

CRYSTALLOGRAPHY NEWS

British Crystallographic Association
No. 87 December 2003

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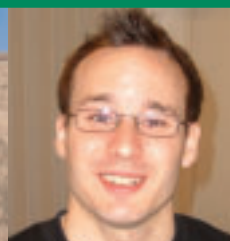


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QUARTERLY





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**NEXT ISSUE OF
CRYSTALLOGRAPHY NEWS**

CRYSTALLOGRAPHY NEWS is Published quarterly (March, June, September and December) by the British Crystallographic Association. Submissions on any subject related to crystallography are most welcome. If possible, please send text electronically without special formatting. Pictures are most welcome, but should be sent as separate, graphic files. Items for inclusion in the **March 2004** issue should reach the Editor by **25 January 2004**.

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As required by the DATA PROTECTION ACT, the BCA is notifying members that we store your contact information on a computer database to simplify our administration. These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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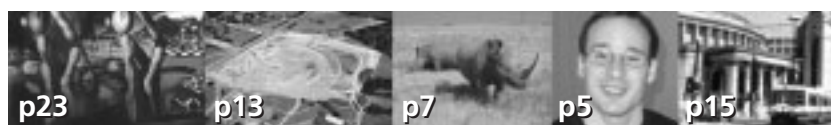
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President's Remarks

You will find in this issue of *Crystallography News* the outline programme for the 2004 BCA Spring meeting, to be held in Manchester next April. I am sure you will agree that an interesting and diverse programme is forming, and hopefully you will find plenty there to tempt you along to UMIST. Why not also spread the word to colleagues who would not normally attend the Spring Meeting, to help us grow the meeting as an annual focus for crystallography and related structural science in the UK. The Plenary/Review Symposium theme this year is *Catalysis in its many guises*, and it is anticipated that this theme will be developed in further sessions, including some relevant talks in aspects of the *Molecules in Medicine* sessions. Suggestions of topics or sessions for our Spring Meetings are always welcome, and we will be pleased to hear your ideas. The 2005 SM, incidentally, will be held at Loughborough, in the excellent conference facilities at the University there.

You will also note that on the day before the SM, we are planning a Young Crystallographers satellite meeting. The details of this are still being formed, but will be organised by our younger colleagues and

largely consist of talks/contributions from them. This is partly a successor to the highly successful "oral poster" sessions, but also an experiment in empowering the many Young Crystallographers who already contribute vigorously to the BCA and allowing them more of an active role within the Spring Meeting. We will also take this opportunity to revive the Lonsdale lecture, which has not been given for several years. This fits extremely well, since the original vision for that lecture was for it to be delivered to an audience of younger people. We hope that the Young Crystallographers meeting will also provide an important focus for those arriving early for the main meeting.

I would like to note (though probably too late to encourage you to attend by the time you read this) the extremely strong set of Autumn meetings organised by the subject groups. In parallel with our overall focus of the Annual Spring meeting, these group meetings are one of the main academic outputs of the BCA, and I would hope to continue seeing the successful science and strong attendances at these meetings.

Speaking of meetings, it was clear that the UK presence at the ECM-21 in Durban was significant and prominent. After some teething troubles the conference was generally enjoyed by the 500 or so delegates present. This number is of course lower than usual for an ECM, which is largely explained by the remoteness of the location from the European mainstream. However, our South African hosts are to be thanked for working so hard to make the meeting a success, in particular Jan Boeyens and Andre Roodt. The cultural experiences of South Africa were a much appreciated bonus for this delegate

who had also attended a satellite meeting "up country" beforehand. Next year's ECM returns to continental Europe, and will be held in Budapest in late August.

On a more organisational note, you will have noticed from a recent circular that we have apparently lost some members this year. We in Council are sure that much of this apparent loss is forgetfulness on the part of some of our members. Let me reiterate that a strong membership is vital to the BCA and what we are trying to achieve in terms of projecting UK crystallography. So if you know of someone who has not renewed their BCA membership, please remind them that they are valuable to us, and also that we believe the continuing low level of our general membership fees make the BCA a real bargain to join! On the membership note, it was agreed at Council in September that we would try to set up a network of contacts out there in University Departments, who will hopefully help us in targeting likely members and in publicising BCA activities. Our local BCA Reps can really play an active role in helping to promote what we do, in terms of our charitable Education remit, our organisation of a range of diverse scientific meetings, and generally promoting and projecting UK crystallography. We will be aiming to set up this network of Reps soon, volunteers are of course most welcome!

Finally, we have slightly updated our presence on the Web, and the BCA Web pages can now be accessed through www.crystallography.org.uk, which seemed to us rather appropriate for the UK organisation for crystallography.

Chick Wilson

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The British Crystallographic
Association is grateful to Birkbeck
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who host and manage the server
for our website.



Editor's Remarks



Welcome to the December Issue of Crystallography News. As the group autumn meetings have not yet taken place as we go to press, there is little to report locally, but we have some lively

reports from our Bursars at various meetings. Many thanks to them for the reports they write! The major crystallographic event since the last issue was undoubtedly the ECM in Durban. As the President says, the British contingent was very prominent, and we have reports from a few younger crystallographers at this meeting. There should be more in the March issue.

Sadly, we have to report the death of one of our honorary members, Professor William Cochran, who combined brilliance with gentleness in a wonderful degree. Michael Woolfson has written an obituary in this issue. In another sense we are also saying good-

bye to Euan Woodward, who has moved from Northern Networking. I should like to express my personal gratitude to him for his great good cheer and ready help with matters relating to *Crystallography News*.

I have now completed two years as Editor, and again want to express thanks to all who write for us – sometimes even without prodding! If you have an idea of something interesting, do let me know about it – our acceptance rate is far higher than *Nature's*! Comments about the appearance of the magazine are also most welcome, and there are some in this issue. Please let us know what you think.

Bob Gould

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BCA Corporate Membership

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

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

The cost of this membership is £600.00 per annum

To apply for Corporate Membership, or if you have any enquiries, please contact:

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Communications to the Editor from Dr Jeremy Karl Cockcroft and Mrs Kate Crennell

Dear Bob,

While going through my old copies of *Crystallography News* recently, I decided to scan in the front covers. While doing so I was struck by the fact that the new A4 size ones look nice and glossy (and colourful being in bold colours), but lack impact and curiosity value. In the older A5 versions, the picture on the front was a story leader that was an encouragement to open the front cover. In the A4 version, this has now been relegated to a series of postage stamp sized pictures at the bottom. Much of the discussion in Council in September 2000 (I think) concerned whether the magazine should be A5 versus A4, glossy versus matt, and little was discussed about cover content. In fact, I actually opened more of the old ones, though I accept this was also driven by having more curiosity of distant as opposed to recent past things as well as curiosity about the front cover story!

Best wishes, Jeremy Karl.

Dear Bob and Jeremy,

I too worry about the changing face of *Crystallography News*: look at no 81, June 2002 and you see that the typeface used was a clear and easy to read sans-serif font where the line of text 'CRYSTALLOGRAPHY NEWS' is much the same size as 'British Crystallographic Association', but in no 85 June 2003 all the text now uses an old fashioned looking type font with thin and spindly letters for the name of

the Association which is now much less prominent and legible from a distance.

I have never liked the "astronomical background image" because I do not know what it represents. The large logo is not an accurate representation of the BCA Logo, it was clearly redrawn by someone who did not appreciate its crystallographic significance, instead of using the vector drawn logo I sent to Chris Gilmore for the BCA flag for IUCr99 in Glasgow.

The trouble with the 'postage stamps' on the cover is that they are too small to see much detail, so they are not eye catching and there is nothing in the Contents to indicate where you can read more about the topic. There is usually something somewhere, but its position changes from issue to issue; it was in different places in the June and September 2003 issues. This makes it difficult for readers to know where to look for it; they prefer to know where to look for their favourite sections, rather than have to wade through a Contents page. This wouldn't matter if the page number where there is an article about the image, were superimposed on the little image on the cover.

Kate

The Editor replies:

I was very glad to receive these suggestions, and would be happy to change things, if there is a general feeling that a different cover would make *Crystallography News* more attractive, in the magnetic sense of the word! As will be noted, the captions of the "postage

stamps" are now given a page number, and they will stay on page 1. The "astronomical background image" is actually thoroughly terrestrial, and is part of an area-detector exposure. It has had a good innings – does anyone have a good idea for a replacement?

Bob Gould



Euan Woodward

Euan joined Northern Networking in 1999 to undertake the social programme for the IUCr conference which took place in Glasgow August 1999. He remained with the company until September of this year to take up a new life in London. Euan was a valued member of the NN team and over the years spent a good part of his working life on BCA activities. Many of you will know him from the annual conferences where he became very much part of the meeting for both delegates and exhibitors alike. He also undertook work on the BCA membership side and often assisted with *Crystallography News*.

The departure of Euan to new ventures down south has left quite a gap in the NN team.

Gill Moore

Computational Physics Group Annual PhD Thesis Prize

The Committee of the Institute of Physics Computational Group has endowed an annual thesis prize. £500 will be awarded to the author of the PhD thesis that, in the opinion of the Committee, contributes most strongly to the advancement of Computational Physics. The two runners up will receive £250. Applications are encouraged across the entire spectrum of Computational Physics. The competition is open to all students whose PhD examination has taken place in 2003.

Deadline:

December 31st 2003

Value:

£500 (first prize);
£250 (runner-up) x 2

Submission:

4 page (A4) abstract + citation

Format:

(max. 500 words) from PhD supervisor

Please enclose contact details, including an email address. Shortlisted candidates will be requested to submit an electronic copy of their thesis and references from their thesis examiners.

Submission Address:

Prof. A.D. Boardman,
Joule Physics Laboratory,
School of Sciences,
University of Salford,
Salford, M5 4WT

European Crystallographic Association: 4th European Crystallography Prize

The European Crystallographic Association (ECA) invites nominations for the fourth European Crystallography Prize to recognize a significant achievement or discovery in crystallography in the past 5-10 years. Nominees should be affiliated or identified with the European crystallographic community, as broadly defined in the charter of the ECA (see the ECA-news site www.ecanews.org)

The prize, including a monetary award and certificate of recognition, will be awarded at the opening ceremony of the 22nd European Crystallography Meeting (ECM-22) to be held in Budapest, Hungary, 26-31 August 2004.

The previous laureates are:

- 2000** Prof. Ada Yonath, Weizmann Institute of Science in Israel
- 2001** Prof. Jochen R. Schneider, HASYLAB at DESY in Germany
- 2003** Prof. Carmelo Giacovazzo, University of Bari, Italy

Nominations for the prize should include a statement of the contribution for which the prize is to be awarded and a short curriculum vitae of the nominee. They should be sent by e-mail or by regular mail no later than February 28, 2004 to:

Professor Anders Liljas
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Box 124, SE-221 00 Lund, Sweden

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Puzzle Corner

This month we have a **caption competition**. Please find the most interesting way of describing what these three distinguished members of the BCA are doing:



Last month's competition had a record number of entries: The hidden nine-letter word was POLYMORPH. Rules for deciding what words were allowed otherwise were not given, so I have decided to award the prize to the most inventive entrant, Bev Vincent of Rigaku/MSU with a definite trans-Atlantic flavour - or should I say flavor:

Morph, Pholy (some sort of rubber-based cement product), Holy, Orly (Airport), Poly (A whitish woolly plant found throughout the Mediterranean region), Roly (Roly Poly is a brand of sandwich), Prop, Prom (formal dance), Pro, Pry, Pop, Hop, Lop, Roy (proper nouns allowed?), Loy (i.e. Myrna, the actress), Hor (Biblical - mountain on which Aaron died), Mom.

Editor

Bursars reports from ECM21, Durban South Africa, 24-29 August 2003.

[The Durban meeting was a most unusual ECM! Getting there was not easy, but everyone who managed the trip seemed to find it very worthwhile. In addition to the well-planned scientific programme, we enjoyed a remarkable environment and social programme, of which these pictures may bring back some memories: Editor]



Some game-park residents

1. Sophie Dale, Loughborough



The bursary awarded by the BCA allowed my attendance at the ECM-21 meeting in Durban, my first ever

trip outside of Europe. On arrival in Durban with my supervisor, Dr Mark Elsegood, we were pleased to find we had booked into an excellent hotel, central to the facilities we would frequent in the next week - the International Convention Centre, the beach



The Indian Ocean from the Tropicana Hotel



The multi-racial Zulu-Indian dance group

and of course the many shops and restaurants!

The satellite workshop organised by the CCDC, held during the afternoon of the first day of the meeting, proved worthwhile attending, with the latest CCDC products presented and the opportunity to ask the organisers for advice on the use of the databases they maintain.

The conference programme commenced with an opening ceremony in which local dancers performed a collage of traditional dances, a delight to watch. The scientific programme, though compacted into four days,

allowed for great variety in the subjects of the microsymbiosia. Careful planning allowed me to attend the lectures most relevant to my PhD and also allowed me to fit in lectures on subjects that I have not met since my degree, particularly those concerning biological applications of crystallography. The plenary lectures were accessible to all delegates, not just those working in the specialised area, and I found the lectures given by Tom Blundell, on high throughput structural biology and drug discovery, and by Bill David, on structure determination from powders, the most interesting and useful.

It was a pleasure, during the very relevant microsymbioses on hydrogen bonding and structure-properties relationships, to be able to attend two talks given by Gautam Desiraju, a crystallographer who has authored many papers which have formed much of the reference material for the hydrogen bonding aspects of my PhD. Other lectures of interest, related to work carried out within our research group, were given by Len Barbour and Petra Bombicz, who both talked on the host-guest chemistry of calixarenes. A series of lectures on the final day covered the range of computing software available to the crystallographer as well as the latest developments at the EPSRC National Service at Southampton.

At the poster sessions, I presented a poster entitled *"Synthesis and Supramolecular Chemistry of the Complexes of the [Ru(p-cymene)]²⁺ Fragment and Pyridinedicarboxylic Acids"* and also co-presented the poster *"Synthesis and Structural Characterisation of Ruthenium(arene) Fragments Bearing Hydrogen Bonding Ligands"* with my supervisor. I had some interesting discussions with other crystallographers who work in the area of supramolecular chemistry, and I was pleased to receive numerous, useful comments and suggestions on our work which I hope to implement in the coming months. The poster session also allowed students from all over Europe and Africa to chat informally about their work, comparing strategies for getting through the three years successfully!

The closing dinner, held in a large marquee, was fantastic - the food and entertainment were excellent. As with the opening ceremony, traditional African Zulu dancing was presented, and, as it was "interactive", I got dragged up to join in! The rest of the night was thoroughly exhausting - every time I tried to go back to my table, I got pulled back to the dance floor by another gentleman for yet another dance. My toes just about survived; the bruises were only small!

Concerns surrounding delegates' safety in and around the conference were high, but a combination of common sense and making use of the shuttle buses provided by the ECM-21 organisers and the local taxis meant that we were not restricted solely to the ICC and our hotel. Evenings were spent mainly in the hotel, but I did manage to sample Durban's nightlife on two occasions, strangely bumping into a fellow Loughborough resident; now that's a small world!

My first visit to Africa was made even more memorable by the trip to the game reserve on the final day of the conference, providing perfect photography opportunities with the animals only feet away. What will remain in my mind for a long time to come is the sincere friendliness of the local people that I met in Durban; from the hotel staff to the taxi driver just nipping you down the street, nothing was too much trouble.

I am very grateful to the bursary committee for providing me with the funding to make the trip to Durban a reality, and I look

forward to my next crystallography meeting to renew the contacts I have made at ECM-21.

2. Robin Owen, Molecular Biophysics, Oxford



The 21st European Crystallographic Meeting was held in Durban, South Africa. The

meeting was an opportunity for me to attend my first international conference. The location and line-up promised an eventful and interesting week and Durban did not disappoint. The week started with an opening ceremony hosted by the Mayor of Durban and a traditional Zulu dance which even falling scenery could not interrupt.

The week's academic programme started with a session on crystallisation, though of particular interest to me was the afternoon session on synchrotron radiation and radiation damage. Zbigniew Dauter spoke on the positive effects radiation damage can have, explaining how radiation damage induced structural changes which can be used for phasing, while Gunnar Berglund talked about how X-ray irradiation changes the active site in horseradish peroxidase. The session closed with Edward Mitchell introducing a (nearly) fully automatic beam line at the ESRF.

Of direct relevance to my own work was the session on diffraction image processing and

data quality, chaired by Eleanor Dodson. Jim Pflugrath talked about the advantages and disadvantages of different detectors. Rob Hooft talked about data acquisition and image integration and the problems encountered in the automation of these processes, and Italian-minded Harry Powell also offered some solutions to this problem. Zbigniew Dauter spoke again, this time on criteria that should and should not be used for assessing the quality of diffraction data.

My own presentation consisted of a poster which was entitled *A new method for predetermining the diffraction quality of protein crystals*. The poster described a new method which allows quantitative measurement of the birefringent properties of protein crystals, allowing comparison of this optical quantity with the diffractive quality of the crystals. It was well received during both of the poster sessions, generating a lot of interesting discussions and winning the IUCr poster prize. Overall I very much enjoyed both the formal talks and the opportunity to meet and talk to other researchers.

3. Simon Coles, Southampton



After 18 hours in transit I found myself walking across the tarmac of Durban

International airport in 25C heat at 9am. It occurred to me that it hadn't been such a bad idea to leave the current heat-wave in

Europe and head for the South African winter! My hotel didn't disappoint either, being just a hop, skip and jump across the road to the Indian Ocean. Many days were going to be started by removing the previous nights excesses with a dip in the 19C water!

The opening ceremony gave a hint of what a conference in Africa was going to be like when an advertising hoarding toppled over onto the stage, narrowly missing one of the Zulu dancers!

I like ECM's! They are an ideal duration and generally packed with science (5 parallel sessions for 4 days). This was going to be no exception...The International Conference Centre is 'state of the art' and provided an ideal venue, even though much of the technology appeared to work on 'African time'! Monday started for me with two consecutive sessions on Charge Density, which were quite refreshing in that they focussed on applications of the technique. This was split by an excellent Plenary from Bill David, executed with his usual panache! Anticipating a busy schedule over the next few days I joined the rest of my research group (8 of us had decided to take advantage of the departure of the ECM to the southern hemisphere) on a rather exciting boat trip round the harbour!

Tuesday morning was spent ducking and diving between selected talks in various different sessions, the highlight of which was the inimitable Lachlan Cranswick's symposium on programming. It was at this point that the exhibitors saved the day by stepping in to sponsor the coffee breaks! The

day culminated in the first of two poster sessions, which was catalysed by some stimulating posters and a copious supply of equally stimulating wine!

Wednesday was an action packed day, which started with the cross-disciplinary 'Diffraction Image Processing' symposium. In my opinion one of the best and liveliest sessions, with some outstanding talks by Jim Pflugrath, Rob Hooft, Harry Powell, Zbigniew Dauter & Ken Shankland. A projector which refused to display any red certainly added to the atmosphere! The afternoon 'Structure-Property Relationship' session proved a great warm up for part 2 of the poster session.

The final day of the scientific program was to be my busiest... The first 2 sessions were spent running between several different focus areas, namely 'Core Chemical Crystallography', 'Indexing Powder Patterns', 'Crystallography at Extreme Conditions', 'Structural Knowledge to Chemical Reactivity' & 'Polymorphism'.

The final session was to be the one in which I was to give my presentation in 'Automatic Structure Solution: Challenges for the Future'. David Watkin gave a typically compelling talk on how his team are introducing chemical intuition into his refinement software, 'CRYSTALS'. Louis Farrugia then demonstrated the capabilities of his GUI which interfaces to a whole gamut of crystallographic tools. It was now my turn...I outlined our work on the intersection of a number of projects which is aimed at automating the entire chemical crystallography experiment and

introduced a novel approach to a user interface for a web-based interactive crystallography service. Ton Spek closed the proceedings by showing us the automatic solution and refinement procedures of SYSTEM-S, -a module of the infamous PLATON.

The conference dinner was a typically African affair, - held in a marquee in a slightly worrying area of Durban. The atmosphere was generated by a backdrop of exotic spit roasting animals and provided such delicacies as warthog and ostrich stew as well as a fancy dress safari jacket for everyone! The free-for-all dancing session was preceded by some entertaining interactive Zulu dancing. The final (and perhaps best) feature of the conference was the excursion visit to a private game park, - which was superb!

It was going to be very difficult to return to Europe and have to adjust to working on 'real time' as opposed to African time! On the whole this meeting was an eye opening experience and I am indebted to the BCA for partial support of my travelling expenses.

ECM 21 Diffraction image processing and data quality

This symposium was held on Wednesday 26th August. The presentations addressed image processing and data quality in single crystal and powder diffraction, and covered both macromolecular and small molecule applications. The first presentation was given by Jim

Pflugrath (Rigaku/MSC, USA), who focussed on the properties of modern area detectors and their relative advantages and disadvantages. CCD detectors are ubiquitous in small molecule applications, and are now becoming more common for macromolecular structure determinations. These detectors have a short readout time, in the range 1-10 s, with pixel sizes in the range 50-150 μm . However, they have a lower dynamic range than image plates, and are easy to saturate; they also show some energy dependence in their response. Image plates have been used, particularly by macromolecular crystallographers, for many years now. Their 'traditional' disadvantage, relative to CCD detectors, of a long readout time has recently been addressed, and may be as short as 10 s. They have a much higher dynamic range than CCDs, so that both strong and weak data may be reliably recorded on the same image. They also exhibit little energy dependence in their response, and they do not require cooling. Image plates are therefore becoming more competitive with CCDs, and modern developments include addition of some iodine to the phosphor to improve absorption, more powerful lasers to improve and expedite erasure and curved image plates.

Rob Hooft (Bruker Nonius BV, Delft, The Netherlands) described the EVAL series of programs (EVAL14, EVAL15 and EVALCCD) which encode a fundamental parameters approach to integration. Although reflections may be accurately located on a detector, determination of their shapes and boundaries is much more difficult. Even a spherical

crystal may exhibit a range of spot shapes because of factors such as oblique incidence of the diffracted beam on the detector or 1-2 splitting. In the fundamental parameters approach, reflection profiles are derived directly from the shape of the source, the wavelength profile of the radiation, the crystal shape and its mosaicity. Since both the distribution of neighbouring reflections and the reflection profiles are well understood, so too is the background. This applies even in difficult cases, such as twinned or incommensurate crystals. The wealth of background information available on an area detector means that elaborate models can be constructed, leading to improved estimates of standard uncertainties.

Harry Powell (MRC-LMB, Cambridge, UK) described the software written as part of the DNA project, which aims to automate data collection and processing. This is of particular importance at synchrotron beam-lines. The data collection part of the program is based on decisions that might be made by an experienced crystallographer after evaluation of crystal quality and determination of the unit cell. For example, the software automatically selects a crystal to detector distance, exposure time and scan range. Crystal decay and data quality are monitored during data collection. The program MOSFLM forms the data processing part of the DNA software. Once again, the aim is complete automation and the program can index an image, assess mosaic spread, refine the cell constants and integrate the data all without user intervention. SCALA is used for final scaling and merging. Initial

tests show that DNA works well for 'normal' crystals; the modular design of the program will facilitate the incorporation of extra functionality.

Zbyszek Dauter (Brookhaven National Laboratory, Upton, USA.) discussed how data quality may be assessed. Complete coverage of reciprocal space is extremely important and depends on the symmetry of the lattice. The data collection strategy needs to be considered very carefully. For example, though a 90° rotation is in principle enough to measure a complete data set from a crystal in point group 222, if the rotation is started from a position half way between the two-fold axes the data completeness may be as low as 60%. Some reflections may never fall into the diffracting position, though this problem may be minimised by off-setting a symmetry axis from the axis of rotation. Analysis of the quality of the intensity measurements and their associated standard uncertainties may be achieved with a range of statistical descriptors. The conventional R_{merge} is actually rather a poor measure because it tends to improve as redundancy increases. Better measures are those such as R_{meras} , R_{rim} and R_{pim} , which have been given by Diederichs & Karplus and Weiss & Hilgenfeld. These tended to be underused though, possibly because they adopt numerically higher values than the R_{merge} statistics that people are used to. Other measures have been designed specifically for anomalous data sets. Finally, though high redundancy is generally a Good Thing, merging together of data after significant crystal decay could degrade the quality of a data set.

Kenneth Shankland (RAL, Chilton, UK) spoke about data quality issues in powder diffraction, particularly as they relate to structure solution. Powders are studied not only because a material may only be available in this form, but also because a compound will usually be used in this form in industrial processes. Analysis is hampered by the overlap of symmetry inequivalent reflections with similar d -spacings, though collection of data at several temperatures can separate out overlapped peaks caused by anisotropic thermal expansion. Much depends though on measuring data with good statistics. One way in which this can be achieved is to use a variable counting time for data collection, so that data at high angle may be measured for some 20 times as long as those at low angle. If good data are available, however, even relatively subtle effect such as the orientation of a sulfonamide group ($-\text{SO}_2\text{NH}_2$) can be determined. Recent innovations at the ESRF on beam-line ID31 (previously ID16) mean that data suitable for structure solution can be obtained in only a few minutes. However with the move from a bending magnet to an undulator, the beam intensity is now so great that radiation damage is a serious problem even in such short exposure times, and procedures for minimising this, for example summing of many quick scans, are currently under active investigation.

The organisers would like to thank the speakers for five excellent presentations.

Simon Parsons and Eleanor Dodson

ECM-21 Durban - Review of Session : 'Structure Determination from Powder Diffraction Data (SDPD)'

Only ten or twelve years ago the first 'unknown' small molecule crystal structures had just been solved from powder X-ray data. The availability of the 'LeBail' extraction procedure had made the area amenable to those structural chemists, like myself, who had no background in theoretical crystallography or software development, and were prepared merely to plug away with existing 'single crystal' direct methods algorithms, and happily spend a week or two chasing a structure with ten or so non-H atoms.

Since then the field has been revolutionised! This fact was further emphasised at the Durban meeting with, in addition to an oral and poster session devoted to the technique, a prize-winning poster from Andrea Docherty (Strathclyde), a Plenary lecture by Bill David and the ECA Prize-winning lecture itself, by Carmelo Giacovazzo.

Professor Giacovazzo divided his talk into two themes at the extreme scales of molecular crystallography – i.e. macromolecular and powder crystallography, both of which have the challenge of 'insufficient data' to overcome. He described recent developments in the EXPO suite optimised for structure solution from powder data. Bill David's talk, as usual visually superb and scientifically enlightening, provocatively suggested that the '100-atom' threshold from powder data was now a realistic target. After

reviewing the dramatic advances made in both data collection methodologies and structure solution software in recent years, Bill gave examples of complex structures which are now 'regularly' (though not yet 'routinely?') solved. Around 92% of the structures in the Cambridge database fall below the '100-atom' limit, and may therefore 'in principle' be amenable to solution from powder data!

The oral session was chaired by Lynne McCusker and Gerd Kruger, and consisted of four invited talks. The first was given by Christian Baerlocher (ETH, Zurich), who described the deliberate and systematic exploitation of 'texture' in a sample to unravel more optimal structure factors from very severely overlapping powder data. Use of transmission geometry, an area detector and a synchrotron source are all key to the success of the method, which can provide 1296 *different* powder patterns from one sample! Ten years ago, this would have been our worst nightmare - now it is so useful that it has already allowed Bill David's 100-atom threshold to be broken, with the solution of a 117-atom zeolite structure, UTD-1! The second lecture was given by Jon Wright (ESRF, Grenoble), who spoke on another clever, and as yet not regularly used, experimental method to remove some of the ambiguity from powder data - anisotropic thermal expansion. The method relies on simultaneous extraction of 'the same' set of F's from a series of patterns collected over a temperature range of 100°C or so, where key overlapping reflections are systematically separated due to anisotropic cell variations. As an example, Jon showed the 'straightforward' solution of a 48-

atom organic structure with $Z'=4$, for which virtually all non-H atoms were revealed directly from the first E-map. Third up was Vincent Favre-Nicolin (Grenoble), who presented recent developments in his FOX program, which uses direct space, global-optimisation methods to circumvent the peak overlap problem. FOX is specifically optimised to tackle extended lattice structures as well as molecular ones, and several new features have been introduced of late even though Vincent is only pursuing this as a 'hobby' in addition to a full-time position in a different field! Finally, Celeste Reiss (PANalytical) presented recent results on two complex organic molecules solved from lab-based diffractometer data. Optimal strategies for data collection, including sample mounting and use of a new, rapid RTMS detector were emphasised.

These talks, together with a related session which showed some impressive developments in overcoming one of the other major problems in SDPD, that of initial powder pattern indexing, highlight the current strength and vitality of this field. Casual 'users' like myself look forward to the day when all of the current developments in indexing, direct methods and real-space methods are incorporated into one grand, unified, user-friendly (and free!) package which will allow SDPD to become genuinely 'routine'.

All-in-all, this was scientifically a good conference and despite, or maybe because of, the somewhat variable quality of some of the local 'hospitality', one which I shall certainly remember for a long time to come! I would like to thank the PCG for a contribution towards the meeting costs.

Phil Lightfoot

Final Accounts BCA Spring Meeting 2003 University of York

INCOME	£
Sponsorship	4,553.74
Registration	41,694.53
Exhibition	15,899.40
Bursary	960.00
Total	63,107.67

EXPENDITURE	
Accommodation & Meals	16,939.80
Facilities	10,757.70
Catering	3,490.88
Social Event	1,275.70
BCA Speakers Expenses	2,906.02
Refunds	2,282.00
Abstract Book	2,765.45
NN Fee	10,107.35
Administration	3,152.60
Stationery & copying	215.29
Bursaries	4,960.00
Total	58,852.79
TOTAL INCOME	63,107.67
TOTAL EXPENDITURE	58,852.79
MEETING SURPLUS (-DEFICIT)	4,254.88

*Ms C Myers The University of York
Mr D J Taylor BCA Treasurer
October 2003*

Note: These accounts include transactions made through the University of York and the BCA accounts

Treasurer's Note: The major contributions to the surplus were:

- 1. A 25% discount on catering because the kitchens were closed in the allocated accommodation halls and we had to stroll in the sunshine to a distant hall for meals.*
- 2. An exceptional take up of the excellent exhibition space with three exhibitors taking double stands.*

Diamond growing

Construction on the diamond site continues apace helped by the weather. The long hot dry summer in Chilton has allowed the builders continuous working with no interruptions for rain. Read all about it in 'diamondnews', the latest issue of which was published in July 2003. If you did not get a paper copy you can read it on the internet; there have been 3 issues so far, now there is more to

report they hope to have a quarterly newsletter. Look at the web site:

www.diamond.ac.uk/activity/activity=newsletter where previous issues are stored in PDF format and may be freely downloaded.

Current information about the latest status of proposed beamlines can be found on the website too; look at www.diamond.ac.uk/activity/activity=beamlines

Kate Crennell



The floor has to be unusually stable. This is achieved by drilling down to the bedrock using several huge drills like the one in the figure above. The drills have hollow centres, down which concrete is poured.



Aerial view of the construction site showing the floor plan of diamond emerging on the ground in the centre, new roads have been built to the RAL car park, and the new roundabout on the A4185 is just visible at the top of the photograph. Below the diamond ring, the white line is reflection from the construction fence. The circular building is the cafeteria; to its North the old RAL Laboratory creche (Known as 'The Little Stars') has been demolished to make room for the diamond office building, and a new creche building constructed to the Southwest, the rectangular white roof on the right.



While the concrete is wet, reinforcing rods are carefully pushed down into the concrete leaving the final hole ready to support the floor.



There are some 1500 of such piles, each of which is capable of supporting 80 tonnes. The floors will need such a lot of concrete at the same time that a huge special concrete mixing machine has to be built on the site. Meanwhile utilities are being connected: water and electricity mains are now being installed.

Diamond Update: New Crystallography Beamlines

Readers will be pleased to know that the two bids for crystallography beamlines on Diamond that were put to the Open Meeting in May 2003 have both been approved for development subject to final ratification by the Diamond SAC in November 2003. These bids were for a beamline for *Small Molecule Single Crystal Diffraction* (I19) and the *Monochromatic Macromolecular Crystallography Side Station* (I04A). The current order of construction indicates that the Small Molecule Diffraction beamline will be developed in Year 2 of the programme (2008) and that the side Station will be a Year 3 development (2009). This is really exciting news for both the small molecule and protein crystallography communities and will greatly enhance the available facilities for the next decade. Further details of all the approved beamlines and the construction schedules can be found on the Diamond website .

A related matter that will be of keen interest to those within the crystallography community that plan to use Diamond is the discussion that is now taking place regarding the setting up and the development of a Research Complex that will augment the facilities at Diamond. This Research Complex will house scientists working on the beamlines and provide supplementary facilities for them. The nature of the scientific infrastructure, people-centred infrastructure and site related infrastructure are all under

discussion, and the community will be asked for its input at various stages of the process over the coming months.

The next Diamond Special Interest Group Meeting will take place on 6th April at the BCA Spring Meeting at UMIST, and speakers will describe developments at Diamond in both the areas of Life and Physical Sciences. Details of the programme can be found in this issue of Crystallography News under the arrangements for the Spring Meeting. We look forward to seeing you all at the Diamond SIG.

Paul Raithby
Co-ordinator of the Diamond SIG.

Life Science Director at Diamond



Congratulations to Dame Louise Johnson (and to Diamond!) on her appointment as Life Science Director at the Diamond Light Source. Louise continues to be Professor of Molecular Biophysics at Oxford. Of her appointment, she said, "I am delighted to be joining such an exciting scientific research organisation. Since 1981 with the commissioning of the UK's first synchrotron facility at Daresbury, synchrotron light sources have revolutionised biological research. Structural

explanations for such large complexes as the Foot and Mouth Disease virus or the mitochondrial ATPase (the central enzyme in energy conversion) have had an immense impact. Diamond will be a significant upgrade on present resources. It will provide scientists with state-of-the-art research facilities that will allow us to address even more challenging problems. These will include membrane proteins, intracellular protein complexes, the design of new therapeutic agents and a host of other biological targets such as those that have emerged from the human genome sequence. Diamond will also benefit a wide range of disciplines such as engineering, earth science, chemistry and medical diagnostics."

Wanted

Professor Gautam Desiraju is looking for a two-circle optical goniometer. Anyone who has one of these that is no longer needed could find an excellent home for it by contacting him:

Professor Gautam R. Desiraju
School of Chemistry
University of Hyderabad
Hyderabad 500 046, India

Tel
+91 40 23010 510 (extn 4828)

Fax
+91 40 23010 567

E-mail
desiraju@uohyd.ernet.in
<http://202.41.85.161/~grd/>

British Crystallographic Association

Spring Meeting
6th-8th April 2004 - UMIST

The BCA Spring Meeting



The BCA Spring Meeting will take place at UMIST from Tuesday 6th April to Thursday 8th April 2004. The Spring Meeting will run for 3 days finishing with tea

on Thursday at 3pm. A Young Researchers' satellite meeting is also being planned, taking place at the Conference Centre on the day leading up to the Spring Meeting, about which full details will be available later.

The Spring Meeting will take place in the Renold Building, part of the Manchester Conference Centre at UMIST (www.meeting.co.uk); the conference facilities at UMIST are excellent for both delegates and exhibitors. The facilities are centrally located and are easily accessible by both public transport and by car. The proximity of Manchester International airport and associated rail links make this venue particularly attractive for our overseas members. Car parking (£8 per day) for 700 vehicles is available on-site. High quality accommodation, both en-suite and standard, is available and is just a short walk from the conference venue.

All scientific sessions, poster sessions and a commercial exhibition will take place in the Renold Building within the conference centre.

The Commercial Exhibition will run from Tuesday 6th April to Thursday 8th April 2004. For more information on the Exhibition and Sponsorship opportunities, please contact Jackie Sayers at the BCA Administrative Office at the address below.

The BCA Administrative Office will manage all administrative issues relating to the Spring Meeting, if you have any queries please contact Jackie Sayers on 01355 244966 or email BCA@glasconf.demon.co.uk

REGISTRATION

The BCA Council is pleased to announce that One-Day Registrations will be available at the Spring Meeting in Manchester.

Early Registration Costs (before 5th March 2004)

Full Registration Fee:	£130.00
Student / Unemployed / Retired Registration fee:	£65.00
One - day Registration Fee (no concession rate):	£65.00
Non - member surcharge:	£25.00

Late Registration Costs (after 5th March 2004)

Full Registration Fee (no concession rate):	£180.00
One - Day Registration Fee:	£90.00

Deadline for early registrations is 5th March 2004

ACCOMMODATION

Two types of accommodation are available at UMIST:	
Standard B&B:	£25.10 per night
En-suite B&B:	£35.00 per night

All accommodation is located in the Weston and Chandos buildings, a short walk from the Conference Centre. Breakfast and dinner will be served in the nearby Barnes Wallis Restaurant.

Please note that en-suite accommodation is limited and will be allocated on a first-come basis, so early registration is recommended.

CATERING

Morning coffee, afternoon tea and lunch will be served in the exhibition area, close to all lecture theatres.

Breakfast and dinner (including the conference dinner) will be served in the Barnes Wallis Restaurant.

Lunch and Dinner must be booked in advance and will be ticketed.

Packed lunch served in the exhibition area: **£6.50 per day**

SOCIAL EVENTS

On Tuesday 6th April 2004, the Posters' / Exhibitors' Reception will be held in the Exhibition Centre from 18.30 hrs, wine and a buffet meal will be served from 19.00 hrs. Delegates will have the opportunity to chat with exhibitors and poster presenters in a relaxed, informal setting. There is no charge for this wine and buffet reception, but sponsorship is welcomed.

	Monday 5 April	Tuesday 6 April			
08.30 hrs		Young Crystallographers Sessions	BCA Council Meeting 09.30 hrs - 10.30 hrs	Parallel Session: Molecules in Medicine	
10.00 hrs		Coffee/Registration 10.30 hrs - 11.00 hrs			
10.30 hrs				Parallel Session: Biomolecules in Medicine	Parallel Molecules Chemica
12.00 hrs		11.00 hrs - 12.30 hrs - Plenary Session : Catalysis: from metals to macromolecules James Naismith (St Andrews) Guy Orpen (Bristol)			AGM: Crystallog 12.00 hrs
12.30 hrs		Lunch & Exhibition: 12.30 hrs - 13.30 hrs			Lunch & Ex
13.00 hrs					
13.30 hrs	Young Crystallographers Sessions	Plenary Session : Catalysis: from metals to macromolecules Jim Kaduk (BP Amoco) Phil Woodruff (Warwick)	Parallel Session: Methods in Macromolecular Crystallography	Parallel Small Ang Wor	
14.30 hrs			Tea/Exhibition: 14.30 hrs - 15.00 hrs		
15.00 hrs	Tea 15:00 hrs - 15:30 hrs	Tea/Exhibition: 15.00 hrs - 15.30 hrs			
15.30 hrs	Young Crystallographers Sessions	Plenary Session : Bragg Lecture: John Finney (UCL) 15.30 hrs - 16.35 hrs	Parallel Session: Methods in Macromolecular Crystallography	Prize L PCG	
16.30 hrs			AGM: Biological Structures Group 16.20 hrs - 16.30 hrs		
17.00 hrs	Oral Posters	DIAMOND SIG 16.40 hrs - 18.00 hrs			
17.45 hrs				Dorothy H	
18.00 hrs	Dinner				
18.30 hrs					
	Kathleen Lonsdale Lecture 18.30 hrs	Posters/Exhibitors 18.30-22.00hrs			
20.00 hrs	Young Crystallographers Mixer 20.00	Buffet and Wine Reception: 19.00 hrs			

Wednesday 7 April			Thursday 8 April		
	Parallel Session: Incommensurate Structures	Parallel Session: Instrument Calibration: How to be a star!	Plenary Session: Use of International Tables		
Coffee/Exhibition 10.00 hrs - 10.30 hrs			Coffee/Exhibition 10.00 hrs - 10.30 hrs		
Session: in Medicine : al Aspects	Parallel Session: Incommensurate Structures	Parallel Session: Instrument Calibration: How to be a star!	Parallel Session: Non-bonded Interactions	Parallel Session: Small Angle Scattering	Parallel Session: Advanced Aspects of Symmetry
Chemical raphy Group - 12.30 hrs		AGM:Industrial Group 12.00 hrs - 12.30 hrs	Lunch & Exhibition: 12.00 hrs - 13.00 hrs		
Exhibition will run from 12.00 hrs - 13.30 hrs					
Session: le Scattering kshop	Parallel Session: Incommensurate Structures Workshop	Parallel Session: Catalysis in Industry	Parallel Session: Non-bonded Interactions	Parallel Session: Small Angle Scattering	Parallel Session: CRYSTALS Workshop with PCs.
	AGM:Physical Crystallography Group 14.30 hrs - 15.00 hrs		Tea/Exhibition: 14.30 hrs - 15.30 hrs		
Tea/Exhibition: 15.00 hrs - 15.30 hrs					
Lectures: & CCG			BCA Council Meeting: 16.00 hrs - 18.00 hrs		
BCA AGM: 16.35 hrs - 17.20 hrs					
Hodgkin Prize Lecture: 17.30 hrs - 18.30 hrs					
Conference Dinner: 19.30 hrs					

The Conference Dinner will be held on Wednesday 7th April at 19:30 hrs in the Barnes Wallis Restaurant at a cost of £30.00 per person (£15.00 for students).

A fun run around the campus is being planned for the BCA Spring Meeting. It will be sponsored by Rigaku/MSc and will follow the general form of their popular event which has become a regular feature of ACA Meetings.

Further details will be available shortly before the meeting, from Harry Powell (hrp1000@cam.ac.uk)

CAR PARKING

There is ample car parking available at UMIST, charges are £8 per 24 hour period. UMIST is also conveniently located adjacent to Manchester Piccadilly station and the use of rail travel is recommended.

E-MAIL FACILITIES

Access to email and Internet facilities will be available throughout the duration of the Spring Meeting in the main conference building.

ABSTRACT SUBMISSION

Submission of Abstracts will be electronic. For instructions, please visit the website: <http://www.isis.rl.ac.uk/BCA2004>

If you have any queries regarding Abstract Submission, please email: BCA2004@isisa.rl.ac.uk

Please note that the deadline for receipt of Abstracts is Friday 20 February 2004.

BCA BURSARIES FOR BCA SPRING MEETING

A limited number of bursaries are available from the Arnold Beevers Bursary Fund to cover the cost of two nights accommodation, meals (including the Conference Dinner) and registration. The bursary will not cover travel expenses and recipients will be expected to present a poster.

Council is again seeking commercial sponsors of Spring Meeting Bursaries at £150 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 20th February. Only on-line applications from the BCA website will be accepted.

For up to date information on the BCA Spring Meeting, please visit the BCA website:

www.crystallography.org.uk

Further information can also be obtained from the BCA Administrative Office:

Northern Networking
1 Tennant Avenue
College Milton South
East Kilbride, Glasgow
G74 5NA

Tel: ++44 (0) 1355 244966

Fax: ++44 (0) 1355 249959

Email: bca@glasconf.demon.co.uk

CITY OF MANCHESTER

Manchester is a city steeped in history, with a rich culture and cosmopolitan outlook. Whether you are interested in art, theatre, opera, pop music or sport, or if you just want to 'shop 'til you drop', Manchester has it all - and the Manchester Conference Centre is close to all the action! Manchester is a city in motion, a city that blends the cultured with the brash, the cheap with the exotically expensive. The whole place zings with excitement, tensions and contradictions.

2002 was definitely Manchester's year of the century. The Commonwealth Games, which began with a glorious opening ceremony, developed into one of the biggest parties Britain had ever thrown. But 2002 was also about building for the future, with a host of exciting and innovative building projects completing in a period of just a few months. These included the Manchester Art Gallery, Urbis, the Imperial War Museum North, the City of Manchester Stadium, the National Squash Centre, the Indoor Tennis Centre, Piccadilly Gardens, Cathedral Gardens, Cathedral Visitors Centre, Selfridges and the huge Piccadilly Station project, just across the road from the Manchester Conference Centre. The speed at which they were all delivered is a great demonstration of the "Manchester attitude".

SCIENTIFIC SESSIONS

The scientific sessions for the 2004 BCA Meeting will again concentrate on "hot-topics" in the field of crystallography. The main theme and Plenary Session is **Catalysis : from Metals to Macromolecules**; this will lead into a sub-theme on **Molecules in Medicine** covering both chemical and biological aspects and Catalysis in Industry. There will be sessions on **Small Angle X-ray Scattering**, which will be preceded by a workshop on the subject, thus offering a good introduction to this subject and an indication of the state-of-the-art. Similarly, **Incommensurate Structures** will be covered with sessions and a workshop. Another topic of importance to all crystallographers is **The Use of International Tables**. The emphasis will be on symmetry, which will be a plenary session, and for those interested in a deeper insight, this will be followed by a session on **Advanced Aspects of Symmetry**. There will be other more specialized sessions including **Non-Bonded Interactions** and **Instrument Calibration** as well as a workshop on the CRYSTALS software suites. There will be a Special Interest Group session on **DIAMOND** that should be of interest to a large proportion of the crystallographic community.

The **Bragg Lecture** will be incorporated into the UMIST BCA as will the **Dorothy Hodgkin Prize Lecture**. The **Prize Lectures** for the Physical and Chemical Crystallography Groups will take place as usual, as well as the general **Poster Sessions**. Prior to the main meeting there will be sessions organized by the **Young Crystallographers** and these will include the oral poster sessions and the **Lonsdale Lecture**.

Some additional details of speakers are given below:

Further, more up to date details are available via the main BCA Webpage or specifically at:
<http://bca.cryst.bbk.ac.uk/bca/meets/bca04/bca04.htm>

Plenary Session: "Catalysis: from metals to macromolecules"

James Naismith (St Andrews)
Activation of Inorganic fluoride

Jim Kaduk (BP Amoco Chemicals, USA)
Extraframework Species in Zeolite Y at Non-Ambient conditions.

Guy Orpen (Bristol)
Structural systematics of phosphine ligands for homogeneous catalysis

Philip Woodruff (Warwick and FHI Berlin)
Surface Crystallography and its Relation to Catalysis

Plenary Session: "Bragg Lecture"

John Finney (UCL)
Beyond Bragg's Law: crystallography without a lattice

Plenary Session: "Diamond SIG"

Chair Paul Raithby
 John Evans (Southampton/Diamond)
 Liz Duke (Daresbury Laboratory)
 General Discussion

Parallel Session: "Incommensurate Structures"

Vaclav Petricek (Czech Republic)
 Gervais Chapuis (Switzerland) - to be confirmed
 Kenneth Harris (Birmingham / Cardiff)
 Clivia Hejny (Edinburgh)

Parallel Session: "Incommensurate Structures Workshop"

The Jana software package

Plenary Session: "Dorothy Hodgkin Prize Lecture"

Chair: Chick Wilson (RAL and Glasgow)

Plenary Session: "Use of International Tables - Symmetry"

Session Leader: Bill Clegg (Newcastle)

Parallel Session: "Small Angle Scattering"

Mary Vickers (Cambridge)
 Member of Peter Laggner Group (Austrian Acad. Sci.)
 Robert Thomas (Oxford) invited - to be confirmed
 Member of Hecus Braun Company (Hecus Braun-Graz GmbH) invited - to be confirmed

Parallel Session: "CRYSTALS Workshop"

With David Watkin (Oxford)

10th Glasgow Protein Structure Workshop, Heriot Watt University - Scottish Borders Campus, Galashiels, 3rd - 5th September 2003

Neil Isaacs welcomed participants to the 10th Glasgow Protein Structure Workshop with some surprise at having reached ten meetings! Hazel Leith was the opening speaker in the first session on *Tools and Preliminary Studies*, with an overview of Invitrogen's ligation-free, one-tube cloning technology (Gateway) and its application to the cloning of light (the luciferase operon). Adrian Abbots then showcased the ÄKTA 3D, Amersham's solution to the protein purification hurdle at which 50% of solubly expressed proteins currently fall. Adrian also presented 'The Balthazar Project' – a vision of purifying 48 samples per day in parallel - allegedly inspired by a mad Swedish cartoon scientist and not a large quantity of champagne. Having purified our favourite protein, and set down some crystallisation trials, Steve Badger explained how the Oasis1750 imaging system from Veeco, which exploits a laser autofocus system and proprietary illumination technology to "get the image quality right", could search our trays for crystals at 8000 wells per hour. Katie Evans from Daresbury, having had more success with her work on bacterial phytochromes than on tuberculosis targets, changed her talk title and brought us up-to-date with her progress in achieving soluble expression of *R. palustris* phytochromes in *E. coli*. Jenny Paterson, probably our most southerly participant, coming from Keele, introduced

us to the structure of an innate immune system component, surfactant protein D (SP-D), and described her attempts to obtain a complex with the high affinity ligand N-acetylmuramic acid (NAMA). Gareth Williams from St. Andrews continued the theme of innate immune response, and concluded the session with the "halfway there and a bit" story of his work to obtain crystals of the two-domain ArnA protein, a microbial enzyme involved in the resistance pathway of lipid A modification by sugar attachment.

After a short break for tea, the *Membrane Protein* session opened with a talk by Dominic Hunter, Edinburgh, on a novel cytochrome P450 from *Rhodococcus* which, he was quick to point out, "is not a membrane protein". The second speaker of the session, Bob Ford, began a series of contributions from UMIST by introducing himself as one of the senior, "or was it senile", people that Lindsay Sawyer talked about, before going on to describe the structure of a true membrane protein – the multi-drug resistant, P-glycoprotein from CHO cells. Maps derived from analysis of tilted images of 2-D crystals, to a "good" resolution for electron crystallographers (8Å), show the molecules are leaning over to one side at a "slightly jaunty angle" within the crystal lattice. Daniel Wyatt then described his method for purification of microgram amounts of L-type calcium channels from sarcolemmal membranes. We were lucky that Richard Collins remembered his slides for the first time this year (hurrah!), and gave a long-awaited presentation on the structure of the megaDalton PilQ

complex determined from single particle analysis of cryo-electron microscope images. Initial work at 25Å produced a 12-fold symmetric structure that looked "like a melting ice-cream". Steve Prince wrapped up the UMIST contribution with his efforts to understand detergent-protein interactions in the light harvesting complex (LHC2) by collecting neutron diffraction data. Several months in Grenoble (foolishly not learning to ski) later, they had collected a load of data that allowed them to confirm the presence of a "droopy carotenoid", and to hypothesize that detergent binds to the LHC as a preformed micelle. Neil Isaacs from Glasgow drew the session to a close with a heroic 4.5Å structure of the *R. palustris* reaction centre (RC)-LHC core that goes some way to solving the enigma of quinone transfer through the LHC 'wall' and may shed light on the assembly process of this complex of 70 components with no instructions.

After supper, the evening session enticed us away from the bar with the promise of *Exciting Structures*. Konstaninos Beis (St. Andrews) kicked off with three membrane proteins, Wza, Wzi and Wzc, involved in transporting the *E. coli* K30 antigen across the inner and outer membranes, which he has studied by scanning transmission, atomic force and electron microscopies, and X-ray crystallography. Richard Norman (AstraZeneca) then described the structure of human thymidine phosphorylase, a potential cancer target, in complex with an angiogenesis inhibitor. Eric Kong (York) explained how he had used surface plasmon resonance and crystallography to

understand the binding of a novel synthetic peptide to the ligand-binding domain of an isoform of the human oestrogen receptor. Michaela Smolle from Glasgow ended the session with her work towards an understanding of the architecture of the human pyruvate dehydrogenase complex.

The second day of the meeting began with a specialist **Workshop on Structural Genomics**, opened with a philosophical view on the scope of structural genomics from John Moulton of the Centre for Advanced Research in Biotechnology (CARB) at the University of Maryland. John expressed a desire to know the structure of everything, but conceded that a few thousands to tens of thousands of structures would probably be sufficient to give adequate coverage "despite the strange behaviour of sequence and fold space", as estimated using the 'sock method'. Osnat Herzberg brought us back to the realities of experimental science with a review of the program on the structural genomics of hypothetical proteins from the *H. influenzae* genome at CARB. To date they have obtained 38 structures from 308 cloned proteins. Their experience shows that typically no more than 200 crystallisation experiments are needed per protein. In contrast to John's wide-ranging interest in protein structures, Marjorie Harding from Edinburgh is only interested "if there's a metal in it". Marjorie has so far collated information on the first coordination sphere of zinc and calcium binding sites in the PDB. Tony Fordham-Skelton from Daresbury described a novel family of protein tyrosine phosphatases (PTPs) that he has

identified in *Arabidopsis thaliana* ("the 2CV of the plant world"), whose structures are currently unknown. Prayank Patel from the CCP4 at Daresbury demonstrated a number of utilities (some old and some new to CCP4 v5.0) "that probably won't help solve the structure but will aid your progress and fill in the gaps". Ian Boucher used the "nice shiny crystallisation robot cunningly called Mosquito" at York to obtain crystals and determine the structure of a novel iron-dependent superoxide dismutase from the malarial parasite, *P. falciparum*. Nicholas Evans from UMIST presented the low resolution structure of the haemoglobin receptor, HmbR, an outer membrane protein from *Neisseria meningitidis* which fortuitously crystallised in 2 dimensions on an electron microscope grid. And finally, Karen McClusky from Dundee illustrated the ubiquitous nature of mobs with reference to this year's CCP4 study weekend, before focussing on the example of MobB, a small molybdoenzyme whose structure, along with a spot of modelling but "not as most people know it", gave insight into its function as part of a GTP binding site in the MobA/MobB complex.

An afternoon of shinning up the Eildon Hills with Lindsay Sawyer, snoozing by the river Gala, shopping in Peebles and sightseeing in Edinburgh led up to the conference dinner followed by entertainment from Chris Pitt and an edifying crystallographic bar-quiz from the inimitable quiz-master Lindsay

The penultimate session of the meeting on **Databases, Instrumentation and Transition States** was opened by Kim

Henrick from the EBI who introduced aspects of the e-MSD – a whole new and exciting way of looking at the contents of the PDB. Carsten Mang followed on with Hamilton's "total solutions" to automate the crystallisation process from screen setup to image analysis. Having "reached the end of the train(?)" with crystals ready for analysis, Anita Coetzee (Bruker-Nonius) reminded us that we should always try to obtain the best quality data, and demonstrated how to achieve improved signal-to-noise in-house through increased data redundancy, higher flux, and a sensitive detector. Tracey Gloster, York, drew the session to a close with an overview of carbohydrates, an introduction to isothermal titration calorimetry, and the mechanistic surprises revealed in the atomic resolution structure of xylanase.

In the final session on **Really Interesting Structures**, Rachel McMaster from Sheffield managed to explain homologous recombination to a hungover audience, and described work towards understanding the mechanism of the atypical RusA resolvase from *E. coli*. Nick Hopcroft (York) took time off from "desperately" trying to get his thesis written up to continue the theme of nucleic-acid binding proteins, with a talk on the structure of the *B. subtilis* TRAP protein bound with randomness and yet specificity to GAG and UAG mRNA repeats. Simon Bailey (UMIST) outlined his work on another interaction involved in the initial infection process of meningococcal bacteria, that of Neisserial Opacity associated proteins with host CEACAM receptor proteins. Simon Newstead (St. Andrews) showed

how *M. viridifaciens* sialidase appears to have taken domains from different proteins and slotted them together, tempting him to try a "mad" experiment to swap the carbohydrate binding domain. So far, however, he has restricted himself to trapping all the substrates that Garry Taylor managed in 1995! Stefan Gerhardt (AstraZeneca) asked us "why did the stupid German solve another pentameric lumazine synthase structure and why is it in this session of really interesting structures?" The answer: *S. pombe* lumazine synthase binds riboflavin – simple! Paul Blackburn from Glasgow ended the program with enthusiasm at probably achieving the highest levels of over-expression of a 7-TM GPCR in mammalian cells, for the atypical chemokine receptor CCR-D6. Paul successfully convinced us that this project was "heading for glory not death" with pictures of his best crystal, growing next to fluff from his jumper, that disappointingly dissolved in the European heatwave on the way to Trieste.

Neil Isaacs found himself, again with some surprise, supplying the concluding remarks, and was encouraged to find "structural biology in Britain in very good hands given the students coming through". Next year's workshop will again take place at Heriot Watt University – Scottish Borders Campus, Galashiels from September 1st to 3rd, with a new organising trio of John Rafferty, Karen McClusky and Jim Naismith.

Richard Norman, Ludovic Otterbein, Siân Rowsell, and Julie Tucker

Perovskites Modern and Ancient

Roger H. Mitchell, University Almaz Press, Thunder Bay ON, 2002
Price US\$70 from www.almazpress.com
ISBN 0-9689411-0-9 (HB); 318 pages.

This book covers the great structural variation of the perovskites and related phases. It is set out in ten chapters dealing with the different structural types of perovskites: "true" perovskites, ordered perovskites, non-stoichiometric perovskites, such as the bronzes and bronzoids and the hexagonal perovskites. Later chapters cover layered perovskites, including Ruddleston-Popper compounds, high T_c superconducting cuprates, and the hydrogen-bonded organic-inorganic halide structures. The great variety is increased as within many of these "structural types" it is possible to find polar transitions in which the central ions in octahedral coordination are driven off-centre, to pure tilting transitions of the framework of octahedra. The final chapter of the book betrays the origin of the author in the earth sciences, and covers the variety of natural perovskites, their compositional ranges, and their importance in the mantle and in meteorites.

Mitchell has deliberately and sensibly avoided covering topics such as superconductivity and magnetism associated with the phases, which would require several volumes of their own to cover in the same detail. What he has produced is an almost encyclopaedic structural work, which should be of great benefit to many solid-state chemists and physicists, materials scientists and mineralogists.

The book is timely in that in the last several years there has been

considerable progress in both the group theory underlying, e.g., the potential tilt systems, limiting the number of possible space groups for tilting transitions, as well as progress in the crystal chemical predictability as to which distortion will occur, for certain cases.

The quality of production in this book is excellent: there are over 300 pages of high quality, glossy paper. The book is illustrated with over 250 figures, all reproduced in colour, covering representations of structures, cation ordering, diffraction patterns, phase diagrams etc, and 36 tables of space groups, possible tilt systems and compositions of natural perovskites.

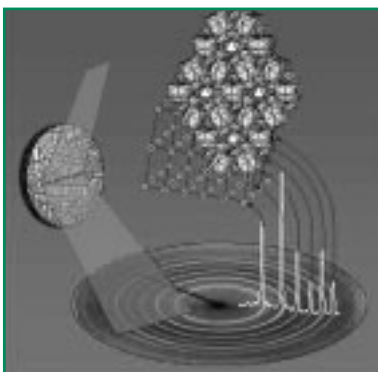
Two things, in my opinion, make this book very valuable: the first is the very large and highly up-to-date reference list provided. This makes the book a truly useful reference and enables the reader to rapidly examine the literature in any corner of the perovskite world. The second is the context that is provided by such a work. In spite of modern databases and internet searches, where one is capable of finding a great deal of information for free, it is only a book such as this in which one can find a global overview of a topic. There is no way one could get such a broad swathe of information in context anywhere near as rapidly even from the most modern databases.

The great scope of this book makes it a highly valuable reference resource for people who deal regularly with, or have an interest in the perovskites. If you think that you have even a slight interest in buying such a book, you probably should purchase a copy of this one.

*Ian Swainson,
NRC, Ottawa.*

Fundamentals of Powder Diffraction and Structural Characterization of Materials

Vitalij K. Pecharsky and Peter Y. Zavalij, University of Iowa and State University of New York at Binghamton
 Kluwer Academic Publishers, Boston USA, 2003
 Price: US\$163.00 (hardback)
 ISBN 1402073658 xxiii+713 pages and CD.



In this publication Pecharsky and Zavalij aim to produce a text that will provide both undergraduate and graduate students with a thorough grounding in the practical aspects of powder diffraction, methods for structure solution from powder data, and in the technique of Rietveld refinement. As such the book aims to cover material that might traditionally have been found in classics such as the texts by Klug and Alexander or Cullity, as well as introducing areas covered in more depth by specialist publications such as the IUCr monographs edited by Young and David/Shankland/McCusker/Baerlocher. The stated entry level is that of students with a "general scientific and mathematical background of the order of the first two years of a typical...college". The book is a well produced and well illustrated text and includes a CD featuring colour figures, the numerous data sets presented in



the text and solutions to the end of chapter problems. The cover deserves special note being apparently inspired by Dali's depiction of Narcissus falling in love with his own reflection and metamorphosing via an egg into a flower – represented here by an intermetallic compound seeing a diffraction pattern, transforming to a reciprocal lattice before becoming an inorganic mixed metal oxide!

Chapter 1, as is common with many texts, covers elementary aspects of symmetry in the solid state, though also includes a nice "taster" of more exotic aspects of symmetry such as incommensurate modulation and quasicrystals to whet the reader's appetite.

Chapter 2 (160 pages) is an ambitious attempt to cover the "Fundamentals of Diffraction" from the production and monochromatisation of X-rays, their detection, simple diffraction theory through to the intensity corrections required for analysing powder data. I must confess that this was by far my least favourite chapter of the book as I personally found the arrangement of material peculiar. For example, monochromators are described

before the phenomenon of diffraction has been introduced. The geometry of diffraction is then described (pleasingly to me via use of the Ewald sphere); however, there are then some 60 pages covering intensity corrections and powder peak shapes before structure factors are introduced. Whilst there is nothing inherently wrong with the material, I can't help feeling that the approach could be confusing to beginners. I also felt that the level at which diffraction is introduced might be slightly daunting to the stated target audience.

Chapter 3 covers "Experimental Techniques" starting with a historical description of powder diffraction methods and instrumentation before moving on to consider sample mounting and how to optimise hardware and data collection parameters. There is also a useful section on the safety aspects of using ionising radiation. Common errors such as an inappropriate choice of slit size for a given experiment are covered in depth. I did feel that there was rather too much overlap between some of this material and that covered in chapter 2, particularly regarding e.g. monochromators

and the choice of slits/detector set ups for different experiments.

Chapter 4 describes the "Preliminary Data Processing and Phase Analysis" of materials and essentially deals with the "everyday" aspects of routine powder diffraction work including peak searching, peak profile fitting and phase identification – in essence the analysis a diffractionist might perform "at the instrument". The material is covered in an exhaustive fashion with detailed descriptions of the various stages of the process. Practical examples of the pros and cons of different background fitting, smoothing, α_2 -stripping and peak search algorithms are described which will be of use to inexperienced operators.

In chapters 5, 6 and 7 this text perhaps comes into its own in that it switches to an example-based format to cover the topics of indexing, structure solution and structure refinement. A large number of real examples, drawn from the authors' own research, and backed up with a CD of data and input files for readers to play with, are provided. The approach adopted falls somewhere between that of a classical text book and a lab manual/interactive course. Chapter 5 deals with the problems of indexing and refining unit cells. Although indexing is now largely automated the authors describe some traditional methods of manual indexing to set the scene. The use of the "classic" software packages ITO, VISSER and DICVOL is then described in depth with several practical examples. Methods for refining cells are then described, along with an outline of the least squares method. This particular section feels slightly out of place in this chapter as it's a

technique that permeates much of the book, and could perhaps have been dealt with separately elsewhere, particularly as a similar treatment of non-linear least squares pops up in the middle of chapter 6. This is perhaps a chapter which will date rapidly as there has been a significant resurgence of interest in the science of indexing recently, and many new techniques/software packages are appearing to supplement the classic methods. This is, of course, no fault of the authors!

The final two chapters concentrate on methods of solving (chapter 6) and refining (chapter 7) structures. After brief introductory sections both chapters present examples from the authors' own labs. In addition to examples solved by Patterson and direct methods it's nice to see cases quoted where "crystallographic common sense" and a thorough knowledge of the literature have proved as important as using "black-box" software packages. The authors have chosen an approach in which the crystal structure of each example is solved in chapter 6 and then details of its refinement given in chapter 7. Whilst this works extremely well from the viewpoint of completeness it does lead to a slightly illogical order in chapter 7 where later examples are often less complex than earlier, and introduce no particularly significant new features. My only criticism of these two chapters is that it would have been valuable, considering the huge current interest in the area, to include a worked example in the text of the use of real space methods to solve an organic structure and illustrate the specific pitfalls that can be encountered during refinement of molecular species. It might also have been nice to illustrate

(perhaps in comparison to the methods already described) the use of an alternate programme, such as the widely used EXPO.

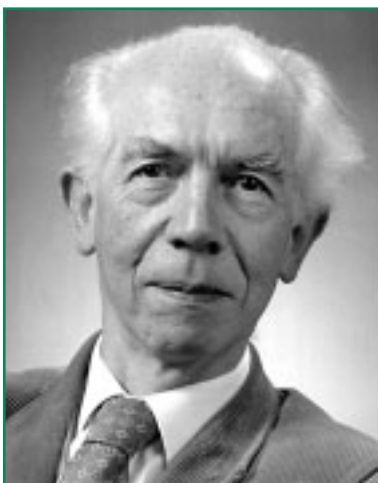
Overall this is a useful, generally accurate and relatively comprehensive text that provides a good coverage of this area of crystallography. It is perhaps slightly long to be suitable as an introductory text for students and contains some annoying repetitions when read sequentially, but will provide a valuable reference source for any lab involved in powder work. There are areas I feel could have been usefully included, though these are clearly my personal bias. They would include non-ambient diffraction; more on topics such as the problems involved in combined neutron/x-ray refinements – how, for example, were data sets weighted in the combined refinement in chapter 7?; and more examples based on synchrotron/neutron data sets.

It's a relatively expensive text (£98 from Amazon though in the US Kluwer offer significant discounts if several copies are purchased as a course book) to expect students to buy, though this is perhaps justified for a 700+ page hard-backed book with extensive additional material on compact disk. My only caveat to potential purchasers is to think before they fly - this was the first book ever to put my travel plans in jeopardy when it tipped my Easy Jet carry-on luggage over the weight limit! Rest assured though, that the simple act of removing the book from the bag in one's right hand and carrying it through the departure lounge in one's left is sufficient to satisfy check-in requirements!

John Evans

WILLIAM COCHRAN

July 30, 1922 -
August 28, 2003



Bill Cochran was born on a remote sheep farm, some 15 miles south of Glasgow. Forebears of the Cochran family had farmed in the area continuously since the middle of the seventeenth century, but Bill's father took the family to a new farm, some eight miles west of Edinburgh in 1928. As Bill himself said 'It is surprising, particularly as I have no brothers, that I did not become a farmer.' Had he done so, it would have been a sad loss to science.

Bill was educated at Boroughmuir High School where his first interest was in languages, but the fortunate gift of a Mecanno set turned his interest first to engineering and later to physics. He entered Edinburgh University in 1939 to read physics, graduating in 1943. He made repeated efforts to become involved in the war effort, but he was always directed towards academic activity and from his graduation until 1946 he was an Assistant in the Edinburgh Physics

Department, mainly involved in teaching electronics. For the first part of that period, he worked under the direction of Professor C G Barkla who had won the Nobel Prize for Physics in 1917 for his work on the characteristic emissions of X-rays. When Professor Barkla died in 1944, Bill moved to the Chemistry Department to do research in X-ray crystallography under the guidance of Arnold Beevers. After an exhaustive, but unsuccessful attempt to solve the native sucrose structure, Bill succeeded in solving the isomorphous NaCl and NaBr adducts of sucrose, which enabled him to obtain his PhD.

In 1946 Bill moved to Cambridge as Research Assistant to the Cavendish Professor, Sir Lawrence Bragg. The research group was under the direction of W H Taylor and also contained June Broomhead and C J B Clews. Professor Alexander Todd of the Chemistry Department had suggested to Bragg the problems of solving the structures of pyrimidines, purines, nucleosides and nucleotides as a way of throwing light on the structure of DNA. Cochran and Broomhead found that they could determine the electronic structures of pyrimidines and purines sufficiently accurately to find the positions of hydrogen atoms, and Bill found that this was greatly improved by the use of an ($F_0 - F_c$) Fourier synthesis that removed the effect of termination errors. Later he built a Geiger-counter diffractometer with which he measured the electron density in salicylic acid to reveal the presence of hydrogen atoms and electron density associated

with covalent bonding. In 1949 Bill met David Sayre, an Oxford-based American postdoctoral worker, and this began his interest in direct methods of solving the phase problem. As early as 1948 papers on inequality relationships by Harker & Kasper, Gillis and others had appeared in *Acta Crystallographica* but such relationships were restricted to very small and simple structures. In 1952, in one issue of *Acta Crystallographica*, there appeared three papers separately written by Sayre, Cochran and Zachariasen that could be said to be the starting point of modern direct methods.

In 1951, after an extended visit to the USA, Bill was promoted to a full Lecturer in Cambridge and so obtained the tenure and stability he needed to anchor his subsequent research career. Travelling home by ship from Stockholm after the second International Congress on Crystallography in 1951, Bill met his future wife, Ingegerd Wall, and they married in Sweden in 1953. Also, at about this time, he collaborated with Henry Lipson in the production of *The Determination of Crystal Structures*, a very influential text for many years.

In the 1950s Bill acted as a consultant to the protein crystallography group in the Cavendish Laboratory, and in 1952 he, Francis Crick and Vladimir Vand published a notable paper on the diffraction pattern of atoms on a helix. It was this paper that enabled Crick and Watson to interpret Rosalind Franklin's diffraction photographs of the A-form of DNA.

Bill saw quite early the potential of computers as a crystallographic tool, and in 1955, with Sandy Douglas, he applied EDSAC, a primitive early computer, to a direct method for solving centrosymmetric structures. This pointed the way to the subsequent development of computer applications in this field, which had an important impact on structural crystallography.

In the mid-1950's Professor Dingle had created a bit of a stir by expressing doubts about the validity of the 'twin paradox' in relativity, and for some time Cochran and Dingle carried out a lively public debate which ended in Cochran's favour. During this period, Cochran was becoming somewhat disenchanted with direct methods and had concluded, incorrectly as he later conceded, that they could not solve more than very simple structures. Protein crystallography was clearly the future, but, having decided early on that it too was unlikely to succeed, he was reluctant to 'climb on the bandwagon' now that it was rolling successfully. By 1958 Cochran was ready to embark on a new field.

In 1957, at the fourth International Congress on Crystallography in Brookhaven, Bill had attended a lecture by Bert Brockhouse on neutron diffraction applied to lattice dynamics. He arranged to spend a year at Chalk River, funded by Atomic Energy of Canada, where Brockhouse, later to win a Nobel Prize, was just using his newly-designed triple-axis spectrometer to measure phonon dispersion curves for sodium iodide. Bill

spotted a theoretical paper by Dick and Overhauser on the dielectric constant of alkali halides and he realized that their shell model was just what was needed to explain the lattice dynamics of sodium iodide. Later he extended the theory to germanium and two papers he wrote at this time became classics in the field. Later development, while he was still in North America, led to the idea of the soft-mode concept for the onset of ferroelectricity.

On returning to Cambridge in 1959 he briefly dallied with the phase problem once more but then turned his full attention to lattice dynamics. He was fortunate in having two gifted research students, Stuart Pawley and Roger Cowley, later to become colleagues at Edinburgh. In the next few years, work was done on the lattice dynamics of molecular crystals, the theory of the lattice dynamics of sodium, and the shell model was extended to GaAs. At this stage Bill was at the forefront of the lattice dynamics field, and it was almost inevitable that, at the comparatively early age of 40, he was elected a Fellow of the Royal Society in 1962.

In 1964 he was appointed Professor of Physics at Edinburgh and quickly established a research group on Condensed Matter Physics. Further work was done on phase transitions leading to the onset of ferroelectricity, mainly using the Chalk River facility for neutron spectroscopy. For the next ten years Bill and his group established a leading position in the general field of lattice dynamics. He also

developed a new model for the structure of amorphous materials.

In 1975 Cochran succeeded Norman Feather as the Professor of Natural Philosophy and Head of Department in Edinburgh. Although his research activity continued for a while, it quickly tailed off as he bore an increasing administrative burden.

Cochran's work was recognised by several awards and appointments to scholarly bodies. He was a Fellow of the Royal Societies both of Edinburgh and London and an Honorary Fellow of Trinity Hall, Cambridge. He was awarded the Hughes Medal of the Royal Society, the Guthrie Medal of the Institute of Physics and the Potts Medal of the Franklin Institute. Amongst his many interests were the writing of poetry and tracing the genealogy of his family. He leaves behind his wife, Ingegerd and children Margaret, Robert and Jennifer, to whom he was a devoted husband and father.

Michael Woolfson

Patenting Software

(There has been a lot buzzing about the Net on this subject. The following has been edited from correspondence on *bionet*, and may be of wider interest. For the purpose of this article, Mike Glazer speaks in roman and Lachlan Cranswick in italic – Editor)

I find it difficult to believe that anyone would find patenting our sort of software worth doing, at least as far as small stuff, typical scientific-research oriented software is concerned. It would be incumbent on anyone holding a patent to show:

a) that there is infringement. This would open up the patent holder's software for close examination and without doubt various aspects of their software could be shown to exist in other programs written earlier, in which case they would be likely to lose. They might even then be judged to be infringing someone else's patent! I suspect that anyone holding a software patent is going to be loath to open their own software up for inspection in case they lose everything. Proving infringement in cases like this is exceedingly difficult.

b) that their software is not obvious, i.e. that someone "skilled in the art" at the time of writing could not have done this themselves. It would be extremely difficult for a company to prove non-obviousness in this area, especially since many of us would say that we could equally well have come up with the idea and that therefore it would be obvious.

The result of this is that even if

someone takes out a patent on software we can generally ignore it, because the patent holder would have to pursue a lengthy and very expensive legal case with a strong likelihood of failure. So, while I too think that software patents are a bad idea, I actually think they will in most cases turn out to be unenforceable. They are typical of the muddle and lack of understanding of the real world that we have come to expect from the European Union. Of course it could be that many of the members of the European Parliament are also lawyers: if so, legislation of this sort is going to be of considerable personal profit to them. Or am I just being too cynical?

But it would seem that others do not find it difficult to contemplate and actually patent this sort of "small stuff". There is a non-exhaustive list of current Crystallographic "Software Patents" (also called "computer-implemented business method patents") at the CCP14 website:

They have titles such as:

- *Computer-aided chemical illustration system*
- *Apparatus and method for monitoring the validity of a molecular model*
- *Method and apparatus for determining molecular crystal structures*
- *Process and apparatus for the x-ray diffraction characterization of a material with amorphous phase*
- *System and method for reducing phase ambiguity of crystal structure factors*
- *Maximum likelihood density modification by pattern recognition of structural motifs*
- *Linear prediction of structure*

- factors in x-ray crystallography*
- *High-resolution crystallographic modelling of a macromolecule*
- *Fitting of X-ray scattering data using evolutionary algorithms.*

Another interesting and related area is that of "Crystallographic Business Method patents", where you don't patent an invention, but patent the business method of using an invention, an example of which is:

"Method for determining parameters of a unit cell of a crystal structure using diffraction", which includes:

"A method for determining the parameters of a unit cell of a crystal structure using diffraction is presented. The method includes the steps of repeatedly rotating the crystal at a predetermined angle, while the crystal moves in relation to a detection surface and measuring the position of radiation reflected from the crystal. The resulting combined measurements are utilized to accurately determine the unit cell dimension and orientation of the crystal"

Does this mean that some neutron (or X-ray) single crystal diffractometers might be moving their motors in an unauthorized way that infringes a current US patent monopoly? That would be for the lawyers to decide in a patent infringement case - if you had the funding to defend?

And the US Patent Office even contains such things as: US Patent 6,368,227 titled "Method of swinging on a swing" Filed: November 17, 2000.

It should be noted in the patent text that licenses are available from the inventor upon request!

Again, you may own a piece of equipment (e.g., in this case a child's swing) - but that does not mean you have the right to use it, as someone may have a patent monopoly on part or all of its use, in which you or your children may be infringing. If you extrapolate this type of business methods patent to crystallographic equipment, it seems to be happening already!

Yes of course, you can always find someone who will patent something anytime. There was until recently, for instance, a UK patent on the transmutation of elements i.e. by alchemy. But simply having a patent issued does not necessarily mean that you are correct. Remember that all that a patent does for you is to give you the right to sue. In most cases in practice it is too costly to bother. So manufacturers usually rely on holding a patent simply to frighten off others for fear of being sued.

Your example of the patent for cell-dimensions could be challenged by anyone skilled in the art (the abstract description makes it sound like the Weissenberg technique, and one has to read the actual patent to see that it is not, by the way) and is clearly one in which a manufacturer is trying to protect itself from its competitors. No doubt a competitor could easily see this off if it wished to spend the money. But for us lesser mortals, writing software for ourselves and our friends, is there anything to fear? I doubt it. After all, the patent holder in this case (a well known X-ray

company) is hardly going to want to alienate its customer base, i.e. us!

There is, of course, nothing to stop someone trying to enforce the "swinging" patent, but it would be unenforceable and in any case up to the commercial company to deal with, not us practising crystallographers. Then again, the above patents are not strictly software patents but patents on methods, so are not really the issue here. The dividing line between methods and actual software is fuzzy.

The real question it seems to me is this. If I write a piece of software, publish it in a journal and give it to my crystallography colleagues for free, do I have anything to fear? In theory someone holding a relevant patent could sue me for loss of potential earnings. If I had copied my software from a company patent, say that of an X-ray diffraction company, and by distributing it I was then wilfully harming the sales of that company, then I **deserve** to be sued and take the consequences. On the other hand, most of the software we produce as working crystallographers is not in this category, and if it is worthwhile software, it is more likely that a commercial company would want to pay us for the rights to the software copyright.

So my conclusion is, again, that I think software patenting is a silly idea, and I doubt if it would have any real effect on non-commercial software writers in crystallography. But then I have been proved wrong before!

Mike Glazer and Lachlan Cranswick

The Younger European Chemists' Conference, 26th - 29th August 2003, Grenoble, France

At the end of August 2003, I attended The Younger European Chemists' Conference at the ESRF in Grenoble, France. This is the third such conference in an annual series designed to bring together young researchers, both academic and industrial, from throughout Europe working not only in the traditional chemistry fields, but also in chemical engineering and technology. A wide range of chemical science was represented at the conference, from traditional organic synthesis, through physical and inorganic chemistry, to the use of nuclear magnetic resonance imaging to optimise fluid flow in chemical reactors.

The conference consisted of a mixture of keynote lectures, shorter lectures, and poster sessions, and was attended by over 140 people. All conference attendees presented a poster, and 35 people were selected (from a list of over 70 people who had expressed an interest) to give a 20 minute lecture on their work. With the exception of the keynote lecturers, everyone involved in either presenting a poster or giving a short lecture, was under 35 years old. The poster presentation sessions were simultaneously entries into a competition for the most original work presented by poster as decided by a panel of five judges. The prize for the best poster was the Europa Medal and €1000 in cash.

The main keynote lectures were

given by Dr Volker Trauz, CEO of Basell Polyolefins, Professor Jon McCleverty of Bristol University, and the recently-appointed Director of Research at the ESRF, Professor Sine Larsen. Professor Larsen's lecture was of particular interest, in which she discussed the many and varied uses of third-generation synchrotrons - not just in structural chemistry - from medical imaging to archaeology. It was followed by an afternoon touring the facilities at both ESRF and ILL.

The vast majority of the conference, however, was made up of short lectures and poster sessions. As with all conferences, these were an excellent way not only of hearing about many different areas of research, but also a chance simply to talk with other people, not always about chemistry. One particularly nice aspect of the short lectures was that each lecturer spent the first couple of minutes discussing their own home town, illustrated with pictures, and in some cases music. With speakers coming from such diverse places as Cyprus, Estonia, Egypt, Canada, Ukraine and Singapore this was a very interesting way to start a talk. The only exceptions to this were the two speakers from Southampton, both of whom skipped this section, confessing that "there are no nice photographs of Southampton".

My own contribution to the conference was my poster, which detailed some recent synthetic and crystallographic results in my work on s-block complexes with pyridones and cyanuric acid. It was clear from reading many of the other

posters, and attending all the lectures, that X-ray crystallography is heavily relied upon to provide key information which cannot be obtained by any other method. In particular, one speaker - an organic chemist - admitted that he would have been lost without crystallography as the NMR spectra of his compounds were too complicated. Unfortunately many of those who illustrated their talks and posters with pretty ORTEP drawings had very little idea how those structures were obtained at all.

Interspersed amongst the science were recreational sessions, including a boat trip, conference dinner at a nearby chateau, several visits to the bars of Grenoble, and even a visit from Sir Isaac Newton! These were an ideal way to relax after a very long day of science, even if I did once find myself at half past midnight explaining to a natural product chemist why anomalous dispersion is needed to determine an absolute configuration - I think I'd had a bit too much vin blanc at the conference dinner!

In closing, this conference was well-attended and well worth attending. I would recommend to anyone that they consider attending future conferences. I am grateful to the BCA for providing a grant to cover my travel expenses, to EPSRC for providing a bursary to cover the conference fees, and to my supervisor Bill Clegg for meeting miscellaneous expenses.

Gary S Nichol

European Congress and Exhibition on Advanced Materials and Processes - EUROMAT 2003, Lausanne, Switzerland

Engineering progress essentially depends on the availability and the intelligent use of materials. For many key industry areas, Europe constitutes a premier place for the development of new materials and their applications. In order to demonstrate an even more dynamic European character, Euromat 2003 was jointly run by the French, German and Swiss materials societies. Euromat 2003 covered fifteen sections in materials domain.

In the frame of these 15 congress topics that were substructured into 47 symposia, the programme included a total of 1283 highly innovative, scientific and technical contributions presented by 1080 speakers. The international group of chairpersons selected 133 Invited Lectures. Together with the 587 Lectures, they were presented in 179 sessions that were arranged in 13 parallel groupings. Further, the chairpersons invited 51 reputed experts to present a Keynote Lecture in the frame of their symposium. 508 contributions were on display as posters in two poster sessions. The scientific programme was particularly enriched by four Plenary Lectures given by well-known experts from both industry and academia, among whom was the 1996 Nobel Prize winner in Chemistry, Harry Kroto (Royal Society Research Professor at the University of Sussex in Brighton).

The exhibition organized during the congress was the platform for the top-development in the field of materials science and technology, reflecting the topics of

the congress. It was good to see representation of the famous manufacturers, such as Bruker AXS, Wiley VCH, NETZSCH, HWL Scientific Instruments, which are essentially from the top 100 blue chip companies.

The congress was huge and it was not possible to attend all parallel sessions. The most interesting and useful for my research I found Symposia on "Advances in Light Alloy Technologies", "Defects in Materials studied by Advanced Analytical Techniques", "Modelling Microstructure Mechanics Across the Length Scales" and "Solid State Transformation, Heat treatment". The poster session was organized over 2 days, so there was plenty of time to attend.

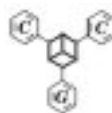
My contribution to the congress took the form of a poster presentation, the subject being "Experimental Study of the Phase Transformation and the Evolution of Microstructure with Temperature in Gamma TiAl Alloy". Taking into account that the congress hosted more than 150 sessions, the poster presentation was of real benefit to me, as it provided a high density interested audience during the 2 days. My poster presentation was well attended, and generated many questions. It was extremely fruitful and motivating to hear the comments of the top experts in my field. I would like to mention first of all the discussion with Prof. David G. Morris, Centro Nacional de Investigaciones Metalurgicas (CENIM), Madrid, Spain, who chaired the "Nanostructured Materials" Symposium. His positive assessment of the results I presented at the congress was a great endorsement for me. As a result of attending poster session, where Dr. Peterson Ferrandini from University Centre FEI, Sao

Bernardo do Campo, Brazil and Prof. Igor M. Rasumovskii from Institute of Metals, "Kompozit", Korolev, Russia gave presentations I have been able to identify opportunities for future collaborative work.

There are few occasions as beneficial as this for any materials scientist in the European materials arena to present and to discuss his/her work, and it was a most constructive, rewarding and interesting experience for my future career.

Tatiana Novoselova

Chemical Crystallography Group



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

Call for Nominations

Elections will be held at the CCG AGM in Manchester for the posts of Secretary/Treasurer and one ordinary member of the Committee. The present incumbents (Secretary/Treasurer: Harry Powell, Member of Committee: Simon Coles) will have each served a full term and will not be eligible for re-election to the same posts (see rules 12 and 15 of the Constitution).

The deadline for nominations is seven days before the CCG AGM in Manchester. Names of the current members and the Constitution of the Group can be seen on the CCG website.

CCDC Chemical Crystallography Prize for Younger Scientists 2004

Nominations are invited for this award, to be made at the BCA

Spring 2004 Meeting. The award is sponsored by the Cambridge Crystallographic Data Centre. The award is for:

'Original research in the field of chemical crystallography or the application of crystallographic information to structural chemistry. This definition shall include advances in instrumental, experimental, theoretical or computational techniques that contribute to this field.'

The CCG Committee will select the award winner on the basis of the published research papers of nominated candidates. Candidates should not have reached their 35th birthday by 1st January 2004, but candidates up to five years older may be considered under exceptional circumstances. The award winner will receive a commemorative item and a monetary prize, and will give a lecture on his/her research at the BCA Spring Meeting which will be held at UMIST in Manchester in April 2004.

Previous winners of the award are Dr Jacqueline M. Cole (Cambridge, 2000), Dr Claire Wilson (Nottingham, 2001), Dr David R. Allan (Edinburgh, 2002) and Dr Ivana Radosavljevic Evans (Durham, 2003).

Further details and a nomination form may be obtained from me (Dr H.R. Powell, MRC Laboratory of Molecular Biology, MRC Centre, Hills Road, Cambridge, CB2 2QH, e-mail: hrp1000@cam.ac.uk fax 01223 213556), or on the CCG website.

Nominations must be received by Friday January 9th, 2004.

Harry Powell, Secretary

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. The help of Dr Simon Parsons and the IUCr listing is gratefully acknowledged.

1-2 December 2003

Validation of Macromolecular Structures and Structure Determination Steps., Trieste, Italy
[<http://www.elettra.trieste.it/um11/sat1.html>]

3-4 December 2003

The Molecular Basis of Life: is Life Possible without Water?', The Royal Society, London
[http://www.royalsoc.ac.uk/events/discussion_meetings/level_2/dec_water03.htm]

4-7 December 2003

High Pressure Structure and Reactivity: The Science of Change. Lawrence Berkeley National Laboratory, Berkeley, California.
[<http://www-esg.lbl.gov/esg/meetings/IUCrCHP0903/index.html>]

8-9 December 2003

PCG Autumn Meeting: Probing Structure at the Nanoscale - Fact, Fiction or Hype? Abingdon, Oxon
[<http://bca.cryst.bbk.ac.uk/bca/pcg/meetings.htm>]

9-13 December 2003

International School on Crystal Growth and Characterisation, La Pedrera, Rocha, URUGUAY
[<http://www.iscgcha2003.fq.edu.uy/>]

10-12 December 2003

The First International Workshop on Advanced Superhard Materials University Paris Nord, Villetaneuse, France
[<http://www-lpmtm.univ-paris13.fr/Workshop/Workshop.htm>]

19 December 2003

BSG Winter meeting and 21st AGM, London
[<http://bca.cryst.bbk.ac.uk/bca/bsg/welcome.htm>]

8-10 January 2004

XXXIII National Seminar on Crystallography, India
[<http://www.ncl-india.org/events/main.html>]

9-16 January 2004

LANSCE Neutron Scattering Winter School on Magnetism, Los Alamos NM, USA
[<http://lansce.lanl.gov/neutronschool/index.html>]

13-16 January 2004

Joint Meeting on Neutron Optics and Detectors, Tokyo, Japan
[<http://www.nop2004.jp>]

27-28 January 2004

Workshop on Polarisation Analysis and Inelastic Cold-Neutron Scattering at Australia's Replacement Research Reactor, Lucas Heights, Australia
[<http://www.ansto.gov.au/ansto/bragg/workshops/workshop10.html>]

14-18 February 2004

Biophysical Society 48th Annual Meeting, Baltimore, MD, USA
[<http://www.biophysics.org>]

23-27 February 2004

International Conference on Dynamics of disordered materials on the nanometer scale, Daewoo Hotel, Hanoi, Vietnam
[<http://www.engconfintl.org/4ah.html>]

23-25 February 2004

PPXRD-3, The 3rd Pharmaceutical Powder X-ray Diffraction Symposium, Sponsored by the International Centre for Diffraction Data Hilton Head Island, SC, USA
[<http://www.icdd.com/ppxrd>]

15 March 2004

2nd Annual Biomaterials Workshop, Cranfield University, Shrivenham
[<http://www.cranfield-biomaterials.com>]

30 March-1 April 2004.

Neutron Scattering in Materials, at the IOM3 Congress in Carlton House Terrace, London
[<http://www.iom3.org/congress2004>]

6-8 April 2004

BCA Annual Meeting, UMIST, Manchester
[<http://www.isis.rl.ac.uk/BCA2004>]

10-14 May 2004

The Second Moroccan School of Crystallography, EMC2, El Jadida, Morocco
[www.ucd.ma/fs/emc2]

2-4 June 2004

13th Annual CCP13/Fibre Diffraction & Non Crystalline Diffraction Workshop, ILL/ESRF, Grenoble, France
[<http://www.ccp13.ac.uk>]

6-10 June 2004

American Conference on Neutron Scattering, College Park MD, USA
[<http://www.ncnr.nist.gov/acns>]

9-20 June 2004

Electron Crystallography: Novel Approaches to Structure Determination of Nanosized Materials, Erice, Italy.
[<http://www.crystalalice.org/2004/EICryst2004.htm>]

9-20 June 2004

Polymorphism : Solvates and Phase Relationships. Erice, Italy,
[<http://www.geomin.unibo.it/orgv/erice/bernstei.html>]

1-10 July 2004

XVI International School on the Physics and Chemistry of Condensed Matter: Structural Aspects of Solids, Bialowieza, Poland
[<http://alpha.uwb.edu.pl/schoolXVI/>]

17-22 July 2004

American Crystallographic Association Meeting, Chicago, IL, USA
[<http://www.hwi.buffalo.edu/ACA/index.html>]

19-23 July 2004

20th General Conference of the Condensed Matter Division , European Physical Society, Prague, Czech Republic
[<http://cmd.karlov.mff.cuni.cz/CMD/>]

21-23 July 2004

4th European Workshop on Piezoelectric Materials (4th EWPM), Montpellier, France
[<http://www.lpmc.univ-montp2.fr/~4ewpm>]

2-6 August 2004

53rd Annual Denver X-ray Conference
Steamboat Springs, CO, USA
[<http://www.dxcicdd.com/>]

20-28 August 2004

32nd International Geological Congress, Florence, Italy
[<http://www.32igc.org/>]

22-24 August 2004

Satellite meeting on "Mathematical and Symmetry Aspects" (ECM-22) Budapest, Hungary,
[<http://www.lcm3b.univ-nancy.fr/mathcryst/satellite.htm>]

26-31 August 2004.

22nd European Crystallographic Meeting, Budapest, Hungary
[<http://www.ecm22.mtesz.hu/>]

31 August - 10th September 2004

Synchrotron Radiation Summer School Daresbury, UK
[website not yet ready]

2-5 September 2004

EPDIC-IX, European Powder Diffraction Conference, Prague, Czech Republic
[<http://www.xray.cz/epdic>]

5-10 September 2004

3rd International and 28th European Peptides Symposium - Prague, Czech Republic
[www.kenes.com/28eps]

7-10 September 2004

X-TOP 2004 - 7th Biennial Conference on High Resolution X-Ray Diffraction and Imaging, Pruhonice (near Prague), Czech Republic
[<http://www.xray.cz/xtop>]

4-7 October, 2004

Analysis of Functionally Graded Materials (1st SOTAMA-FGM) Krakow, Poland
[<http://www.imim-pan.krakow.pl>]

17-21 November 2004

SGO International Conference on Structural Genomics 2004 (ICSG 2004), Washington Hilton & Towers Hotel, Washington, DC, USA
[no website yet given]

19-29 May 2005

Evolving Methods in Macromolecular Crystallography, Ettore Majorana Centre, Erice, Italy
[<http://www.crystalerice.org/futuremeet.htm>]

23-31 August 2005

XX Congress of the International Union of Crystallography, Florence, Italy
[<http://www.iucr2005.it>]

28 November-2 December 2005

2005 International Conference on Neutron Scattering (ICNS 2005), Sydney, Australia
[<http://www.sct.gu.edu.au/icns2005/announce.html>]

9-18 June 2006

The Structure Biology of Large Molecular Assemblies, Ettore Majorana Centre, Erice, Italy
[<http://www.crystalerice.org/futuremeet.htm>]

7-17 June 2007

Engineering of Crystalline Materials Properties: State-of-the-Art in Modeling, Design, and Applications, Ettore Majorana Centre, Erice, Italy,
[<http://www.crystalerice.org/futuremeet.htm>]

Kate Crennell writes:

In response to my request for further news of events associated with the 50th anniversary of the discovery of the structure of DNA I have received a letter full of news of events from Professor Herbert Wilson who worked with Maurice Wilkins at Kings' College, London and helped to demonstrate that the phosphate groups were on the outside of the DNA helix. He later became Professor of Physics at the University of Stirling. He wrote this poem for the special occasion.

On the 50th anniversary of the double helix

Let's wish many happy returns of the day
To the double helix of DNA.

Five decades have passed since Watson and Crick
Unveiled their model - like a conjuring trick!

Five decades since Wilkins and Franklin days
Gave support for the model using X-rays.

Five decades in which The Code was broken,
And dogma was an information token!

Five decades when we have also seen
The sequencing of every human gene.

But these advances raise ethical issues
In bioengineering cells and tissues.

In the era of GM crops and Dolly,
Some see great hopes but others folly.

Let's hope that in all the applications
Wisdom prevails when making decisions.

But these are topics for future debate,
For today is a day to celebrate!

Herbert Wilson



*And in honour of the year
that came and went,
Here's the offering from
the Royal Mint!*

Olga Kennard Research Fellowship 2004

Applications are invited for the Olga Kennard Research Fellowship for research in crystallography or structural molecular biology.

Eligibility: Applicants must have a PhD or equivalent research experience and have at least three years' postdoctoral experience by 1 October 2004. Career breaks such as maternity leave, EU national service and voluntary service overseas can be discounted, but teaching experience and/or time spent in industry since the award of a PhD should be included in the total amount of postdoctoral experience. Part-time work will be counted *pro rata*.

Applicants must be citizens of the EU, Norway, Israel or Switzerland but there are no residency requirements for this fellowship. Persons holding a permanent post in a European Union university will not be considered.

Length of tenure: This appointment is tenable for five years only from 1 October 2004 and there is no possibility of renewal.

Place of tenure: The fellowship must be held in a UK university or recognized research institute.

Value: The Olga Kennard Research Fellowship is designed to be particularly beneficial for women as it includes additional funds for family support, conversion for a period to part-time working and maternity leave if required. The fellow will be paid on the non-clinical academic and academic-related staff (Lecturer A and B) salary scale which currently runs from £22,191 to £33,679. Starting salaries will be set at a point on this scale, with London Allowance where appropriate, and will rise incrementally each year. A limited number of merit increments will be awarded each year to reward outstanding performance. Annual research expenses (up to a maximum of £13,000 for the first year and £11,000 thereafter) will be available together with relocation expenses and a contribution to baggage costs for successful applicants from overseas and their families.

Number offered: 1 only.

Closing date: 9 January 2004. Past experience suggests that the results of the competition will be available about five months after the closing date. Please note that interviews are not held for these fellowships.

Applications can only be submitted online on the Royal Society's new electronic Grant Application and Processing (e-GAP) system (<https://e-gap.royalsoc.ac.uk>, or via the e-GAP logo on the front page of the Society's web site). **Applications can no longer be submitted on paper.** If you would like any further information on these schemes, about the e-GAP process, or the submission of your application, please contact the Research Appointments Department, The Royal Society, 6-9 Carlton House Terrace, London, SW1Y 5AG (Tel: 020 7451 2545 or email: e-gap@royalsoc.ac.uk).

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