Kopf**. Until 1992, software for indexing could fail on some 10% of samples because of non-merohedral twinning; the program DIRAX solved the majority of these problems. Indexing could also be problematic with area detector data because reflection positions were less accurately determined. A method for auto-indexing of area-detector data was introduced by Steller & Rossmann in 1997, where the periodicity of the lattice was determined using fast Fourier transform. The program QTRECLAT combines the power of links with DIRAX with visual optimization of indexing data sets. The human eye is very effective at spotting patterns characteristic of lattices, and diffraction patterns can be 'cleaned-up' prior to indexing. Input to the program is via a .p4p format file familiar to users of Bruker instruments. The program is written in C++ using the Qt graphics library. It is open-source and has been tested with Linux, though it should compile and run under Windows as well.

There is substantial interest in developing a method for quantitative comparison of crystal structures. Desirable characteristics for comparison measures are that they should be based on crystal packing, applicable to very different structures, physically meaningful and unbiased. In another symposium **Rene de Gelder** had described a comparison method based on matching simulated powder diffraction patterns; in this symposium **Andy Parkin** described a method based on Hirshfeld surfaces. Spackman and co-workers have shown that Hirshfeld surfaces are a means to partition crystal structure into regions belonging to individual molecules; packing information related to distance or electronic properties can be mapped onto the surface to encode information on crystal packing. Hirshfeld surfaces can be reduced to two-dimensional 'fingerprint' plots. Crystal structures can be compared by correlating pairs of fingerprint plots, with a correlation coefficient forming the measure of similarity. The method was illustrated using the series of salts $\text{Cu(en)}_2\text{X}$ where $\text{X} = \text{SCN}^-$, SeCN^- and ClO_4^- ; the thio and selenocyanate salts are easily recognizable as being isostructural, and this similarity was shown to be reflected in the high correlation coefficient between these structures. In another example the crystal structures of naphthalene was shown to be more similar to anthracene than to benzene. Recent developments in Hirshfeld surface software map specific interactions to the fingerprint plot, and this will enable comparisons to be made of H-bonding or π -stacking networks.

Simon Parsons & Gabor Oszlányi



*From left to right:
Gabor Oszlányi,
Simon Parsons,
Andy Parkin, Lukas
Palatinus, Jürgen
Kopf, David Watkin
and Oleg Dolomanov*

Making Crystals by Design

Eds. Dario Braga and Fabrizia Greponi, University of Bologna

Wiley VCH, 2007

Price: £100.00 (hardback)

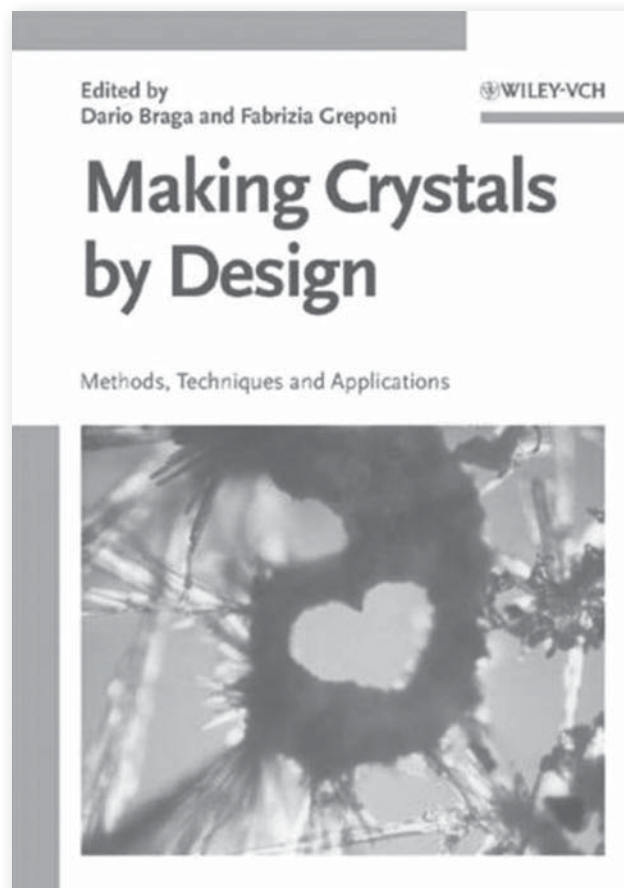
ISBN 978-3527315062, xiv + 346 pages

THIS book attempts to provide an overview of the field of crystal engineering, both as an entry point to the fundamental methods and techniques required for a successful investigation of crystalline solids, and as a snapshot of the current state-of-art. It is a book that is full of good things, with an impressive list of contributing authors and a wide-ranging subject matter attempting to capture the current climate across the field, rather than a narrow focus on one particular area. The book is divided into three sections under the general titles of **Geometry and Energetics, Design and Reactivity, and Characterisations and Applications.**

The Geometry and Energetics section contains a very good description of the various methods for calculation of properties of materials in the solid state, and notably includes an excellent summary of the PIXEL method. The second chapter collects together useful information on intermolecular interactions from other theoretical methods, and the third chapter tackles the description of networks and topological arrangements.

The Design and Reactivity section contains three chapters on various aspects of solid-state reactivity, and covers this fascinating and fashionable area in some detail. There is a particularly good description of topochemistry, as well as numerous examples of solid-state reactions and crystal-crystal transitions. This section finishes with two very good general chapters on the philosophy and approaches to making coordination frameworks and to the design, engineering and building of molecular crystals.

In the Characterisations and Applications section it is particularly pleasing to see emphasis on multiple methods of characterisation, with chapters on diffraction techniques (without focussing solely on standard single crystal methods) and solid-state NMR. The diffraction chapter includes sections on single crystal X-ray and neutron diffraction, and on the increasing use of high pressure and multiple temperature single crystal work. There is a section describing the use of powder diffraction and structure solution using powder data, and some discussion of the potential of charge density work in this area. The Solid State



NMR chapter is an excellent description of this underused technique, and the inclusion of it in a book such as this illustrates the increasing recognition of the importance of complementary methods of characterisation. Other chapters briefly mention the uses of techniques such as atomic force microscopy and IR spectroscopy in that particular area. The final two chapters of the book comprise an introduction to polymorphism, and a section on nanoporosity, gas storage and gas sensing. The book therefore finishes on an emphasis of two areas of potential industrial importance of the field.

There are, however, a few areas where the book does not fare so well. The book may be rather intimidating and unsettling to the uninitiated reader, (the time dependent Schrödinger equation makes an appearance at the top of page 2) and lacks an opening chapter giving either historical perspective, or a general review of where the field is before launching in to the descriptions of the different areas. There are a few peculiarities in chapter 1.2; some of the fine distinctions on whether or not a bond is actually a bond made in the section on a theoretical perspective on understanding the intermolecular interactions are rather

unhelpful, and confuse more than they clarify. A particular stand-out example is a short hydrogen bond between two oxalate anions that the authors tell us is not a hydrogen bond, but that might still be better included within the hydrogen bond class! It is rather frustrating to see both $\text{kJ}\cdot\text{mol}^{-1}$ and $\text{kcal}\cdot\text{mol}^{-1}$ being used in adjacent chapters, so that interconversion is constantly necessary, and I would also like to have seen an additional chapter on crystal structure prediction included in the Geometry and Energetics section.

Overall this work provides a useful handbook to those in the area, and I have thoroughly enjoyed reading it. Each chapter stands alone and explores a different area of the field. This is both a strength and a weakness; the book will provide a valuable resource to those already in the field, but may not be quite as accessible to newcomers to the area. It is not (and nor does it claim to be) an exhaustive account of work in the area, but it does give an excellent and enjoyable snapshot of the field as it currently stands.

Andy Parkin

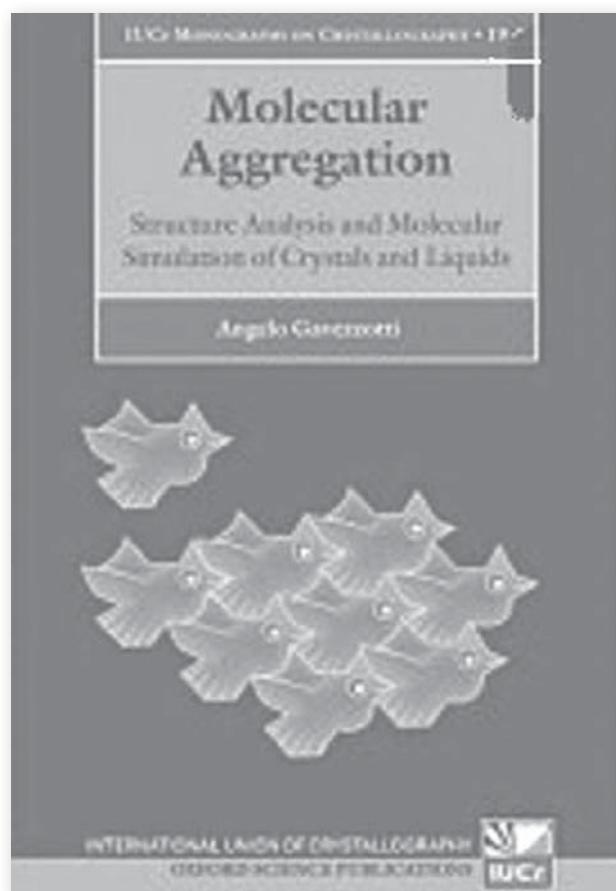
Molecular Aggregation

Angelo Gavezzotti, University of Milan

Oxford University Press, 2007

Price: £65.00 (hardback)

ISBN 0-19-857080-5, xv+425 pages



THIS is an ambitious book, which aims to cover the theoretical concepts and computational methods used to study the structure and energy of organic condensed matter at the molecular level. It succeeds in clearly describing the range of methods used by computational chemists interested in molecular materials, with insight into their development through a series of interesting historical portraits at the end of several of the chapters.

The chapters are grouped into two sections - 'Fundamentals' and 'The Frontier' - the first of which consists of ten chapters, progressing from molecular descriptors of size and shape (chapter 1) to force fields and molecular vibrations (chapter 2) and the basics of quantum mechanics, summarising some of the approximations used by quantum chemists to allow its application to molecular systems (chapter 3). These fundamentals are extended to periodic systems in chapter 6: vibrations in crystals (lattice dynamics) and the quantum mechanical treatment of the electronic structure of solids. Bridging these are chapters on the nature and modelling of intermolecular interactions (chapter 4) and crystal symmetry (chapter 5). The order and structure of these first chapters is carefully planned and the topics are covered in a clear and accessible manner. The remainder of the first section covers key thermodynamic concepts and measured values of thermodynamic quantities of molecular crystals (chapter 7), correlations in structure and energy in large sets of crystal structures taken from the Cambridge Structural Database and their calculated lattice energies (chapter 8), liquids and their modelling via molecular dynamics and Monte Carlo simulations (chapter 9) and finishes with a short chapter on computers and computer programs.

The theory and methods are often described at an intuitive level, leaving the details to more specialised texts. Nevertheless, the material is covered with sufficient depth that readers new to these topics should be able to comfortably move on to reading modern research papers. The first chapters also provide the background for the five chapters in the second section, which explore the author's views on various aspects of the condensed organic state and where computational methods have and will add to our understanding. This section starts with a swift overview of relationships between structure and properties in molecular organic crystals (chapter 11), touching on dissolution rates, thermal, mechanical and electronic properties. The topic then shifts to the nature of specific intermolecular bonding and chapter 12 is largely devoted to describing the author's semi-classical density sums (SCDS) or Pixel method as a powerful tool for evaluating specific intermolecular interactions and crystal energies. This is followed by a chapter discussing phase equilibria and the prospects of molecular simulation for studying melting, crystal nucleation and growth. The penultimate chapter concerns polymorphism, the energy differences between polymorphs and a realistic view of computational methods for crystal structure prediction, using the author's 'Prom' algorithm as an illustration of one of the many existing computational approaches to generating crystal structures used to explore packing possibilities of molecules. The book concludes with a walk through the stages in the crystallisation process itself

and sets out the author's preliminary ideas on a predictive theory of crystallisation.

There are clear illustrations throughout the text, of which very few suffer from the lack of colour. The supplementary material, available from the author's website, includes the OPIX program package, which can be used to perform crystal packing calculations using atom-atom model potentials or the Pixel method, as well as a routine for computer-generating crystal structures. The software is well documented, is provided with example input and output files and might stimulate readers to perform their own computational experiments and perhaps encourage more crystallographers to include such energy calculations as a regular part of crystal structure analysis.

In summary, I found this book to be a valuable account of current computational methods that are relevant to investigations of molecular aggregation and crystallisation, written in a readable and enjoyable style. The emphasis is on the author's own work, but the chapter notes provide pointers into the general literature. A particular strength of the book is to provide a critical view of both strengths and limitations of the various molecular simulation techniques, while pointing to some of the most urgent directions for development of new methods. It is therefore particularly recommended to graduate students whose research involves analysis or computational studies of molecular materials, and will be of interest to anyone with an interest in organic condensed matter.

Graeme Day

Harwell: the Enigma Revealed

Nick Hance

Enhance Publishing, Oxford, 2006

Price: £20 (hardback)

ISBN 0-09553055-0-0 xiv +336 pages

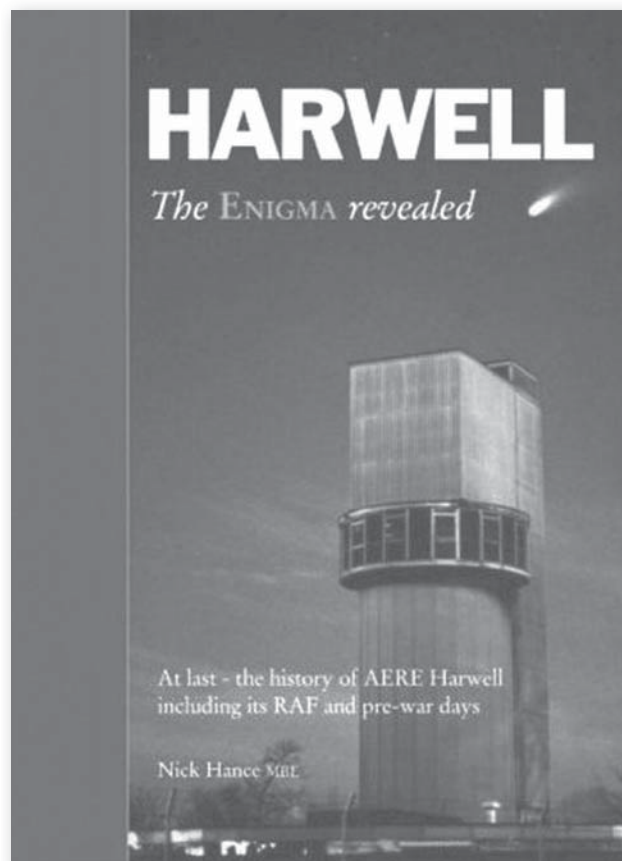
NEUTRON diffraction in the UK began at Harwell, the Atomic Energy Research Establishment, AERE. In publications from 1948, **J. Thewlis, G.E. Bacon & colleagues established guidelines for neutron scattering, including absorption and extinction, in analysis of crystals and powders.** They had to cope with weak neutron fluxes from the first reactor in Western Europe, Graphite Low Energy Experimental Pile (GLEEP) and from British Experimental Pile O (BEPO), the prototype for Windscale. Interesting authorship combinations at this time included Bacon and Pease and Bacon & Curry!

From the late 1950s, scientists in solid-state physics, materials science and metallurgy under **Graeme Low, Ron Dyer, Jane Brown** and others utilized higher flux fixed

wavelength neutrons from the enriched-uranium heavy-water materials-testing steady-state reactors PLUTO and DIDO (shut down in 1990), familiar to visiting crystallographers. University usage was formalised in 1966 by an agreement between the AEA and the research council. Many visitors from the UK and overseas will recall summer schools associated with **B.T.M. Willis**. At present, both ISIS and Diamond are located on the same Harwell-Chilton site.

Why should there have been neutron-producing reactors in White Horse country on the edge of the Berkshire Downs, an area associated with breeding racehorses and growing fruit? (Incidentally, the regularly spaced rows of cherry trees hereabouts could seem like a large-scale illustration of a lattice). **Nick Hance**, who has spent his working life at Harwell - first on nuclear accelerators, then with **D.H.C. Harris** on reactors and later in information and media relations - has tried to answer this in his book and to continue the story up to the present-day multi-tenanted science park on the Harwell-Chilton campus. The book is based partly on his local history lectures and on AERE records and newsletters. I still have a copy of a 1973 users guide by **N.J.Hance** for the Badger (neutron) diffractometer on the 6HGRIO hole in DIDO, labelled "not for publication", though the Ferranti four-circle instruments had been installed in the 1960s.

Hance has certainly not recorded the story of neutron scattering at Harwell - Bacon gets only a brief mention - but his book has a much wider appeal. He sketches the historical significance of the site, describes the construction and World War II activities of the RAF bomber station and



its post-war transition to AERE. He then recounts the successive changes over the decades to the organisations on the site reflecting different emphases of scientific and technological research.

Historically, the Harwell-Chilton plateau is at the intersection of the 4000 years old Ridgeway Path and the Icknield Way with the Roman Straight Street. In 1935 it became the site for one of the many RAF Expansion airfields constructed by Laings before WW II. The selection of Harwell (rather than Chilton or East Hendred) as the name of the RAF station, and hence of what became a nuclear research centre recognised worldwide, was said to have arisen because the CO's house was in that parish. From being a pre-war airfield initially for open-cockpit biplanes, Harwell went on to train 1200 bomber crews and then was the base from which Horsa gliders were towed off on the evening of 5 June 1944 to initiate the D-day invasion of Europe. RAF Harwell even figures in a Dermis Wheatley novel.

When a site for a UK atomic energy research establishment was discussed in 1945, Sir **John Cockroft**, then Director of the Anglo-Canadian Laboratory at Chalk River, Ontario, thought it should be close to either Oxford or Cambridge and have convenient access to London. A former active RAF station would possess many facilities, ready-made hangers (for reactors) and sound accommodation buildings, but the Air Ministry would not release aerodromes in East Anglia. Of 15 active airfields, in and around Oxfordshire, Harwell, with its high water table and low-mineral-content water supply was chosen. Its entrance was right on the A34, linking Southampton with Oxford and points north, and it was near to Didcot (ironically the site later of a large coal-fired power station) on the London-Bristol railway line.

Visitors will recall the prominent water tower (now supporting microwave antennae), one of the few remaining RAF buildings. Of the hostels used by visiting scientists, the former RAF B Mess is now an innovation centre while at least the name of Ridgeway House (A Mess) lives on in a new hostel. The other big post-RAF landmark, the Tandem Van de Graaff Generator tower, with its corrugated walls looking like a giant cigar lighter, ran from 1958 to 2002 before being collapsed by explosives and demolished.

Cockroft, to become a Nobel Prizewinner in 1952, was the first Director and soon encouraged neutron beam research. He attempted to give the former RAF station (denuded of trees) a secure but more academic ambience with tree-planting among the prefabricated housing and new redbrick buildings (still described by numbers, RAF style). From the 350 staff growing to 600 envisaged by Cockroft, AERE grew to employ 6000 staff at its peak in 1958. Earlier, two notorious employees of the secret nuclear establishment were Klaus Fuchs, a naturalised British subject convicted of espionage in 1950 and the Italian physicist Bruno Pontecorvo who defected to Moscow.

By 1965, changes in attitudes to national R and D centres led to broadening of AERE's nuclear power remit to

embrace non-nuclear activities such as marine and energy technologies and to engage in increased industrial liaison. One group of neutron scatterers retrained to become part of a large non-destructive testing team. Staff numbers declined markedly, but in 1989 AEA technology became a consultancy and scientific services business, subsequently privatised. Organisations for fusion and high-energy physics and for radiation protection had been successively hived off.

From the outset, computing was important to AERE; the brilliant neutron-scattering head of theoretical physics, **Walter Marshall**, became Deputy and then Director of AERE 1966-1975. Ferranti computers gave way to IBMs, to Ferranti Atlas, IBMs again and Crays; Atlas, in a separate building "outside the wire", merged into the Rutherford-Appleton Laboratory (RAL), on the former airfield site but using the Chilton address, in 1975.

In more recent times, neutron scatterers have moved on to the ISIS spallation pulse source with target station 2 at RAL. The most prominent structure on the Harwell-Chilton site is now the Diamond synchrotron source, controversially built here rather than at Daresbury, just visible like a giant flying saucer from the new dual-carriageway A34 shifted to the east.

Visitors to Harwell and some former staff may be surprised at the vast range of problems tackled over the years by Harwell scientists: from dating the Turin shroud to explaining how the 1987 Kings Cross Underground fire was generated. Backed by reference footnotes on each page, 300 historic photographs and a useful glossary, Hance's 35 topic-based chapters provide an informative and entertaining account. It should appeal to a wider audience as well as to those with a Harwell connection.

Derry W Jones

Aperiodic Crystals: From Modulated Phases to Quasicrystals, IUCr Monographs on Crystallography number 20

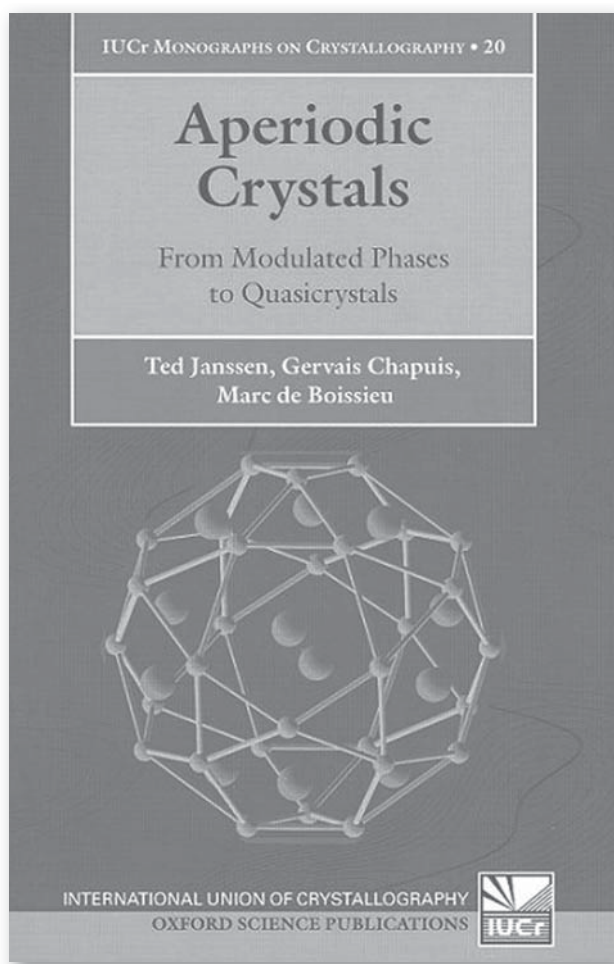
Ted Janssen, Gervais Chapuis & Marc de Boissieu

Oxford University Press, 2007

Price: £75.00 (hardback)

ISBN 0-19-856777-6, 480 pages

A crystal is defined as a material whose diffraction pattern contains Bragg reflections. A periodic crystal is one that also has three-dimensional translational symmetry. An aperiodic crystal is a crystal in which the translational symmetry has been lost in one or more dimensions. The authors of this book divide aperiodic crystals into three classes: modulated structures in



which the positions or occupation numbers of the atoms are modulated by a wave whose wavelength is incommensurate with the crystal lattice, composite crystals composed of two or more components whose lattice translations are incommensurate in at least one direction, and quasicrystals often described in terms of two kinds of tiles (unit cells) that are assembled according to a set of rules that ensure that the resulting solid does not have translational symmetry.

What all of these have in common is a mathematical description of their structures and reciprocal lattices in a space with more than three dimensions. This book explores these spaces for the three kinds of aperiodic crystal. The mathematics of each differs in detail but the use of higher dimensional space is common to all. It is the mathematics that is the focus of this book and the authors expect the reader to be already familiar with, among other concepts, space group theory, matrix algebra, gauge transformations and Lie groups as applied to the description of periodic crystals. In each case the mathematical description of periodic crystals is used as the starting point for developing the multidimensional theory that follows. Once the aperiodic theory is developed its application to each of the three kinds of aperiodic structure follows.

The Introduction describes the discovery of aperiodic crystals and how their theory was developed, providing a

foretaste of what is to follow. The subsequent chapters deal with the extensions required to the theory of space groups, the models that are used to describe aperiodic structures, aperiodic diffraction theory and structure determination, the causes of aperiodicity in crystals, their physical properties (specially lattice dynamics), and finally their morphology and surfaces. Two appendices deal with higher-dimensional space groups and the magnetic symmetry of quasicrystals.

Although the mathematical theory forms the core of this book, it is illustrated by a good number of examples, starting with simple models (especially the one dimensional Fibonacci chain) and moving on to a judicious selection from the wonderful zoo of real aperiodic structures. The book is not without its errors both of substance and typography. Some mislabelled terms in the mathematical sections could well confuse a less-than-confident reader. Others are more harmless but egregious - for example the CsCl structure is described under the heading NaCl on p.8 and on p.41 the popular name of iron pyrites, 'Fool's gold', is given to the compound $\text{Hg}_3\text{-}\delta\text{AsF}_6$, which the original authors nicknamed 'Alchemist's Gold'; alchemists may have been misguided but they were no fools!

Almost anything one would want to know about the theory of aperiodic crystals is compressed into this book's 450 pages making it an essential reference for anyone working, or planning to work, with these compounds. However, this is no introductory text for the beginner, and those who prefer a descriptive to a mathematical approach will find themselves fully challenged. Nevertheless this book will be a valuable addition to many researchers' shelves; it is likely to be the aperiodic crystallographer's bible for many years to come.

I. David Brown
McMaster University

Macromolecular Crystallography - conventional and high-throughput methods

M R Sanderson and J V Skelly, editors

Oxford University Press, 2007

Price £65.00 (hardback)

ISBN 978-0-19-852097-9.

HAVING been involved in what was commonly known as 'protein crystallography' for a fair number of years, I must admit that the same techniques have been being applied to nucleic acids for almost as long and so the title 'macromolecular crystallography' is certainly a more accurate description. Couple to that the advances reached in the past decade in which rapid and high resolution

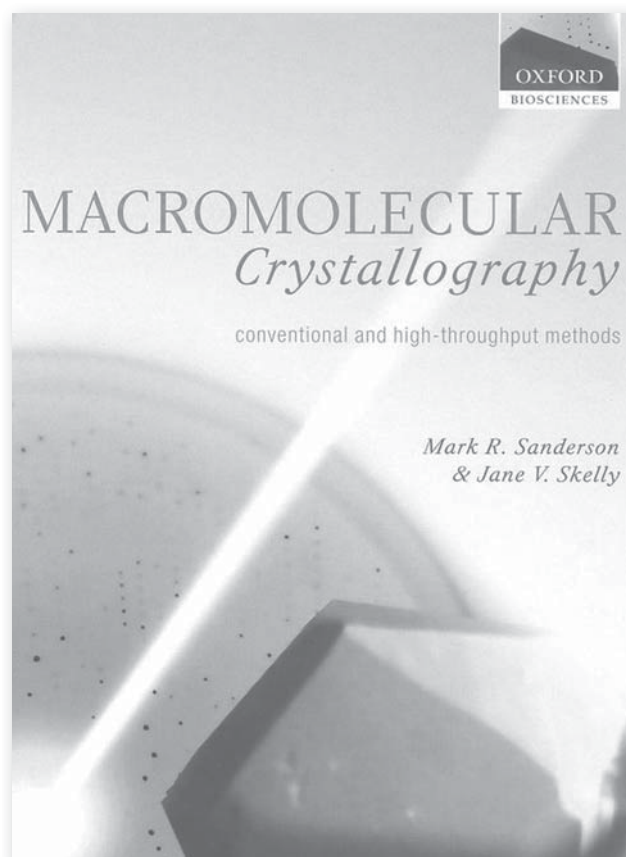
structure determination of biological macromolecules is almost commonplace, particularly as regards the high-throughput methods demanded *inter alia* by the pharmaceutical industry, then there is undoubtedly a need for a book such as *Macromolecular Crystallography*.

The approach adopted by the editors is to bring together experts who are involved in the application of X-ray crystallography to the solution of biological problems and the result is a volume that will enthuse both graduate students and more senior researchers alike. Beginning with the essential, and now rate-limiting, steps of cloning and over-expression, the opening chapters provide well-referenced descriptions of methods for both normal and high-throughput production and purification of soluble protein in quantities sufficient for its structure determination. Chapters on crystal growth, the initial X-ray analysis, and in-house data collection follow, each containing protocols and tips which all will find useful. A short review of isomorphous replacement, the original phasing method now verging on the quaint, precedes chapters on molecular replacement, MAD-phasing, the applications of direct methods, and phase improvement by density modification. A good phase set will provide an interpretable electron density map and the next chapters deal with the modern methods for model building and refinement including automation of the process. Interestingly, between the two chapters dealing with model building and refinement, is one on high-throughput data collection at synchrotrons, which deals principally with the system developed by the Structural Genomics Research Consortium using the APS at Argonne. The book then moves to chapters on RNA crystal growth, protein-DNA interactions as studied by X-ray crystallography followed by the protein-nucleic acid tour de force, virus crystallography. The final chapter is on structure-based drug design.

The editors say in their introduction that the book is not intended to serve as a text book dealing with crystallographic theory, although there is some. Rather it seeks to bring together the methods and techniques

as they are currently applied, with special emphasis on automation and/or high-throughput. In this aim, it is more than successful, and most, if not all, who dip into it will be rewarded by learning things they did not know, or possibly had forgotten. It is well produced, contains a comprehensive reference list and indeed many URLs, and is largely error-free although in a few places the use of colour would have clarified the figures. This is a minor criticism of a book that will surely find its place in every crystallographic lab whether protein or macromolecular.

Lindsay Sawyer



Meetings of interest

FURTHER information may be obtained from the website given. If you have news of any meetings to add to list please send them to the BCA Web Master cockcroft@img.cryst.bbk.ac.uk or to the Editor, gould@ed.ac.uk.

17-20 December 2007

Rayons X et Matière - RX2007.
Dijon, France
www.ext.impmc.jussieu.fr/sincris_fr/

18 December 2007

BCA BSG Winter Meeting 2007,
The School of Pharmacy, London
www.bmsg.ulsop.ac.uk/BCA/index.html

6-11 January 2008

6th NCCR Practical Course
on Biomolecular Modelling.
Kandersteg, Switzerland
www.structuralbiology.unizh.ch/course2008.asp

14-17 January 2008

Magnetic Structure Determination
Workshop 2008, Abingdon, Oxon
www.isis.rl.ac.uk/conferences/magneticdiffraction/2008/index.htm

21-23 January 2008

ANKA - School on Synchrotron
X-ray and IR Methods Focusing
on Environmental Sciences,
Karlsruhe, Germany
<http://ankaweb.fzk.de/conferences/EUN2school/>

2-3 February 2008

3rd TOPAS Users' Meeting,
Melbourne, Australia
www.bruker-axs.de/uploads/media/Zirkular_1_Lo_TOPAS3.pdf

2-6 February 2008

16th International Biophysics
Congress, Long Beach, CA, USA
www.biophysics.org/meetings/2008

3-6 February 2008

ICDDD 2008 Dubai, UAE
www.icddd.com/

4-8 February 2008

Australian X-ray Analytical
Association (AXAA) 2008
Schools, Conference and
Exhibition. Melbourne, Australia
www.pco.com.au/axaa2008

11-15 February 2008

School on Advanced Neutron
Diffraction Data Treatment, ILL,
Grenoble, France
www.ill.fr/dif/FPSchool/

3-6 March 2008

16th Annual meeting of the
German Society of Crystallography.
Erlangen, Germany
www.conventus.de

5-7 March 2008

ARC 2008: International
Symposium on Pulsed Neutron
and Muon Sciences, Mito
www.ips08.com

9-13 March 2008

The Minerals, Metals and
Materials Society (TMS) 2008
New Orleans LA USA
www.tms.org/Meetings/Annual-08/AnnMtg08Home.html

8-10 April 2008

BCA Spring Meeting, York
www.crystallography-meetings.org.uk

27 April - 3 May 2008

Summer School on Mathematical
and Theoretical Crystallography.
Gargnano, Garda Lake, Italy
www.lcm3b.uhp-nancy.fr/mathcryst/gargnano2008.htm

6-9 May 2008

ICCBM12 2008 International
Conference on the Crystallisation of
Biological Molecules. Cancun, Mexico
www.iqumica.unam.mx/ICCBM12/

18-23 May 2008

7th Symposium on High
Temperature Corrosion and
Protection of Materials. Les
EMBIEZ, France
www.htcpm-2008.uhp-nancy.fr/

18-25 May 2008

IWCGT-4 Fourth International
Workshop on Crystal Growth
Technology. Beatenberg, Switzerland
www.beatenberg.ch/IWCGT-4

21-23 May 2008

Surfaces and Interfaces in Soft
Matter and Biology: the impact
and future of neutron reflectivity,
ILL, Grenoble, France
www.ill.fr/Events/rktsymposium/

31 May - 5 June 2008

ACA Annual Meeting - Knoxville,
TN, USA
www.hwi.buffalo.edu/ACA/

8-13 June 2008

IWPCPS-10: 10th International
Workshop on Physical
Characterization of Pharmaceutical
Solids, Bamberg, Germany
www.assainternational.com/

6-11 July 2008

ICQ10 - 10th International
Conference on Quasicrystals.
Zurich, Switzerland
<http://icq10.ethz.ch/>

13-18 July 2008

Gordon Research Conference:
Diffraction Methods in Structural
Biology, Lewiston ME USA
www.grc.org/programs.aspx?year=2008&program=diffrac

21-26 July 2008

XRM2008 9th International
Conference on X-ray Microscopy.
ETH Zurich, Switzerland
<http://xrm2008.web.psi.ch/>

23-31 August 2008

21st Congress of the International Union of Crystallography 2008. Osaka, Japan
www.congre.co.jp/iucr2008/greeting.html

31 August - 4 September 2008

ECTP2008: 18th European Conference on Thermophysical Properties. Pau, France
<http://ectp.univ-pau.fr>

1-11 September 2008

EPDIC-11 European Powder Diffraction Conference Warsaw Poland
www.epdic-11.eu/

7-12 September 2008

BCA/CCP4 Summer School in Macromolecular Crystallography, Oxford
www.biop.ox.ac.uk/www/bcasummer2008.html

9-14 September 2008

WATOC-08 World Association of Theoretical and Computational Chemists. Sydney, Australia
www.ch.ic.ac.uk/watoc

20-24 September 2008

ICSG 2008: International Conference on Structural Genomics, Oxford
www.spine2.eu/ISGO

17-20 November 2008

14th International Conference on Thin Films. Ghent, Belgium
www.ICTF14.UGent.be

25-30 July 2009

Annual Meeting of the American Crystallographic Association 2009. Toronto, ON, Canada
www.amercrystalassn.org/meetingspg_list/futuremeetings.html

7-9 August 2009

Symmetry and Crystallography in Turkish Art and Culture: Satellite Conference of ECM-25, Istanbul, Turkey
www.lcm3b.uhp-nancy.fr/mathcryst/istanbul2009.htm