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**NEXT ISSUE OF
CRYSTALLOGRAPHY NEWS**

CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association. Text should preferably be sent as MSword documents (any version - .doc files) or else as .rtf or .txt on a PC disk or electronically. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (e.g. awards, honours, retirements etc.), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews. Please ensure that items for inclusion in the **March 2003** issue are sent to the Editor to arrive before **17th January 2003**.

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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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President's Remarks

Well, I survived the bears and mountains of Wyoming (although eternally hungry chipmunks were another matter) to make it to an early Council meeting in mid-September with a lot of material to discuss. We offered three new honorary life memberships of the BCA to Professors Michael Woolfson at York, Andrew Lang at Bristol and Jane Brown at ILL, all of whom have accepted. These are in honour of a lifetime of achievement and service in crystallography. The constitution allows up to 20 honorary life members at any time, and we have not currently reached that number. If you have suggestions for suitable eminent candidates feel free to contact me or any member of Council with your ideas.

There is another issue on which the views of the BCA are sought: Council discussed at length the possibility of a two-tier membership scheme. One level would encompass the standard membership that we all currently enjoy (at a very modest fee). The other level would be a premium one for those who would be designated 'Foundation Members' (or a similar title - this is not really the issue yet). Such members would be crystallographers of over 5 years standing, and who would pay a double membership fee. There would, of course, be no formal letters after one's name, but such members could refer to themselves as Foundation Members and would, perhaps, be listed on our web site. We will discuss this at the AGM, but your views are solicited before then.

The AGM will also be the scene of new elections (including the President). I am a great believer in elections rather than simply filling posts by default, so please make nominations for all our vacancies. Details can be found elsewhere in this issue of Crystallography News. This is something the ACA have enshrined in their constitution, and it works.

The York Spring Meeting is shaping up very well with high throughput as its plenary theme. York University is very accommodating in its booking schemes for conferences, and this has made it relatively easy for us to pass on flexibility to delegates (Although there is a considerable financial risk involved here.) This means you can book for any number of days and nights as you see fit during the meeting. It is also shorter than usual: we are all under great pressures of time these days, and conferences are getting shorter in response to this, even the IUCr. The next triennial congress in Florence in 2005 will last 7 days with an optional excursion as a final extra day. The 2008 congress will be in Osaka.

Finally, the BCA web site is in the process of a major upgrade to modernise its look and feel, and to provide information more easily. Give your opinions to our webmaster, Jeremy Cockcroft.

Chris Gilmore
November, 2002

Cover pictures left to right:

PCGlogo? Can you do better?

Streamlining at Diamond

Crystallography at low temperature

Lovely weather in Geneva

Cross-linking at CrystEngComm

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This is my fourth issue as Editor, and so brings me to the end of my first year. I hope that you have liked what you got – there have been few complaints, and I am looking forward to my second year. Keep the material flowing! In fact, it has been necessary to hold back some material for the next issue. A particularly interesting article to look forward to is one by Lachlan Cranswick on the importance of Patents to Crystallographers, and it isn't quite what you might think, either! I am particularly grateful to those who have taken on Book Reviews. If, as Michael Woolfson said in his Ewald prize

address at Geneva, a journal can be known by the quality of its Book Reviews, we are not doing badly!

While your chances of getting published in *Crystallography News* are much greater than your chances of getting into *Nature*, we do not, in fact, publish everything we are sent. In particular, there are two types of submission that require editorial judgement. One consists of articles which take extreme standpoints on scientific matters. We are not, for example, looking for arguments that matter is not atomic in nature, and that our experiments only find it that way because we are biased. The other is more difficult, and I may have made mistakes here. That is the "press release" from a firm, which may be considered (particularly by other firms!) as a disguised advertisement.

The main item in *Crystallography News* number 83 is the new, streamlined programme for the York meeting in April, and how to apply for a Bursary to get there! There are also accounts of

several meetings during the summer, some of which are reports written by our bursars, to all of whom many thanks for their submissions.

Nothing has turned up worthy of an agony column this month, but "Can you believe it?" has encountered some amusing bits of crystallography in the press and elsewhere.

An apology for a careless mistake in the last issue must go to Dr Giovanna Cicognani, of the ILL. She wrote, thanking us for mentioning the ILL Annual Report 2001, but then adds: 'However, may I draw your attention on the correct spelling of my first name: "GiovannA" and not Giovanni, and on the fact that I am a not a "he" but "she" ? ' And she sent me a photo too!

With very best wishes for Christmas and the New Year, and let me hear from you by January 17!

Bob Gould
November, 2002



Acknowledgements

BCA Sponsors

The British Crystallographic Association is grateful to Birkbeck College, University of London, who host and manage the server for our Website.

Arnold Beavers Bursaries In 2003

BCA Council gratefully acknowledges several generous donations to the fund and welcomes further contributions to this worthwhile cause. A donation form can be downloaded from the Membership section of the BCA web site.

Applying for Bursaries in 2003

Bursaries for York Spring Meeting (15-17 April 2003):

A limited number of bursaries are available from the Arnold Beavers Bursary Fund to cover the £155.90 cost of two nights accommodation, food and registration. The bursary will not cover travel expenses and recipients will be expected to present a poster.

Council is seeking commercial sponsors of Spring Meeting Bursaries and it is hoped to again offer some "Named Bursaries" at this meeting.

The **closing date** for all applications is **10th February 2003**, applicants should ask for an Arnold Beavers bursary application form from the BCA Administrative Office or download one from the membership section of the BCA website (details below).

Bursaries for other BCA Meetings and Schools:

These are administered directly

by the organisers of the Meeting or Teaching School. They will publicise the procedure for their bursary applications, whether funded by the BCA itself or a constituent group.

General Bursaries:

Arnold Beavers Bursaries are available to members, (see point (a) below) who wish to attend relevant scientific meetings in the UK or abroad which are not organised by the BCA.

All applications are considered by the BCA Bursary Committee, comprising the President, Vice President, Treasurer and Secretary and are guided by the following considerations:

(a) The bursaries are primarily intended to support bona fide research students and postdoctoral workers who are BCA members. Applications from those with more senior non-tenured positions, and from those in junior permanent positions where university or industrial funds are unavailable, may be supported at the discretion of the BCA Bursary Committee if BCA funds are available.

(b) Applicants must normally have been a BCA member for 6 months before applying.

(c) Applicants will not normally be considered if they have been awarded a general bursary in the previous two years.

(d) Preference will be given to applicants who have attended a BCA meeting. Applications must be received at least 6 weeks

before the date of the meeting/visit. No retrospective applications are possible.

Successful applicants are expected to submit a word-processed short scientific report on the meeting/visit soon after their return; this should include details of the sessions attended and of the applicant's presentation. The reports may be submitted via electronic mail to the BCA Administrative Office and may be published later in 'Crystallography News' or the BCA website.

In short, applicants should ask for an Arnold Beavers bursary application form from the BCA Administrative Office or download a copy from the Membership section of the BCA web pages.

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Dr Frank H. Allen appointed as Executive Director of the Cambridge Crystallographic Data Centre

The Board of Governors of the Cambridge Crystallographic Data Centre (CCDC) is delighted to announce that Dr Frank Allen has been appointed as Executive Director of the CCDC from 1 October 2002, following the retirement of Dr David Hartley. Dr Allen is currently Scientific Director of the CCDC.

"By combining the Executive and Scientific Director posts, we emphasise the CCDC's commitment to its scientifically driven ethos and our wish to see this continue," said Prof. Peter Willett of the Department of Information Studies at the University of Sheffield, and Chairman of CCDC's Board of Governors. "Dr Allen has played a major role in establishing CCDC's enviable worldwide scientific reputation, and this will be further enhanced in his new combined role."

Dr Frank Allen has worked at CCDC since 1970, following undergraduate and graduate studies (BSc, ARCS, DIC, PhD) at Imperial College, London and postdoctoral work at the University of British Columbia, Vancouver, Canada. He has been involved in most major developments at the CCDC, with a strong accent on creating the Cambridge Structural Database (CSD) of small molecule crystal structures, software development, and applications of the accumulated CSD data for research

purposes. Dr Allen has authored or co-authored more than 200 publications and has edited 16 reference books and conference proceedings.

He became a Fellow of the Royal Society of Chemistry in 1992, was awarded the RSC Silver Medal and Prize for Structural Chemistry in 1994, is a Visiting Professor of Chemistry at the University of Bristol from 2002, and will receive the Herman Skolnik Award of the American Chemical Society Division of Chemical Information in 2003. He has held a range of senior positions in the British and European Crystallographic Associations and in the International Union of Crystallography (IUCr), including the Editorship of *Acta Crystallographica*, Section B from 1993-2002. He is a current member of the Editorial Board of *Chemical Communications*, and of the International Advisory Board of the Protein Data Bank (RCSB, USA).

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David Hartley

Individual Membership of the European Crystallographic Association

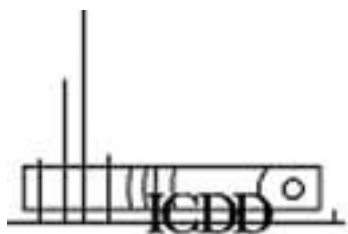
BCA members are invited to become individual members of the European Crystallographic Association (ECA). ECA is the regional organisation representing crystallographers in Europe and Africa, and is the body through which organisation of the major European Crystallographic Meetings (ECM) is carried out. The ECA itself has a vibrant scientific structure, with 13 Special Interest Groups established to date - the programme for ECM meetings is largely constructed around input from the SIGs. Individual Members have the right to elect their representatives for the Council (1 Councillor elected per 100 Individual Members), and can propose to set up a SIG. Individual members also receive substantial discounts on registration fees for ECM meetings.

Equally importantly, for a modest annual fee of 10 Euros (£6.50), you will be helping to strengthen your professional environment within Europe and will help the development of the Association and its work.

The BCA Treasurer has offered to collect individual membership fees from BCA members on behalf of the ECA, and incorporate these into a single payment, which is highly cost-effective. Details and a membership application form can be found on the BCA Website.

More information on the ECA can be found on
<http://www.ecanws.org>

Chick Wilson
ECA Councillor



ICDD Press Release, September 12, 2002 – New Appointment to the Board of Directors

The Board of Directors of the International Centre for Diffraction Data is pleased to announce that David J. Taylor of the United Kingdom has been appointed to the office of Director-at-Large, serving the term 2002-2004.

Effective immediately, this appointment was made in accordance with the bylaws, Section 4.7(b), in response to the vacancy in the Director-at-Large position, formerly held by Ron Jenkins.

Endorsed by strong support of the ICDD membership, Dave brings to the Board extensive experience in XRD and XRF as a senior research scientist in the glass industry. He took early retirement from Pilkington and is now active as a consultant in x-ray analysis to industry and academia. He is the Treasurer and ICDD representative of the British Crystallographic Association and has invaluable experience as an active ICDD member and Regional Co-chair for the United Kingdom.

The 6th International Conference of Ancient DNA and Associated Bio- molecules, Jerusalem, July 21-25 2002.

This conference was a great success because of the quality of the papers presented and the support shown by our many international visitors. We were particularly pleased to note a geographical shift in that apart from North American and Western European delegates we were pleased to see delegates from Eastern Europe, the Indian subcontinent, Latin America and Africa, making our discipline truly international. Those who were not present did miss an excellent scientific as well as social meeting.

At the conference it was decided that the next meeting would be held in Australia at the University of Queensland under the chairmanship of Tom Loy. In view of the enviable reputation Australia has for hosting international events I am certain you will not want to miss aDNA7.

It was proposed that we should form a more formal organization. During the business meeting it was felt that such an organization should have a basis of local chapters which would be country based. Proposals were made on guidelines, ethical and scientific and a position paper. It was decided that position papers will be asked to be presented at aDNA7. Tom Loy was appointed temporary chairperson. He will appoint committees to study the issues involved, and they will present their reports at aDNA7.

Thus it is extremely important that you send him any input you may have, and plan to attend aDNA7.

In the interim I am off for a long rest, but not before thanking the many people who contributed to making aDNA6 a success:

as they say in Israel:
Shalom

Mark Spigelman

European Commission Programmes supporting Neutron Scattering in Europe

Neutron scattering facilities at a number of laboratories are open to European scientists through the Access to Research Infrastructures action of the Improving Human Potential Programme of the European Community. Access is free of charge, and support is given for travel and subsistence costs. The programme also supports networks for research and technical development.

The Neutron Round Table promotes coordination and collaboration between facilities and networks, and activities that spread the use of neutron scattering (conferences, workshops, technical meetings etc. - deadlines for applications for support are April 15 and October 15).

For more information on the Round Table, and links to facilities and networks, go to http://www.risoe.dk/afm/Neutron_Round_Table.htm/

News from the CCG

Ninth BCA/CCG Intensive Course in X-ray structure Analysis

As announced in the last issue, this course will take place in Durham from 7th-15th April, 2003. The course finishes in time for participants to attend the BCA Spring Meeting as well. For registration details and further information please see <http://bca.cryst.bbk.ac.uk/BCA/CCG/index.html> or contact Claire Wilson, claire.wilson@nottingham.ac.uk.

CCDC Chemical Crystallography Prize for Younger Scientists 2003

Nominations are invited for this award, to be made at the BCA Spring 2003 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 2003, 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 the University of York in April 2003. Previous winners of the award are Dr Jacqueline M. Cole (Cambridge, 2000), Dr Claire Wilson (Nottingham, 2001) and Dr David R. Allan (Edinburgh, 2002).

Further details and a nomination form may be obtained from the Secretary of the Chemical Crystallography Group (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: (<http://bca.cryst.bbk.ac.uk/BCA/CCG/ccg.html>).

Nominations must be received by Friday January 10th, 2003.

Chemical Crystallography Group - Call for Nominations

Elections will be held at the CCG AGM in York for the posts of Chairman, Deputy Chairman and one ordinary member of the Committee. The present incumbents (Chairman: Paul Raithby, Deputy Chairman: Sandy Blake, Member of Committee: Jon Steed) 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 York. Names of the current members and the Constitution of the Group can be seen on the CCG website, given above.

9th CCP4 Glasgow Protein Structure Workshop, Galashiels, September 4th-6th, 2002.

Sixty participants from Dundee, St Andrews, Edinburgh, Glasgow, York, Sheffield, Leeds, Daresbury, AstraZeneca & Manchester gathered for this annual northern UK regional protein crystallography meeting - which is free for students and subsidised for non-commercial participants through generous sponsorship from CCP4, Hamilton, Molecular Dimensions, AstraZeneca, Greiner, Bede Scientific and Bruker AXS. The programme accommodates short presentations describing current work as well as a special-topic morning workshop with invited speakers.

On a sunny Wednesday afternoon, Colin Williams (Sheffield) opened the first session on new structures with a talk on aconitaseB from *E.coli*. David Kommander (Dundee) showed how "essential dynamics" can model a neat switch in the PDK1 kinase domain. Bernard Lohkamp (Glasgow) talked on a histidine-biosynthesis enzyme (HisG-PRT) in a surprisingly effective Scottish-German accent. Laura Kehoe (Sheffield) discussed an inhibitor complex of streptogramin A acetyltransferase, a protein which confers resistance to certain macrocyclic lactones in *E. faecium*. Iain Kerr (Dundee) presented a challenging MAD (SeMet) structure solution, complicated by twinning, of an

archaeal single-stranded DNA-binding protein—reminding us that the de-twinning process destroys the anomalous signal. Dominic Hunter presented a splendid review of flavocytochrome B2 structures.

After a well-deserved coffee break (during which we saw the new Hamilton crystallisation robot), there was a lively session on preliminary results. Konstantinos Beis (St. Andrews) demonstrated the potential pitfalls of believing the mosaicity estimation in data processing programs. Hayley Patterson (York) has been purifying spore coat proteins from Anthrax! Alistair McEwen (Glasgow) presented his collaboration with Aventis on a Tau-class GST from rice and the implications for anti-herbicide structure-based drug design. Steven Glynn gave us a taste of the Structural Genomics efforts at Sheffield aimed at novel antibiotics: by using the inducible knockout plasmid pMUTIN it has been possible to identify essential genes of the menaquinone biosynthesis pathway in *B. subtilis*. Paul Blackburn (Glasgow) presented progress on the structure determination of a GPCR, surely one of the more challenging projects discussed at the meeting. Impressive protein quantities are being obtained for the chemokine receptor D6 - 1mg of soluble D6 per 6 litres of insect cell culture! Simon Newstead (St Andrews) presented the structure determination of nanH, a large sialidase from *C. perfringens*.

Karen McLusky (Dundee) introduced our “vintage

speakers” for an after-dinner session, making polite analogies to quality malt whiskeys. The evening kicked-off with Garry Taylor’s (St Andrews) presentation on the structure of Alba (appropriately, the old name for Scotland), an archaeal chromatin protein modulated by acetylation. Andy Freer (Glasgow) offered the interesting hypothesis that myelin can be used as an MS marker. He described the interactions of some myelin-specific proteins, such as MBP, MAG and MOG and their possible use as MS targets. For the last talk of the evening, Dundee Daan (with graphic aid from PyMol) took us on a white-knuckle roller-coaster ride around and through chitinase - three different ChiB inhibitor-complex structures enabled elucidation of the reaction mechanism and provided insights for the design of specific antibacterial drugs. The day’s talks had clearly generated much excitement - judging by the hours of discussion that followed in the bar.

The following morning was dedicated to “High-throughput crystallisation”, this year’s special-topic workshop. We started with inspiring presentations from our two AstraZeneca-invited guest speakers, Janet Newman (SGX, California) and Dave Stuart (Oxford). Janet, introduced by Richard Paupit as “seriously into power yoga”, shared lessons learned from her experience on ~1000 proteins tested at SGX in ~2.5 years. She stressed that automated optimisation should be based on improvement of

crystal diffraction rather than crystal “gorgeousness”, and that this can be implemented. Janet’s views on NMR were positive if it could increase the probability of crystallisation. Dave provided an overview of the high-throughput setup at the new Oxford Protein Production Facility (from protein cloning to crystal imaging). He emphasised that high-throughput requires a powerful LIMS database (in his case the commercially available Nautilus). Jason Breed (AstraZeneca) presented a list of considerations for automating crystallisation. Since the bottleneck is tray-gazing, not making drops, he maintained that the priority for automation must be image capture and analysis rather than automated liquid handling, which appears to dominate current focus. Gabriela Juarez-Martinez (Glasgow) discussed microtechnology applications to crystallisation; particularly impressive were crystallisation studies in which an accurate temperature gradient could be applied across a chip. The new Hamilton crystallisation robot was then introduced by Carsten Mang. An open discussion session followed, in which best current methodology was debated and also pertinent questions were put to our expert guests.

During the free afternoon, Joe Jaeger planned a walking trip which was curtailed by bad weather and good beer, arguably more on target than Lindsay’s previous ventures. Others explored great cities such as Edinburgh and Galashiels. In the evening, Janet Newman rounded off a superb conference

dinner with a recital of a crystallographic poem. This was followed by an impromptu-composed scientific paper (somehow, frogs featured highly) to which every participant contributed (might not make it to *Nature*, but maybe *Crystallography News*?). We even sang "My Bonnie" for Arnold Beevers; it seemed appropriate. (Mainly) scientific discussion continued in the bar and around the pool table, juke box, and the Risk quiz-machine which we all swore took serious liberties with the truth.

The last morning started with a session on complexes: Neil Paterson (Glasgow) told us of his enviable crystals that grew effortlessly and diffracted beyond 1 Å, but mysteriously did not have his expected Huf activity. Jon Read (AstraZeneca) reported on LDH inhibitors, work done at Bristol University as part of the WHO "Medicines for Malaria" initiative. Douglas Houston (Dundee) clearly explained the different affinities of two natural cyclic pentapeptides (argadin and argifin) for chitinase B. Ludovic Otterbein (AstraZeneca) reported on work done during his time at the Boston Biomedical Research Institute on the actin scavenger system and on the complex of actin and vitamin-D binding-protein, the "jaws of life". After a revitalising coffee break, the emphasis shifted slightly to methods. Huanting Liu (St Andrews), unfazed despite lack of title in the programme or in his title slide, discussed high-throughput expression using TEV protease cleavable His-tags. Peter

Wood (CCP4/Edinburgh) gave us a tantalising glimpse of early work into LIMS tailored for protein crystallography. Alun Ashton entertained us royally whilst delivering the sad message that "CCP4 can't help you crystallise your protein". His award-winning use of PowerPoint and masterful "mouse"-control deserves special mention. Aleksander Roszak (Glasgow) gave the latest instalment in the epic structural characterisation of photosynthesis, and David Hargreaves (Sheffield) closed both session and meeting with the structure of Kid toxin protein from *E. coli*.

The next Galashiels meeting will be the 10th anniversary, and promises to be very special. It takes place September 3-5, 2003, again at the Galashiels Campus of the Heriot Watt University. We've booked the larger lecture theatre to allow more participants: if you are interested please contact any of the organisers (neil@chem.glasgow.ac.uk, l.sawyer@ed.ac.uk, richard.pauptit@astrazeneca.com)

J.Breed, L.Otterbein, R. Norman & J.Read (AstraZeneca)

IUCr meeting in Geneva Switzerland, August 2002: Three reports

Attending such a large and diverse conference serves not only to develop my own research but to obtain a wider picture of what is happening at the frontiers in crystallography, meet other crystallographers from around the world and sample some of the local culture. Although concerns about personal safety meant that the venue had to be switched from Jerusalem, a fantastic venue culturally and historically, we were welcomed to Geneva. We were treated to Israeli folk dancing as well as to Swiss cheese fondues and delicious biscuits at coffee time. This account gives an overview of just a fraction of what was on offer at the IUCr meeting in Geneva. I am a crystallography service provider and have found that as the field of supramolecular chemistry has grown, synthetic chemists are increasingly aware of the relevance of crystal engineering and polymorphism to their own research and are now more appreciative of what crystallography can do for them. Many presentations emphasised the vital role polymorphism has to the pharmaceutical industry. The control of crystal growth to obtain the best polymorph for a drug draws together many crystallographic areas, such as crystal structure prediction. Sally Price showed us some of the theory bringing in kinetic as well as thermodynamic factors and Sam Motherwell looked at crystal structure prediction from the perspective of looking for similar

molecules in the CSD and using their crystal packing motifs. Finding polymorphs with high throughput polymorph screening using a multiwell crystallisation plate on a powder diffractometer was illustrated by Christian Lehmann. In his overview of polymorphism on the final day of the meeting, Guatam Desiraju described the nemesis of crystal design being understanding and controlling the phenomenon of polymorphism.

Just some of the topics on the crystal engineering side included the application of Hirshfeld surfaces to "fingerprint" crystal packing by Mark Spackman, informative as well as visually stunning where the difference in Hirshfeld surfaces for two polymorphs was clearly shown. Guy Orpen used platinum group metal complexes as synthons or tectons in building up organic-inorganic hybrid frameworks.

Light and thermally induced spin state transitions of several compounds related to $[\text{Fe}(\text{NCS})_2(\text{phen})]$ was another popular topic in chemical crystallography. Lasers have been incorporated with diffractometers for data collection and coupled with fast low temperature data collection. I first heard about this at Phil Coppens' excellent talk at the BCA meeting in Reading in 2000 and several speakers including Andreas Goeta told us more at this IUCr. There was a whole session devoted to real time probing of structural changes and excited molecules which I was sorry to miss but this was



blocked against the polymorphism session.

I presented a poster on "Bridging the Z-macrocycle, Consequences for conformation and reactivity" which contained comparisons of shape and size of 16-membered macrocycles with substituents on opposite sides of the macrocycle (*trans* position) with those with *cis* substituents made by Daryl Busch and co-workers. The cavity sizes of the *cis* and *trans* are identical but the *trans* species have taller and narrower cavities and ESR studies showed that the *trans* is less effective in reversibly binding dioxygen. Two of our *trans* species gave polymorphs which gave us a feel for the influence of packing forces on the cavity size and shape. I look forward to finding more polymorphs when we have our in-house CCD diffractometer and the chance of finding the twin laws for crystals that would fail to index on our serial detector diffractometer. In the session on Twins, Disorders and other Demons we heard from Simon Parsons about programs and tips

on how such difficulties can be overcome in more user-friendly ways such as ROTAX incorporated into the Crystals program and also by using the Bruker-Nonius program, Gemini.

Progress on other frontiers also caught my eye: Michael Woolfson reminded us that there are still key challenges for direct methods, namely solving macromolecular structures with resolution poorer than atomic resolution. Current improvements have been made by applying dynamic density modification as employed by the program ACORN. George Sheldrick told us more about new strategies for solving macromolecular structures with SHELXE such as treating the electron density as a spherical surface. If single crystal aren't forthcoming, developments in structure solution from powders by direct methods using direct space techniques and utilising the whole digitised powder pattern were shown by Kenneth Harris and other speakers.

To sum up, meetings like this encompassing the breadth and depth of our subject remind me of why I am a crystallographer.

Georgina Rosair
Heriot Watt University

The Congress and General assembly of the International Union of Crystallography is held every 3 years and draws delegates from a wide variety of backgrounds. It was apparent that all have a keen interest in applying a diverse range of crystallographic techniques to their research. Even though the congress location was switched from Jerusalem to Geneva it was fully staffed and run by the Israelis, who managed to keep their own individuality and give a flavour of traditional custom and dancing on a special 'Israel evening'. Geneva, a city heavily influenced by the presence of the United Nations, provided an ideal location for such a multicultural gathering of academics and industrialists alike. Held at Palexpo, the congress was on a grand scale with a few thousand delegates, 6 halls running simultaneous programs of lectures, many exhibitors and over 400 posters. Of course, subdivision into similar areas of interest meant in practice most delegates mixed with only a smaller, more selective group of colleagues. However, the 10 day conference duration gave everyone the opportunity to meet new people, relax and make those all important contacts that may prove useful for collaborative research in the future.

Throughout the week various social events were organised for the delegates including a classical concert, banquet and importantly early on, a student mixer with complementary drinks. This enabled the younger contingent to meet and greet each other, preventing, as is often the case with such a large international conference, segregation into individual nationalities or just a feeling of being overwhelmed for those on their own.

Overall there was a strong showing for protein crystallography in terms of both the number of dedicated sessions, 2 simultaneous events per day, and quantity of posters on display. However, coming from a background of solid state chemistry with industrial application, the program presented some interesting sessions for myself and all those interested in this theme. Starting on the first morning, with possibly the most applicable session in relation to my project on salt selection in the pharmaceutical industry, was a series of lectures on the preparation of crystals for pharmaceutical applications. A strong emphasis was placed on high-throughput and combinatorial techniques. All speakers emphasised the requirement in industry for complete characterisation of potential solid state pharmaceuticals at the preformulation stage of development. The need for polymorph, salt and hydrate screens to become more automated and which techniques are subsequently required for a

full analytical profile, was indicated from an industrial perspective (Storey). Crystallographic analysis was discussed in relation to polymorphs (Lehmann) and the afternoon session showed the importance of powder diffraction, specifically to structure solution when a suitable single crystal is unavailable (Tedesco).



In-situ monitoring of crystal growth processes was the session in which my supervisor (Davey) spoke about the potential use of SAXS and WAXD for gathering key information on nucleation of crystal clusters from liquid phases. Molecular dynamics and its application to the successful prediction of all possible structures of polymorphic systems was demonstrated (Gavezzotti and Price), but overall this area is still in its initial stages of development. Using the Cambridge Structural Database as an aid to polymorph prediction and selection of the most stable form was outlined (Motherwell), but the need for more industrial and academic collaboration and the publishing of more structures was highlighted.

On the final day a full program of interest began with a keynote



lecture (Lahav) on stereochemical approaches to crystal nucleation. This was preceded by a session on polymorphism, in which an initial, clear and concise overview was given (Desiraju), followed by more specific examples of this phenomenon (Brock and Zaworotko). An afternoon session dedicated to the subject of crystal engineering allowed many of the world leaders in this field to demonstrate their work. For example an interesting lecture was given on engineering organic-inorganic hybrid solids (Orpen), which showed the potential for inducing electronic and magnetic properties in an organic solid by the inclusion of a transition metal species.

During the second week I was able to present my work during 4 days of dedicated poster sessions. My poster, entitled 'A Crystallisation / Crystal Engineering Approach To Aid Salt Selection – Anions', was well received and I obtained some valuable feedback to my research. I also made some useful acquaintances, to add to the list of those I previously met during the evenings' dining with my supervisor, Prof. Roger J. Davey.

Edwin A. Collier
UMIST

The XIX IUCr Congress had many highlights which were of significance to my research. These included several demonstrations of the power of X-ray crystallographic techniques to elucidate even the largest subcellular structures in atomic detail. There were also several talks on powerful new developments in methods.

David Stuart described his group's work on the crystal structure of the bacteriophage PRD1. This is an icosahedral virus with a lipid bilayer. The crystals have 66 MDa in the asymmetric unit and the structure was phased with a low resolution cryoEM map. This was a tour de force of X-ray crystallography.

The Ribosome Symposium consisted of talks by Tom Steitz, Ada Yonath and Venke Ramakrishnan on their respective ribosome structures. Many years of work has led to the structures of the 30S and 50S subunits at almost atomic resolution.

K. Namba gave an overview of the work done on the bacterial flagellum. Crystallographic work on the flagellar proteins was used to explain different coil states of the flagellum as observed under the optical microscope. This talk was illustrated with stunning movies.

K. A. Nugent talked about the non-crystallographic phase problem and opportunities presented by free electron lasers. The theory is in place to take advantage of the

data that will be collected at free electron laser X-ray sources.

Tom Terwilliger gave a talk on his impressive work on RESOLVE, a software package to automate structure solution using statistical maps and pattern recognition. He estimates that at high resolution and with 70% solvent, his program could solve structures ab initio.

Art Olsen gave a talk on "tangible interfaces in molecular biology", illustrated with three-dimensional models from the PDB.

Of interest to me was the session on "MAD, SAD and difficult" which included tales of heroic phasing, such as Frank von Delft's location of 160 Se atoms in KPHMT, and talks on methods development such as Gordon Leonard on de novo phasing using softer X-rays, and Z. Otwinowski on improved techniques for data analysis and scaling and the possibility of phasing using radiation decay.

A topic discussed at several sessions was that of radiation damage, and the importance of at least recognising it. Several speakers mentioned radiation induced disorder in the structures they presented (e.g. Titia Sixma in the Acetylcholine binding protein). Raimond Ravelli and Zbyszek Otwinowski talked about the possibility of using the isomorphous differences caused by specific structural damage to phase crystal structures. Better data processing algorithms will enable us to extract more information from radiation-

damaged data and even enable us to use this more extensively for phasing.

A Session was organised on Fundamental and Applied Aspects of Radiation damage in memory of Jan Kroon. In it, Elspeth Garman gave an introductory talk on radiation damage and ended with some of our work on free-radical scavengers. Martin Weik spoke about his work on the effect of cryotemperature on radiation damage, which linked appropriately with Sean Parkin who spoke on his investigation of a phase transition in a protein crystal. Mitch Miller introduced the automated crystal mounting system at SSRL. Raimond Ravelli presented his experimental work on using phasing using radiation damage, including a DNA structure solved entirely using this method.

My own presentation was a poster (C279) entitled "Investigation of Possible Free Radical Scavengers in Protein Crystallography". There was a lively interest in this poster, which presented a possible method to improve the radiation damage problem in cryocooled crystals by adding scavengers to the protein crystal. I gave away many preprints of our paper (J. Synch. Rad. Nov. 2002) on this topic, and have already received a testimonial from a crystallographer who has successfully applied the technique.

James Murray
Laboratory of Molecular
Biophysics, Oxford

XIX Congress and General Assembly of the International Union of Crystallography, Geneva, Switzerland, August 2002. Report of the Education Sessions.

The first session was held on Monday, August 12th 2002. The co-chairs were **Karimat El-Sayed** (chairman of the Education Commission) and **Carolyn P. Brock**, who had provided a varied program of talks, which attracted an audience which filled the lecture hall.

The session was dedicated to the memory of **Charles A. Taylor**, a former chairman of the teaching commission who died earlier this year at the age of 79. (An obituary was published in the June 2002 issue of 'Crystallography News').

K. Kantardjieff, from the Center for Molecular Studies in Southern California, spoke on the problems of setting up a 'virtual laboratory' for the study of both small molecules and macromolecular structures with remote access to a central diffractometer from the 23 campuses of the California State University system which are predominantly undergraduate institutions.

She found that much of her time was taken up in communicating what crystallography is to people from other disciplines. She runs an American Chemical Society annual 3 day workshop for faculty members from the Californian State system. These workshops concentrate on

showing students where crystallography is useful in the modern world, for example in drug design where ignoring the presence of polymorphism can be disastrous.

In conclusion she mentioned her incomplete survey of United States Undergraduate Courses; preliminary results show that many pre/post doctoral graduate chemists have no crystallographic training; their education has failed to give them the crystallography courses they will later need.

The second speaker, *T. Ito*, from Japan, described their approach to teaching a specific subject using commercially available graphics software. He showed a movie running on a Mac, which tries to teach the mechanism of epitaxial crystal growth using a quantum mechanical approach based on computer simulations using 'ab initio' calculations and a kinetic Monte Carlo approach. It is essential to simplify the calculations to keep the students' interest, and to try to convey just the main ideas in the movie.

A similar problem but aimed at a different audience confronted the next speaker, *Th. Tschentscher*, from the HASYLAB at DESY in Germany. The Laboratory has proposed a novel accelerator which will enable new X-ray scattering experiments in many scientific domains. Dr. Tschentscher is trying to explain the principles and applications of X-ray free electron laser (XFEL) radiation to the funding agencies. The new design generates FEL radiation at

short wavelength with intense pulsed radiation where the pulses are typically 100 fs duration. It will allow new experimental techniques such as scattering using coherent Xrays, femtosecond time resolved studies or looking at single molecules in the fields of biology, physics and chemistry. For example it may be possible to determine the 3D structure of a large molecule more quickly than with current MAD methods.

Education over 30 years of the 'Erice' courses was described by *P. Spadon*, Padua University, who described the advantages of running a course in a beautiful, small centre where informal communications between students and more senior scientists can take place in a social setting. Erice is an old remote town in Sicily, on top of a hill, where the whole town is used for the course. Meeting rooms are often in disused monasteries and churches which have been restored for teaching purposes. The 1st course was held in 1974, organised by Michael Woolfson on 'Direct methods'. Now the daily timetable is that invited speakers give lectures in the mornings, in the afternoons there are small group tutorials and Poster sessions including short talks from some of the young researchers who present their poster topic. There are 'Round table discussions' mostly towards the end of the courses. With such an intensive course it is important to organise some social events as light relief; one of the most popular is the singing of national folk songs,

ably led by one of the organisers, *Ludovico di Sanseverino* from Bologna who updates his '*Crystallographers song book*' for every course. Student selection is based on qualification, age, and geographic distribution. Students have come 84 different nationalities; grants are available for students from developing countries. Further information can be found on their website at: <http://www.crystalerice.org>

The last speaker was *Kate Crennell*, BCA Education officer, who spoke on the importance of starting to teach crystallographic ideas to very young children. New born babies have an intense interest in their surroundings, we should make use of this to show them interesting crystallographic shapes to look at from their cradles. If you want to raise protein crystallographers give them mobiles of brightly coloured isocahedra over their cradles instead of model teddy bears or butterflies. Toddlers can be taught symmetry by cutting shapes from folded paper. Older children can be engrossed by 'playthings' such as building blocks which are not just boring rectangular blocks and yet can be made to fill space. As their manual dexterity improves they can learn to cut out planar nets and build them into 3D models of crystallographic shapes for themselves. Such models can also be useful to undergraduates from any discipline struggling with understanding of rotational symmetry. A4 pages of model kits can be found on the BCA web site at: <http://bca.cryst.bbk.ac.uk/ed/model.htm>

The session ended with *K. El-Sayed* demonstrating some sequences from her CD used to teach the principles of symmetry to primary school age children with images of tourist attractions such as the Taj Mahal and interactive games where the child manipulates shapes to make diagrams of a given rotational symmetry. IUCr web staff are looking into the problems of making this CD available over their website. The CD was mounted on the PCs of 'The Software Fayre' for delegates to try for themselves during the Congress.

The second session was the *Open Meeting of the Commission on Crystallographic Teaching* chaired by *Gervais Chapius*, University of Lausanne, Switzerland; its 4 planned talks were on the single topic of "Macro-molecular teaching", which described two intensive residential courses held in the USA and two British 'distance learning' over the Internet courses.

W. Furey from the University of Pittsburgh School of Medicine described how theory was integrated with 'hands' on 'experience in the annual two week Cold Spring Harbour Laboratories Course, which is intended for students with a working knowledge of protein structures but none of macromolecular crystallography. They aim to provide a stimulating and supportive environment with no distractions. This requires a high ratio of experienced instructors to students. The course also

benefits by having access to all the facilities of the Cold Spring Harbour Laboratories, including a nearby restaurant and dormitory accommodation. They try to cover all practical aspects from growing and mounting crystals through data taking to structure determination, including running an experiment at the National Synchrotron Light Source, a 45 minute drive from Cold Spring Harbour. The course is limited to 16 students who have to show that they have enough background knowledge and a need for this course.

J.P.Rose described how protein crystallography is taught as part of the ACA Summer Course held annually since 1992. Originally this was limited to fundamentals of crystallography and determination of small molecule structures. More recently the course has changed to a 12 day one, the first 7 days are still devoted to fundamentals of crystallography, now the last 5 days concentrate on applying crystallography to macromolecular molecular structure analysis. He listed the keys to success as:

- making the learning fun and interesting
- organisation
- provision of course materials
- local facilities
- plenty of enthusiastic instructors
- support from the hosting institution
- accommodation within easy walking distance

Students have a choice of accommodation either low cost

college dormitories or moderately priced hotels. All students receive a copy of the textbook "*Crystal Structure Analysis*" by Clarke and Trueblood with their course materials.

J.K. Cockcroft, Birkbeck College London, outlined how they have used the Internet for teaching since 1993. In 1995 they pioneered an Advanced Certificate in protein structure run entirely on the Web, in 1999 they started a Powder Diffraction Course and since 2000 they have offered a part time M.Sc course. Course prerequisites are a B.Sc in a science subject, experience of the use of email and browsing the Internet. Course materials are mostly prepared 'in house' with a strictly enforced simple 'house style' for the web pages. This preparation took much longer than expected. One difficulty with 'on-line learning' is how do the teachers know who is actually doing the learning and writing the web pages as part of the two projects which students have to complete.

Details of Birkbeck Courses are at: <http://px.cryst.bbk.ac.uk/>

R.J.Read, University of Cambridge, described their use of the Web as a teaching resource for protein crystallography. Their aim was to link together useful web pages from other sites to form an informal introduction for non-crystallographers and in time a deeper treatment for future crystallographers. They presented a series of Web Pages as a lecture series ; the intention was to provide a teaching resource for

the community and recycle their old lecture notes, which in future would be freely accessed from anywhere. As the previous speaker emphasised it is essential to conform to a 'style guide' for these web pages if students are not to be confused. One problem was how to display equations, a standard web language, MathML, is coming but since it is not yet here equations were displayed in images. Simple animations can be made using 'animated GIFs' which can be displayed by any browser. In conclusion he offered 3 pieces of advice to those considering making such a course, it is a lot more work than you think, to make it worthwhile a Web course needs a large audience and we are only just starting to realise the great potential of such courses.

Finally, in an extra presentation, Bob Sweet from Brookhaven National Laboratory, USA said a few words about their 5 day practical course at the NSLS 'Data Collection and Structure Solving'. This is now held in April, 6 months away from the Cold Harbour Course. Students use 6 beam lines of the NSLS round the clock; the 48 students are divided into teams of 8 to work shifts on the beam line. They have about 20 helpers and instructors. Students seem to enjoy it, some even use vacation time to attend. This is an international course, about half the students are foreign, the others are about equally divided between US students and foreign students currently working in the USA.

Kate Crenell

International Mineralogical Association Meeting, Edinburgh, 1-7 September 2002

Despite its seemingly narrow specialisation, mineralogy is a very broad discipline, closely related not only to geological and environmental studies, but also to materials science and crystallography. This was particularly obvious from this year's International Mineralogical Association (IMA) meeting in Edinburgh. Such meetings are held only once in four years and have a very high profile.

At this conference I presented an invited lecture "Theory of MgSiO_3 Perovskite: Towards a Thermal and Mineralogical Model of the Earth's Mantle". MgSiO_3 perovskite, metastable at ambient conditions, becomes thermodynamically stable at high pressures (>24 GPa) and turns out to be the most abundant mineral in the Earth (~40 vol. % of the whole planet). Understanding the properties and behaviour of this phase, one could greatly advance the understanding of the deep Earth. Using quantum-mechanical simulations, my collaborators and I have obtained a number of important results, ultimately leading to the formulation of a detailed thermal model of the Earth's mantle. In brief, this was the topic of my talk.

Of particular interest to me was the symposium "Crystallography of high-pressure minerals and

ultra-high pressure research", organised by the IMA jointly with the European High-Pressure Research group. The first invited talk of this symposium was given by L. Dubrovinsky (Bayreuth, Germany), who presented experimental evidence for novel high-pressure phases of silica, based on the hexagonal close packing of the oxygens with silicon atoms statistically filling the octahedral and sometimes the tetrahedral voids. Such phases are most likely metastable, but due to a high degree of disorder may become thermodynamically stable at high temperatures. Another invited talk, by J. Loveday (Edinburgh), described applications of high-pressure neutron diffraction to methane and ammonium hydrates, which are believed to be important components of the giant planets' satellites. Experimentally constraining the compressional behaviour of these materials is vital to formulating reliable models of such satellites.

Experiments at high pressures and temperatures rely on pressure standards, and there is a significant international effort towards calibrating an accurate MgO pressure standard. MgO is a very simple and cheap material with high melting point and no phase changes up to ultrahigh pressures (510 GPa as indicated by the best theoretical calculations), which makes it ideal as a pressure standard. M. Matsui (Hyogo, Japan) demonstrated in his talk how, using molecular dynamics

simulations with an accurate description of the interatomic forces, he derived a theoretical MgO pressure scale and argued that the often used Au scale may be inaccurate at high temperatures.

The plenary lecture 'New windows on Earth and planetary interiors' was given by R. Hemley (Washington, USA) and described the latest experimental and theoretical advances in studies of planet-forming materials. This remarkable lecture included a very wide range of topics, such as methodological novelties in the high-pressure research (SiC anvil cells, MgO primary pressure scale) and a number of new results (anisotropy of the lowermost mantle, magnetoelastic coupling and magnetic collapse in transition metal oxides, and new chemistry of molecular solids subjected to high pressures).

In addition to the formal lecture programme, the meeting was also very exciting and fruitful in terms of meeting other people and discussing future collaborations. It has certainly been one of the most remarkable meetings that I have attended.

Artem R. Oganov
(University College London).

Win a Top Holiday or £££'s Cash Prize in the PCG Logo Competition!!

This is your chance to go down in the crystallography history books!

The physical crystallography group are organising a grand competition to design their new logo for the 21st Century. The lucky winner will be able to choose from a staggering array of prizes on offer including £100 in cash, free student registration/accommodation at the York Spring meeting or a signed photograph of the newsletter editor [Not the editor of *Crystallography News!* – Ed].

All you have to do is design a simple, eye catching logo for the



PCG which can be used on its web pages, in publications and in *Crystallography News*. The winning design should reproduce well in both colour and black and white publications, should capture some aspect of physical crystallography, and shouldn't infringe any copyrights! You might want to bear in mind the group's dual function as both the "Physical Crystallography Group of the British Crystallographic Association (PCG of the BCA)" and the "Structural Condensed Matter Physics Group of the Institute of Physics (SCMPG of IoP)". A sample logo is reproduced above to give an

idea of what we're after, though an approximately square shape would be desirable.

Entries can be produced electronically and sent by email in vector format (.ps postscript or .cdr coreldraw preferred) or pixel format (.gif) to the PCG Secretary/Treasurer john.evans@durham.ac.uk or hand drawn and posted to John Evans, Department of Chemistry, University of Durham, DH1 3LE, UK. The deadline for mailed entries is 1st April 2003.

The judging and prize presentation will occur during the York Spring meeting. The judges' decision is final. No correspondence will be entered into. No purchase necessary.

Puzzle Corner

The illustration represents the labyrinth on the floor of Chartres Cathedral, and copies of it are frequently used as an aid to meditation, as one reflectively walks it. People are often surprised by what comes into their heads. What came into mine was a simple puzzle: How many fixed (integral) constants and how many adjustable parameters must one know to construct such a labyrinth? Let us assume that anything that looks like an arc of a circle is an arc of a circle. The usual prize of a £10 book token for the best answer!

Last month's cryptogram read:

Talc is commonly found in association with serpentine often in veins with magnesite or quartz, or along faults. It also forms by the low grade metamorphism of siliceous dolomites, and talc schists are not uncommon. Talc is the first mineral with which the student comes into contact.

The first solutions came from Frances Bernstein and John Malone (who wrote from different time zones, so I'm not clear who was first!) Only one solver recognised the text: "Mineralogy for Students" by M.H. Battey, and this quote contains one of the only two jokes I ever found in the book. Unfortunately, I have misplaced the letter (s)he sent – Please identify yourself to claim the prize!



*British Crystallographic Association**Spring Meeting 2003 -
The University of York***THE BCA SPRING MEETING**

The BCA Spring Meeting will take place at the University of York from Tuesday 15 April to Thursday 17 April 2003. The Spring Meeting will now run for three full days – the same amount of science, but only two nights accommodation required. We will also be offering one-day registrations!

The Spring Meeting will take place in the University of York's Exhibition Centre which is part of the main Heslington campus, a 200-acre landscaped park. The conference facilities at the University of York are amongst the best in the country, offering state of the art facilities for both delegates and exhibitors. The accommodation is of a high quality and is a short walk from the Exhibition Centre.

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

The Commercial Exhibition will run from Tuesday 15 April to Thursday 17 April 2003. For more information on the Exhibition and Sponsorship opportunities, please contact The BCA Administrative Office at the address below.

The BCA Administrative Office will manage all administrative issues. Any queries should be directed to Euan Woodward, Project Manager:

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

REGISTRATION

The BCA Council is pleased to announce that One-Day Registrations will be available at the Spring Meeting in York. Please note that the deadline for early registrations is 10 March 2003.

Non Member surcharge£25.00

Early Registration - before 10 March:

Full Registration£120.00

Student/Unemployed/Retired£60.00
(students require the signature of a Head of Department)

One-day Registration£60.00
(per day - no concessions)

Late Registration - after 10 March:

Late full registration fee£180.00
(no concessions)

Late one-day registration.....£90.00
(per day - no concessions)

ACCOMMODATION

Two types of accommodation are available at The University of York:

Standard B&B:.....£27.50 per night

En-suite B&B:£40.50 per night

All accommodation is located in James College, a short walk from the Exhibition Centre. Breakfast and dinner will be served in Goodricke College, located close to James College.

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

CATERING

Morning Coffee (Wednesday 16 and Thursday 17 April), Afternoon Tea (Tuesday 15, Wednesday 16 and Thursday 17 April) will be served in the exhibition area, close to all lecture theatres.

A packed lunch (sandwich, biscuit, packet of crisps, piece of fruit and soft drink) will be served in the exhibition area between 12.30 and 13.30 on each full day of the Spring Meeting. Please note that lunch will be ticketed and must be booked in advance.

Breakfast and dinner (including the conference dinner) will be served in Goodricke College.

Lunch and Dinner must be booked in advance.

Lunch.....£5.30 per day

Dinner£10.00 per day

SOCIAL EVENTS

On Tuesday 15 April 2003, the Posters/Exhibitors Reception will be held in the Exhibition Centre from 19.00 hrs. Delegates will have the opportunity to chat with exhibitors and poster presenters in a relaxed, informal setting. This is included in the registration fee.

The Conference Dinner will be held on Wednesday 16 April at 19:30 hrs in Goodricke College 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

Car parking is available in car parks Campus West and Campus South. Please note however that car parking at the University of York is not free.

Car parking permits can be purchased in advance at a cost of £2.00 per day - a saving of £1.00 per day on pay-and-display rates.

EMAIL FACILITIES

Access to email and Internet facilities will be available throughout the duration of the Spring Meeting. Further information will be available on-site.

ABSTRACT SUBMISSION

Submission of Abstracts will be electronic. For instructions, please visit the website:

<http://www.isis.rl.ac.uk/BCA2003>

If you have any queries regarding Abstract Submission, please email:

BCA2003@isisa.rl.ac.uk

Please note that the deadline for receipt of Abstracts is Friday 28 February 2003.

BCA BURSARIES FOR BCA SPRING MEETING

A limited number of bursaries are available from the Arnold Beevers Bursary Fund to cover the £155.90 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 seeking commercial sponsors of Spring Meeting Bursaries and it is hoped again to offer some Named Bursaries at this meeting.

The **closing date** for all applications is **Monday 10 February 2003**, applicants should ask for an Arnold Beevers bursary application form from the BCA Administrative Office (details on previous page).

THE UNIVERSITY OF YORK

The University of York was founded in 1963 with 200 students in two city-centre locations and Heslington Hall. Now in its 39th year, it has expanded to over 9000 students and has over 30 academic departments and research centres.

York boasts several major attractions including the stunning Cathedral, an award-winning Railway Museum and the famous Jorvik Viking City. For further information on the University of York and the town itself, please visit their website:
<http://www.york.ac.uk>

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

<http://bca.cryst.bbk.ac.uk/BCA/>

Further information can also be obtained from the BCA Administrative Offices.

As the programme evolves, the information will appear on the website, and the final programme will be in the March issue of *Crystallography News*.

SCIENTIFIC SESSIONS:

The scientific sessions for the 2003 BCA Meeting will continue last year's emphasis on "hot-topics" in the field of crystallography. The programme will cover a large range of interesting sessions including "**High Through-put, Databases and Data Mining**," which is the topic of the 3h plenary session and a 4.5h parallel session, which should be of interest to all groups. These sessions will form the basis for the 2003 BCA Review Symposium issue of *Crystallography Reviews*. Crystallography is very important in the advancement of technology (e.g. in the area of magnetic, optical, semiconductor materials) and there is a 3h session on "**Crystallography for Technology**" this year. To probe materials deep into the bulk there are advantages in using "**High Energy Diffraction**" and 3h is devoted to this subject. Crystallography has always been concerned with the molecular structure and when a good single crystal cannot be grown powder diffraction is the only feasible method, so again in York we will have sessions on "**Structure Solution from Powders**" (3h) and a discussion on the Rietveld method (1h). "**Quantitative Phase Analysis**" is a very important tool for industry, e.g. for the analysis of cement and metal ores, and there are 3h covering this subject. We have sessions on the complexities of modeling and interpreting data from structures with more than one independent formula unit "**Structures with Z' $>$ 1**" (1.5h) and the advances in "**Synchrotron Radiation**" (1.5h) for structure determination.

At York there is a Max Perutz Memorial Lecture to be given by Venki Ramakrishnan as well as the long established prize lectures. As usual, we are also running workshops at this conference with more interactive presentations on "**Introduction to Powder Diffraction**" (2h) and a series on "**Phase Identification**" (4h). There are also workshops on the CCP4 (1.5h) and the CRYSTALS (3h) software. Special Interest Groups (SIGs) are an important part of the BCA activities and the new "**DIAMOND SIG**" (0.75h) is becoming established along with the "**Education SIG**" (0.75h). The posters, as always, are an important part of the BCA conference and as usual to give greater coverage we will be running the popular "**Oral Poster**" session and in the evening you can scrutinize the "**POSTERS**" (3h) with a glass of wine in your hand!

I think you must agree that much of the activity in the world of crystallography is covered by this conference and with its new condensed format this is an event you should not miss!

DETAILED PROGRAMME:**"High Throughput, Databases and Data Mining"**

Crystallography has moved a long way from its early days of lengthy structure solutions and database searching with books, etc. Now all crystallographic activities benefit from rapid computer searching and fast data collection and this has led to quite different ways of working and of course the automation of the growth and selection of crystals. Rapid data collection methods eventually create vast databases of structures that can benefit drug design, for example, by rapid search for structural analogues. The databases and extracting the right data from them (data mining) have now become very important topics. The identification of structural phases by X-ray diffraction has long been important, and building quality databases is essential. This session will cover aspects of rapid data collection and handling large quantities of data, the use of databases and the use of new synchrotron diffraction methods capable of simultaneously monitoring multiple grains within a single bulk sample as a function of time, temperature and 3 dimensional space.

Tuesday 15 April**11:00 - 12:30 and 13:30 - 15:00****Plenary Session:**

Chair: Paul Fewster (PANalytical)

Henning Poulsen (Risoe)

3DXRD: grain maps, grain dynamics and grain refinement

Mike Hursthouse (Southampton)

High throughput Chemical Crystallography: Meeting and Greeting the Combichem Challenge

John Faber (ICDD)

ICDD's New PDF-4 Databases: Search Indexes, Full Pattern Analyses, and Data Mining

Christian Cambillua (CNRS Marseille)

*Structural Genomics in a Medium Sized Laboratory***Wednesday 16 April****08:30 - 10:00 and 10:30 - 12:00 and 13:00 - 14:30****Parallel Sessions:**

Organisers: Gideon Davies, Sandy Blake and Dave Taylor

Julie Wilson (York)
Automatic evaluation of high throughput crystallisation trials

Richard Storey (Pfizer) - to be confirmed

David Rendle (The Forensic Science Service, London Lab.) - to be confirmed
Database Use in Forensic Analysis

Frank Allen (CCDC)

Marek Brzozowski (York)
Low-cost alternatives for nano-crystallisations

Herman van Tilbeurgh (Paris)
The Yeast Structural Genomics Project

Robert Esnouf (Oxford)
Information Management for High Throughput Structural Biology

Victor Lamzin (EMBL Hamburg)
Developments in ARP/WARP and Automated Building of Protein Models

George Sheldrick (Göttingen)
Some innovations for high throughput SAD and MAD phasing

Tom Oldfield (EBI)
Data Mining Approaches and Successes

"High Energy Diffraction"

The high energy diffraction session organised by the PCG will develop the themes in Henning Poulsen's plenary presentation by showcasing different uses to which high energy X-ray sources can be applied. These will range from in-situ studies of chemical reactions to probing engineering materials.

Wednesday 16 April 08:30 - 10:00 and 10:30 - 12:00

Parallel Session :

Chair: Steve Collins (Daresbury Lab)

Paul Barnes (Birbeck)

Peter Hatton (Durham)

Alexander Korsunsky (Oxford) - to be confirmed

"Introduction to powder diffraction"

Powder Diffraction is a widely used technique for identifying phases of polycrystalline materials in industry and academe. This session introduces the Phase Identification Workshop by explaining some of the fundamentals of the technique so that those who are not fully versed in the method will gain the necessary background to get maximum benefit from the Wednesday sessions.

Tuesday 15 April 16:05 - 17:45

Parallel Session :

Organisers: Judith Shackleton and Dave Taylor

Principal Instructor : John Faber (ICDD)

"Phase Identification Principles, Practice and the Use of PCs"

This modular workshop spanning the first two days of the Spring Meeting has emphasis placed on the practical use of powder diffraction phase identification. The modules are linked to give a good grounding in best practice for phase identification and are suitable for both novice and experienced practitioners. You can choose to attend any of the modules that fit into your meeting schedule. For those who attend all the sessions, an optional certificate of attendance is available for your professional development file. The purpose of this workshop is to build proficiency in the interpretation of experimental powder data, especially in the application of the Powder Diffraction File (PDF) and new relational databases: On the type of information the database contains; its history; the way this information is organised; how data may be retrieved and interpreted; how to collect experimental data; how interpretation is affected by accuracy of experimental data; how to detect and understand common instrumental and specimen induced errors; how new relational databases extend search options. Hands-on work sessions will allow you to become familiar with the application of both printed and computer media to phase identification.

Wednesday 16 April

08:30 - 10:00 and 13:00 - 14:30 and 15:30 - 16:30

Parallel Session :

Organisers: Judith Shackleton and Dave Taylor

Principal Instructor: John Faber (ICDD)

"Quantitative Phase Analysis"

Quantitative Phase Analysis is a very powerful X-ray diffraction analysis tool and is widely used in many industries from pharmaceuticals to cement. There is a range of methods from the comparison of peak intensities of different phases through to full profile fitting. Complexities of texture, micro-absorption and for some methods finding suitable pure phases for standards. This will lead on from the Phase Identification Workshop, i.e. now I know how to find what phases I have, what is proportion of each in my sample?

Thursday 17 April

08:30 - 10:00 and 10:30 - 12:00

Parallel Session:

Organiser: Chris Frampton

"Structure Solution from Powders"

The ability to perform full structure solutions from powder diffraction data has perhaps been one of the most significant crystallographic advances of the past decade. Continuing advances in computational methodologies mean that structures of increasing complexity can be successfully tackled by powder methods. In this joint session between the CCG and the PCG the speakers will highlight how a variety of different approaches (simulated annealing, genetic algorithms, combined annealing and refinement) of different data (lab/synchrotron X-rays, time-of-flight and constant wavelength neutrons) can be used to target both molecular and extended systems of pharmaceutical and technological relevance.

Thursday 17 April

13:30 - 15:00 and 15:30 - 17:00

Parallel Session :

Chair: John Evans (Durham) and Paul Raithby (Bath)

Maryjane Tremayne (Birmingham)

Replicate, Divide, Mutate, Survive: Evolving crystal structures from PXRD

Ivana Evans (Durham)

Structure Solution of Complex Oxides from Powder Diffraction Data

Alastair Florence (Strathclyde)

"Discussion on Rietveld Method"

The Rietveld discussion session will follow the format successfully trialed in Nottingham whereby those who have attended the pre-meeting Rietveld workshop, and any others interested, will be given a chance to "ask the experts" any burning questions they have on the practice of Rietveld refinement. A "distinguished" panel of some of the UK's leading practitioners of Rietveld methods will be assembled and questions from participants encouraged to provoke an informal discussion of topics ranging from data collection and indexing through to refinement and publication.

Wednesday 16 April 13:30 - 15:00

Parallel Session :

Chair: Jeremy Cockcroft (Birkbeck) / Chick Wilson (RAL)

"Max Perutz Memorial Lecture"

Max Perutz (1914 -2002) was an outstanding scientist and crystallographer, and in honour of his major contributions to our subject we have introduced the Max Perutz Memorial Lecture preceded by a short introduction.

Wednesday 16 April 17:30 - 18:45

Plenary Session :

Chair : Chris Gilmore (Glasgow)

17:30 Introduction by David Blow (Imperial College)

17:50 Venki Ramakrishnan (MRC)

18.45 Close

"Prize Lectures PCG and CCG"

This session sees the presentation of the PANalytical Prize and the CCDC / CCG Prize, both for outstanding young crystallographers. The award presentations are followed by the Prize lectures.

Wednesday 16 April 15:30 - 16:30

Parallel Session :

Chairs: Pamela Thomas and Paul Raithby

The PANalytical Prize :To be announced at the presentation

The CCDC / CCG Prize for Younger Scientists

"Structures with $Z' > 1$ "

"Structures having more than one independent formula unit are interesting because they are unusual; only 8% of the structures in the CSD have $Z' > 1$ and fewer than 1% have $Z' > 2$. In some $Z' > 1$ structures the pseudosymmetry is so strong that the structures are best described as modulated; in others the molecules have such different orientations and/or conformations that an analogy can be made with co-crystals. Because $Z' > 1$ structures are exceptional they can provide new insights into crystal packing. They also present interesting technical problems. As a group these structures are wonderful and informative puzzles that too often remain unpublished. Consideration of $Z' > 1$ structures is timely because anecdotal evidence suggests they are more likely to be recognized when a CCD or image-plate detector are used."

Professor Carolyn P. Brock
Department of Chemistry
University of Kentucky

Thursday 17 April **08:30 - 10:00**

Parallel Session :

Organiser: Sandy Blake

Sam Motherwell (CCDC)
Packing energy patterns in CSD for $Z' = 2$

Ton Spek (Utrecht)

Richard Cooper (Oxford)
 $Z' > 1$: just a nuisance, or something more interesting?

"Crystallography for Technology"

The science and methods of crystallography are widely applied across disciplines for the investigation of materials with technological applications, both potential and realized. Our aim is to demonstrate the widespread and continuing importance of crystallography and its methods to current materials research through a varied programme of talks, which are intended to be accessible and interesting to the wider audience of the BCA. This session brings together in the programme a number of expert speakers who are united by their use of diffraction and scattering methods to address problems in the physics and chemistry of technologically important materials.

Thursday 17 April

08:30 - 10:00

Parallel Session :

Chair: Pamela Thomas

Tom Hase (Durham)
Investigations of Materials showing Giant / Colossal Magneto-resistance

Petra Pernot (ESRF)
Periodically poled non-linear Optical Materials investigated by New X-ray Imaging Methods

Stephen Lee (St Andrews)
Scattering Studies of Magnetic Media

Tricia Kidd (PANalytical)
Crystallographic studies of Semiconductor Thin Films

Don Paul (Warwick)
Superconducting Crystals

"Synchrotron Radiation"

The role of synchrotron radiation in the structural chemistry community has developed greatly over the last decade, and now synchrotron-based experiments are vital to many areas of research from biology, through physics and chemistry to materials science. In this session several snapshots of current 'cutting-edge' science that is carried out using synchrotrons will be highlighted, and future possibilities for the development of 'new' exciting science discussed.

Thursday 17 April

10:30 - 12:00

Parallel Session:

Organiser : Paul Raithby

Paul Raithby (Bath)
Exciting Synchrotron Experiments on Luminescent Materials

"Diamond SIG"

The meeting will provide an update on the development of beamlines that are of interest to the crystallographic community, and include a discussion of the lines that have been approved and of those that are currently under consideration. There will also be an overview of exciting new science that could be undertaken on DIAMOND that is not possible at the moment. There will also be a general open discussion on matters of interest.

Thursday 17 April 12:00 - 12:45

Plenary Session :

Chair: Paul Raithby (Bath)

Jeremy Cockcroft (Birkbeck)

Update on the high-resolution powder diffraction station

Paul Raithby (Bath)

The bid for a single crystal beamline

Chick Wilson (RAL)

New, Exciting Science at Big Facilities

"Education SIG"

This session will report the results of the BCA survey on UK Undergraduate Courses in Crystallography, it will include all questionnaires returned by February 2003. Send in yours now. There is a form on the BCA website if you have mislaid yours. Find it at: <http://bca.cryst.bbk.ac.uk/ed/survey/Survey.html>

This year everyone is encouraged to submit a POSTER ON EDUCATION.

I will also show new BCA educational web pages, and as usual have a general discussion, bring along your ideas of what the BCA should be doing to improve crystallographic education.

Tuesday 15 April 17:00 - 17:45

Parallel Session :

Chair : Kate Crennell

"Oral posters for all groups"

Tuesday 15 April

15:30 - 16:00 and continued at 16:02 - 17:00

Plenary and Parallel Session :

Organisers : Chris Frampton, Pamela Thomas, Paul Raithby and Richard Pauptit

Oral Posters: IG, PCG, CCG and BSG

Presenters of posters from all Groups have the opportunity to publicise their poster in this session. Each presenting author is expected to speak for 2 minutes in order to sum up the important points of their poster and encourage people to view it during

the formal poster session in the evening. Always a fun and enjoyable session, but with a serious point.

"Poster Session IG, PCG, CCG and BSG"

Tuesday 15 April 19:00 - 22:00

The poster session will take place in the main Exhibition Centre and please be present throughout this time.

"CRYSTALS Workshop"

Thursday 17 April 13:30 - 15:00 and 15:30 - 17:00

Parallel Session :

With David Watkin (Oxford)

The CRYSTALS Workshops attached to previous BCA (and other) meetings have proved astonishingly popular. A similar workshop has been scheduled into the York meeting. It will include a brief presentation on new and changed features, followed by hands-on experience of the current release using up to 69 PCs available to us.

"CCP4 Workshop"

Thursday 17 April

08:30 - 10:00

Parallel Session :

Software demonstration including recent developments and overview of CCP4 software.

BCA Spring Meeting York 2003 Timetable

	Tuesday 15/4	Wednesday 16/4				Thursday 17/4			
08.30 hrs	BCA Council Meeting 09.30 hrs - 10.30 hrs	Parallel Session High Throughput, Databases and Data Mining in Chemistry and Biology	Parallel Session High Energy Diffraction		Parallel Session : Phase Identification principles	Parallel Session Crystallography for Technology	Parallel Session Structures with Z>1	Parallel Session Quantitative Phase Analysis	CCP4 Workshop
10.00 hrs		Coffee/Exhibition				Coffee/Exhibition			
10.30 hrs									
11.00 hrs	Plenary Session : High Throughput, Databases and Data Mining - Henning Poulsen Mike Hursthouse	Parallel Session High Throughput, Databases and Data Mining in Chemistry and Industry	Parallel Session High Energy Diffraction	Parallel Session High Throughput, Databases and Data Mining in Biology		Parallel Session Crystallography for Technology	Parallel Session Synchrotron Radiation	Parallel Session Quantitative Phase Analysis	
12.00 hrs			AGM Physical Crystallography Group	AGM Biological Structures Group		12:00 to 12:45 hrs DIAMOND SIG			
12.30 hrs	Lunch/Exhibition	Lunch/Exhibition				Lunch/Exhibition			
13.00 hrs									
13.30 hrs	Plenary Session : High Throughput, Databases and Data Mining - John Faber Christian Cambillua	Parallel Session High Throughput, Databases and Data Mining in Chemistry	Parallel Session Discussion on the Rietveld Method	Parallel Session High Throughput, Databases and Data Mining in Biology	Parallel Session : Phase Identification practice	Parallel Session Structure Solution from Powders	Parallel Session CRYSTALS Workshop with PCs.	Parallel Session Quantitative Phase Analysis	
15.00 hrs	Tea/Exhibition	AGM Chemical Crystallography Group			AGM Industrial Group	Tea			
15.30 hrs	Oral posters PCG, IG and CCG and BSG	Prize lectures PCG & CCG		Parallel Session High Throughput, Databases and Data Mining in Biology	Parallel Session : Phase Identification Workshop with PCs.	Parallel Session Structure Solution from Powders	Parallel Session CRYSTALS Workshop with PCs.	Parallel Session Quantitative Phase Analysis	
16.30 hrs	Introduction to powder diffraction	BCA AGM 16.30 hrs - 17.15 hrs							
17.00 hrs	Education SIG	17.30 hrs-18.45 hrs Max Perutz Memorial Lecture				BCA Council Meeting 17.00 hrs - 19.00 hrs			
18.00 hrs	Dinner	19:30 hrs Conference Dinner							
	19:00hrs Poster/Exhibitors Wine Reception								

Memorial Meeting for Max Perutz , Cambridge, 21 September, 2002



Max with H.M. the Queen

Max Perutz spoke on mutant haemoglobins at a meeting in the Royal Society in 1969. The warmth, wit, charm and intellectual rigour of his talk were decisive in directing me into crystallography. The recent memorial meeting for Max was outstanding for the inspiring, heartfelt and moving nature of the many tributes to Max, from his colleagues, collaborators, friends and family. The event included a beautiful performance of a Brahms clarinet trio, with Max's grandson Tim playing the clarinet. John Meurig Thomas, who spoke first in the personal tributes, has very kindly given permission for part of his lecture to be included here. You can read it in full on the [BCA Website](#).

In the universities and academies of the world, Max Perutz was acknowledged both as one of the foremost scientists of the 20th century and as the architect of arguably the most famous and successful research laboratory now in existence. But Max was a multifaceted human being, a citizen of the world deeply immersed in its diverse

cultures. And among his many qualities were:

- the temperament of the artist
- the imaginative sensibility, insight and expression of the poet;
- an extraordinary intellectual energy coupled with a single-minded determination;
- a stylish and incisive author of popular scientific articles and reviewer of books;
- a continuous enthusiasm and youthful voracity for new knowledge;
- an indefatigable warrior passionately committed to social and political justice, human rights, and intellectual honesty .
- a gift for writing charming personal letters
- the old-fashioned virtues of good manners, politeness and respect for others.

He was a gentle, kindly tolerant and forgiving lover of people, particularly the young. Through my friendship with him ever since I came to Cambridge twenty four years ago, I benefited enormously from his wisdom, guidance and humour, which I grew to appreciate during our numerous walks around playing fields adjacent to our homes, while strolling through The Botanical Garden, wandering in Wandlebury or sitting for tea in the intimacy of our respective homes. Max delighted in the beauty of the natural world. He was the kind of man who, before starting his laboratory work at the LMB on a spring morning, would occasionally take a walk on the Gog-Magog hills, filling his heart and soul, in so doing, with pantheistic pleasure.

One of his most devastating and uncompromising book reviews, dealing with a book on Louis Pasteur, was a justified attack on a historian of science, done with irrefutable logic and argument, yet without rancour or vituperation. Max rejected as nonsense the thesis, popular among modern sociologically oriented philosophers of science, that scientific truth is relative and shaped by a scientist's personal concerns including his or her political, philosophical, even religious instincts. Hence the reason for choosing Max Planck's magnificent assertion: *"There is a real world independent of our senses "*. *"The laws of nature were not invented by man, but forced upon him by that natural world. They are the expression of a rational world order. The entire approach emphasising relative truth seems to me "* said Max *"a piece of humbug masquerading as an academic discipline; it pretends that its practitioners can set themselves up as judges over scientists whose science they fail to understand"*.

The opening words of Max's now famous *New Yorker* (1985) article entitled "Enemy Alien", which is an amalgam of the harrowing and the humorous, also begins in an unforgettable way:

"It was a cloudless Sunday morning in May of 1940. The policeman who came to arrest me said that I would be gone for only a few days, but I packed for a long journey. I said goodbye to my parents ".

Although Max would never regard himself as a poet, his peers did. And Rockefeller University bestowed upon him

the Lewis Thomas Prize to honour the activities of the scientist as poet.

"Imagination comes first in both artistic and scientific creation - which makes for one culture rather than two, but while the artist is confined only by the prescriptions imposed by himself and the culture surrounding him, the scientist has Nature and his critical colleagues always looking over his shoulder". Max Perutz ("Is Science Necessary?")

In the September 1978 issue of *Scientific American*, Max begins his wonderfully anecdotal, humorous self-deprecatory article on Haemoglobin with the following arresting opening paragraph:

"When I was a student, I wanted to solve a great problem in biochemistry. One day I set out from Vienna, my home town, to find the Great Sage at Cambridge. He taught me that the riddle of life is hidden in the structure of proteins, and that X-ray crystallography was the only method capable of solving it. The Sage was John Desmond Bernal, who had just discovered the rich X-ray diffraction patterns given by crystalline proteins. We really did call him Sage, because he knew everything, and I became his disciple".

This article is teeming with incidental asides not normally found, even in popular scientific articles, e.g. how he absent-mindedly left a thermos flask full of carp haemoglobin on the platform of a London Underground Station, etc. So when, fifteen years later, I found myself struggling with Jesuitical sub-editors of *Scientific American* concerning my own

article on catalysis, I asked Max how on earth he had succeeded to have published his delightfully evocative account. "Look", he said, *"they re-wrote it completely. It was not what I had written. The science was acceptable, but all the liveliness and asides had been ruthlessly expunged. So when the final proofs arrived, I kept them for a little time. I then told them to publish the article as they had modified it - but NOT under my name. This caused alarm, and they relented; and it was then accepted in its original form".*



Max and Gisela

Max was not only a fine expositor in the written word, he was also an excellent lecturer. His lectures had a mesmeric charm, partly because they were interspersed with literary and historical incidents involving his friends and scientific adversaries. They also charmed you because he was so unpretentious and so passionately, almost obsessively, aroused by the joy of science. In addition, he always injected an element of theatre and drama into his talks. I heard him lecture some thirty times covering a wide range of topics. No two lectures were exactly the same. He took each as a new task with well-defined objectives to be reached. Many were virtuoso performances, like the one we,

at Peterhouse, invited him to give to the Student Science Society (The Kelvin Club) to mark his 60 years as a member of the College - he joined as a graduate student in 1936. I had tried to convince him to speak on the topic "What every scientist should know", but he refused, because he said he did not know what every scientist should know! He suggested a much better title: Science is No Quiet Life. I knew that he spent a great deal of time preparing this lecture, lavishing the care upon it that would be given to such a task by a performing artist. In that context, the following words of Dame Margot Fonteyn appealed to him. They appear in Max's "Commonplace Book", along with other aphorisms: *"I cannot imagine feeling lackadaisical about a performance. I treat each encounter as a matter of life and death. The important thing I have learned over the years is the difference between taking one's work seriously and taking oneself seriously. The first is imperative and the second disastrous".*

No picture of Max would be complete without reference to his letters, which were a huge delight to receive. One Saturday morning in January 1998, I ran into my old friend Aileen Kelly, an expert in Russian literature. She was deliriously happy for she had just received what she described as one of the most charming letters of her life. It had come from Max. He expresses his joy about learning that Chekhov's views on the synonymy of the creative processes in the humanities and the sciences coincided with his



Max with J.M. Thomas

own. Then comes a piece of pure Perutz. He animadverts on Chekhov's plays and short stories and says:

"I find that the people in his plays are trapped by their characters rather than their circumstances".

Then he goes on to quote Shakespeare.

In September 1994 his 80th birthday was marked by a Feast in Peterhouse. He finished by saying he was *"still alive, aged 80, happily surrounded by my family and so many good friends. There are other things to be thankful for: to have lived in a country free from oppression and also from war - Falklands apart - these 49 years; to have worked among the British scientific community where you are judged, not by your origins, nor by your religion, nor by your politics, nor by your connections in high placed, nor by your wealth, but solely by the quality of your work; to have enjoyed and to be still enjoying generous support for my work from both sides of the Atlantic; to be tolerated by my colleagues at the laboratory and here (Peterhouse) with affection and without being made to feel a burden, and finally for having*

received so many honours which in my youth I never expected to come my way, though I used to tease my son when he was little and when peerages were still hereditary that one day I would become Lord Haemoglobin, and he would inherit the title whether he wanted to or not".

That after-dinner speech was a carefully crafted, beautifully presented one.

He was sitting in the front row of the Cockcroft Lecture Theatre when I gave an address to the Cambridge Philosophical Society on "The Genius of Michael Faraday" (Faraday along with Rutherford, Pasteur, Lawrence Bragg, Bernal - as well as George Eliot, Shakespeare, Tolstoy, Manzoni - was one of his heroes). I ended my lecture by showing a slide of a verse in the Book of Job from Faraday's Bible. It was Faraday's favourite verse, heavily marked by him. Four days later, on Saturday 9th November, Max came to lunch at Peterhouse, as he had done regularly for thirty years - he relished conversation there especially with young scholars. Usually he would sit next to a new Fellow, just to be friendly to a new member of the community. But on this Saturday, he came straight to me, handed me a pen and paper and requested that I write out for him Faraday's favourite verse: *"If I justify myself my own mouth shall condemn me; if I say I am perfect, it shall also make me perverse".*

That verse appealed greatly to Max: amongst other things it is an injunction not to boast. Max, like Faraday, never boasted. He was very much like Faraday in

many respects: they each liked talking about and showing science to children; they each kept 'commonplace books'; and they each declined knighthoods. But there were other kinships: they were each prodigiously hard working; they were each exceptional intellects and wonderful experimentalists. Each was a humble, decent human being, kind and respectful of others. His written work, like Faraday's, was refreshingly free of pettiness and full of self criticism. Like Faraday, Max Perutz was a great scientific adventurer; and like Faraday he knew innately which scientific problems to go for. In the florescence of modern science, well nigh every problem that one encounters is interesting: not all problems are important. Max chose the important ones, and that selectivity he taught to those who worked alongside him. Max was probably a better negotiator than Faraday. One example of his supreme skill in this regard is manifest in the creation of the magnificent Laboratory of Molecular Biology, opened in May 1962. You may recall that in 1953, when Sir Nevill Mott was elected Cavendish Professor, to succeed Sir Lawrence Bragg (who moved to the Royal Institution), he made it clear that, notwithstanding its success, the MRC group led by Max, would be expected to vacate the rooms they occupied in the Cavendish. Max pleaded with and tried to persuade many Heads of Departments in Cambridge to find accommodation for his burgeoning team of excellent collaborators - the Heads of Chemistry, Metallurgy, Physiology, Anatomy and many

others were approached. There was temporary accommodation; but nothing really concrete and permanent appeared in sight until Max brought his latent excellent negotiating skills to bear. When I asked him years later how he accomplished such an achievement, he retorted, quoting a former Fellow of Trinity, that, in Cambridge, to reach your goal you must learn to combine the linear persistence of the tortoise with the circuitous locomotion of the hare.

Max had a generosity and nobility of spirit. The warmth of his personality and decency radiated a feeling of human goodness which induced others almost by cultural and intellectual osmosis to behave sanely, especially because he exuded an inner joy that stemmed from a love of knowledge for its own sake and a compassionate concern for others. Max Perutz's monument is to be found in the whole of molecular biology, a subject which, along with a few other individuals, he effectively founded. To those who had the good fortune to know him, he will always be remembered as Max, the quintessence of a great and good man, someone who made you glad to be alive.

Précis by Christine Cardin

Women in Science, Engineering and Technology (SET)

A "great national mentoring scheme for women in SET" should leap forward in a higher gear now that a project manager has been appointed. She is Jan West, working from home with young children. mentoring@wes.org.uk should reach her until a new name and the corresponding internet domain are arranged.

A list of potential mentors and mentees is being compiled – please think about signing up, either for a long-term arrangement or a shorter 2-or 3-session type of quick-boost mentoring. Mentors and mentees will be given training, as well as handbooks etc. Those who have already registered an interest should hear soon about the next stage in getting mentoring happening before Christmas.

Meantime, Baroness Greenfield told an audience at the Royal Institution in October that men will always dominate British science unless the Government introduces family-friendly policies to encourage women to continue with their research. Her speech outlined the preliminary findings of The Greenfield Report, which has been commissioned by the Government.

Dynamical Theory of X-ray Diffraction

André Authier, Université de Pierre et Marie Curie, Paris.
IUCr Monographs on Crystallography, Oxford University Press, 2001
Price: £95.00 (hardback)
ISBN 0-19-855960-7, xviii + 661 pages .

This book has been compiled with meticulous care and attention to detail. André Authier has been very active in the field of X-ray dynamical theory for more than 40 years, testing some of the conclusions through to the exploitation of the theory in topography. The theory is very relevant to the analysis of nearly perfect crystals and the design of high-resolution diffractometers and synchrotron beam lines.

The book is split into four sections; the first is concerned with the basics and the background. The first chapter is historical, explaining some of the conceptual thinking in the development of the theories. Chapter 2 introduces Maxwell's equations, fundamental to all electromagnetic waves, and leads to the concept of polarisability in a crystal and introduces the Ewald and Laue theories; the former is based on a microscopic approach assuming the crystal is a series of dipoles, whereas the latter assumes a distribution of negative charges surrounding positively charged atoms. The geometrical (kinematical) theory is also derived in this section along with the application of the Fresnel equations, used extensively for specular scattering

(reflectometry). This first section is more than 100 pages, and is well illustrated with diagrams of the dispersion surface construction and wave propagation.

Section II describes the theories in greater detail, with many more derivations leading to interesting consequences, from the deviations from Bragg's law to the extreme conditions of back-reflection. These applications are especially relevant to the design of monochromators at synchrotrons. These properties of wave-fields are considered in transmission and reflection geometries and their combinations, and how they form standing waves. Thirty-five pages are devoted to the interesting condition when the exit or incident wave is almost parallel to the surface. The scattering profile is modified since several positions of the dispersion surface now have significant contributions to the scattering. When both waves are nearly parallel to the surface, scattering planes normal to the surface can be accessed; this is becoming an increasingly important technique for probing thin layers and the theory of the method is discussed in this section.

With monochromatic X-ray wavelengths, we generally assume the scattering comes from one set of crystal planes, but when several reflections can be excited simultaneously, fascinating effects occur. Authier has spared us much of the mathematical details but describes the boundary conditions for 3-beam dynamical theory and how it can lead to phase determination in structure

determination. At page 249 the concept of spherical wave dynamical theory is introduced; basically the plane wave theory cannot model distorted structures. Kato's approach of creating a sum of plane waves is discussed first, with all its implications in various geometries, before the more generalised theory of Takagi, and its derivations, is covered in considerable detail. These descriptions are followed by the mathematics of ray tracing in perfect crystals, since the optics used to condition the X-rays will not create a pure plane of spherical wave. Experimental examples are given that illustrate these points.

Section III deals with imperfect crystals, working through the Eikonal approximation and the trajectories of the wave-fields in the plane and spherical wave theories. Twenty-eight pages are devoted to the propagation of waves in highly deformed crystals from the Tagaki theory and statistical dynamical theory. The latter is most relevant when the deformation becomes extreme and the wave coherence is disrupted.

The final section concentrates on applications of the dynamical theories. The description of X-ray optics is well illustrated with DuMond diagrams and the expected profile shapes determined by dynamical theory. The suppression of harmonic radiation and the controlling of the polarisation, focusing mirrors, Fresnel lenses, wave-guides and refractive lenses are all touched upon in this section. X-ray interferometry, developed by

Bonse and Hart provides a very good illustration of dynamical theory leading to phase contrast imaging, Authier then extends this section to the increasing interest in phase contrast imaging by more direct methods. An important consequence of dynamical theory is the standing wave that is created which is periodic with the crystal lattice; it also extends outside the crystal and can be used for probing the atoms from their fluorescence yield. The formulae pertaining to these effects are presented for the diffraction condition and for the specular condition; the latter can probe longer length scales. This analysis becomes more complex with thin layers and is briefly discussed. The largest emphasis on the material applications of dynamical theory is on topography in its various forms, transmission (projection and section) and reflection, with a historical perspective of the important works of Berg and Lang, low and high resolution respectively, right up to the present day. This section is well illustrated with experimental and simulated images. The volume is rounded off with a list of useful formulae derived in the book and a transcript of a lecture given by Ewald in 1975.

This monograph covers a very important subject for today's X-ray scientists which has become a very large field with many applications from the electronics industry to the design of optics for synchrotron beam lines. It is full of references for further reading, and I for one am very pleased that André Authier has put into a print a lifetime of

experience in this field. There will always be sections that one feels should also be included, for example the analysis of thin films, where dynamical theory is widely used; these aspects are, however, covered in other books. The real value of this monograph is that it brings up to date all the fundamental approaches and puts them together and explains them in a very good way.

Paul Fewster

Polymorphism in Molecular Crystals

Joel Bernstein, Ben-Gurion University of the Negev, Beer Sheva, Israel
IUCr Monographs on Crystallography, Oxford University Press, 2002

Price: £75.00 (hardback)

ISBN 0-19-850605-8, xiv + 410 pages.

This book deals with a field that in the past forty years has grown from a curiosity to a major field of study. Joel Bernstein has been one of the main movers in this development, and the book he has produced is both an excellent resource book and a very good read – no small feat! The book makes extensive and relevant use of stereo diagrams. Readers who are unfortunate enough not to be able to focus directly on these should have a pair of spectacles at hand before starting to read.

The word “polymorph”, literally meaning “multiform” or “many-shaped”, is not easy to give a precise definition. Sometimes the word, which is used in many

contexts, seems to describe its own definition! Bernstein adopts the definition of McCrone (1965) that a polymorph is “a solid crystalline phase of a given compound, resulting from the possibility of at least two different arrangements of the molecules of that compound in the solid state.” Thus solvates fall outside the scope of the book as do such pairs as acetylene (C₂H₂) and benzene (C₆H₆) with the same chemical composition but different molecules. Crystals of molecules in different conformations are polymorphs, while those of geometrical isomers are not, and the same borderline cases arise as do in solution or the gas phase. A wide-ranging historical perspective is included, with particular reference to that still amazing mine of information, Groth's *Chemische Kristallographie* (1906-1919).

A chapter on “Fundamentals” includes thermodynamic and other characteristics of polymorphs, including the often confused distinction between crystal form and crystal habit. In the structural fundamentals, the valuable Etter graph sets are introduced. The development of these has been much due to Bernstein's own use and active promotion of them.

Chapter 3 deals with the control of crystallisation and hence polymorph selection, insofar as this is possible. It includes the story of “disappearing polymorphs”, which can no longer be made after once a more stable polymorph has been found. Chapter 4, the longest in the book, is a useful description of

experimental techniques, headed by a splendid quote (from a baseball player) “You can observe a lot by just watching”. In addition to a range of thermal methods and X-ray powder diffraction, solid state nuclear magnetic resonance (SSNMR) is included.

The next two chapters cover conformational polymorphism and structure-property relationships. The possibility of various molecular conformations, differing little in energy, explains the great difficulty in the prediction of crystal structures, and the failure, so far, of computer programs to predict structures of significant flexibility. A number of fascinating examples are given, including a six-polymorph system with a convenient range of colour and habit. The presence (or absence) of significant electrical and magnetic properties distinguishes some polymorphic crystals from one another, and Bernstein makes a distinction, which is useful but must sometimes be arbitrary, between differences in *bulk* and *molecular* properties.

There are three shorter chapters dealing specifically with the importance of polymorphism in pharmaceuticals, pigments and high-energy compounds. The text concludes with some fascinating accounts of the bizarre legal cases have been fought over polymorphs, particularly in the pharmaceutical industry.

The last chapter of the book is a really extensive bibliography, 92 pages in length, which covers literature up to the end of 2000, with a few entries for 2001.

All in all, this book can be recommended strongly both for content and interest. It is expensive. Perhaps it would be a good book to share with a friend?

Bob Gould

Crystal Structure Analysis – Principles and Practice

W. Clegg, A.J. Blake, R.O. Gould and P. Main

IUCr Texts on Crystallography, Oxford University Press, 2001

Price: £49.50 (hardback)

ISBN 0-19-850618-X, xiv + 265 pages .

Crystal Structure Analysis represents the compilation and publication of the material derived from the BCA Intensive Course in X-Ray Structure Analysis, taken largely from the 1999 Course for which the authors were the principal lecturers. The book is focused on the practical aspects of structure analysis, and the succinct introductory chapter advises readers at the outset that a certain level of prior knowledge is desirable. Hammond's earlier volume, *The Basics of Crystallography and Diffraction*, from the same IUCr series would seem to be an ideal companion. The present book follows essentially the path from obtaining crystals through to structure publication. The excellent Chapter 2, dealing with crystal growth and evaluation, is drawn unmistakably from genuine experience and gives the immediate impression that the authors are masters of their profession.

Chapters 3 and 4 provide the necessary conceptual framework for understanding crystal symmetry and the theory of data collection. The introductory sentence of Chapter 4 is beautifully understated: *"Although many crystal structures are determined by people with little knowledge of the theory underlying the subject, success is more likely and problems will be better avoided by some understanding of the fundamental properties of the crystalline solid state, the nature of diffraction, and the relationships between a crystal structure and its diffraction pattern."* Both chapters are necessarily brief, and are perhaps best considered as concise summaries of assumed prior knowledge. The discussion of symmetry is densely packed and may appear a little daunting on first sight. The section concerning data collection theory is somewhat less thorough and I was a little disappointed by the omission of the Ewald construction. My disappointment was rapidly tempered, however, by a clear discussion of the indexing process and orientation matrix.

Chapters 5 and 6 deal with data collection, using serial and area-detector instruments respectively. Although the discussion of area detectors has been augmented slightly from the original Course, the authors have perhaps failed to reflect the increasing prevalence of these instruments. The discussion of serial diffractometers is in itself excellent, and will be valuable for the still considerable number of

four-circle users. The relative balance of Chapters 5 and 6, however, comprising eighteen and eight pages respectively, might be considered to lack vision. While the balance is distorted by initial discussions in Chapter 5 of fundamentals such as the number of independent data, data corrections, etc., which are not repeated in Chapter 6, it would be refreshing to see these issues addressed within a discussion of area-detector instruments. Equivalence of (hkl) and $(h-kl)$ within the monoclinic system, for example, might be better illustrated by a wide-angle CCD frame taken from a monoclinic crystal oriented with the b axis perpendicular to the X-ray beam, rather than a reflection list from a serial instrument. I hope that the emphasis might be reconsidered for any subsequent editions of the book.

Chapters 7 – 10 deal with the fundamentals of Fourier syntheses and structure solution. The chapter on Fourier syntheses is masterful, with the 1-D FeS_2 example providing excellent illustrations of the F_{obs} , F_{calc} and difference syntheses, and of the effects of series termination. Any previous Course attendee will be pleased to see that ammonium oxalate monohydrate retains its rightful prominence in the 2-D examples! Chapter 8, dealing with Patterson techniques, is equally masterful and equally concise, with the introductory section on the nature of the Patterson function being particularly impressive. I would have been pleased to see both Chapters 7 and 8 expanded, but their brevity is consistent with the practical

focus of the book as a whole. Chapter 9 deals with direct methods, in considerably greater depth than the previous chapters. The lucid discussion of the physical basis of direct methods gives genuine insight into what many of us perceive to be intimidating mathematics, and provides as a result one of the more comprehensible descriptions of the technique. Chapter 10 gives an interesting introduction to the concepts of maximum entropy and is a welcome addition to the structure solution discussion.

Chapters 11 – 14, dealing with structure refinement and interpretation of results, are without question the outstanding feature of the book. The discussion of least-squares fitting in Chapter 11 is excellent and should prove generally valuable to a scientific audience much wider than the crystallographic community. Discussion of the effects of restraints and constraints on the least-squares procedure is particularly enlightening. Chapter 12 concentrates more specifically on crystal structure refinement and is filled with helpful practical advice; this chapter in conjunction with suitable example data sets would form the basis of an excellent refinement workshop. Chapters 13 and 14 describe the derivation of secondary results, their statistical significance, the effects of errors and the comparison of results with authority and a healthy realism. As the number of structure determinations performed by non-specialist crystallographers inevitably increases, Chapters 13 and 14 should become mandatory reading.

The closing chapters, dealing with the presentation of results, the CIF format and structure databases, are relatively lightweight in comparison with their predecessors, a reflection of the difficulties associated with presenting such topics in a traditional book format. Nonetheless, each provides a useful starting point and numerous sources of further information. The book also contains three Appendices: useful mathematical formulae, a brief crystallographic dictionary and the answers to Exercises present at the end of each chapter. Inclusion of the Exercises, no doubt remembered with affection by past students of the Course, is most welcome. I suspect that they may find extensive use in lecture courses – I am aware of at least one where that is already the case!

There is of course no question that the book is a valuable addition to the crystallographic literature, and it succeeds in communicating to the reader the extensive knowledge and experience of the authors. The chapters have been admirably edited into a coherent whole that provides an informative and enjoyable account of the practical aspects of the subject. Available initially only in hardback, the price may be intimidating to the average student, but the paperback release should be eagerly anticipated.

Andrew Bond

Structure Determination from Powder Diffraction Data

W.I.F. David, K. Shankland, L.B. McCusker and Ch. Baerlocher
Editors

IUCr Monographs on Crystallography, Oxford University Press, 2002

Price: £70.00 (hardback)

ISBN 0-19-850091-2, xvii + 337 pages.

It is probably best to start this review by declaring some American style First Amendment rights, in that the following is only the personal opinions of an individual reviewer. A reviewer who was less irritated by the promotional blurb and extremely high price would no doubt have very different options, and thus provide a very different review.

This book on structure determination from powder diffraction data is a worthy kindred spirit to the Rietveld book edited by Ray Young and published in 1995, both of which are part of the same series of IUCr Monographs on Crystallography. With the exceptions of peak profiling to obtain peak positions prior to indexing, a chapter on solving structures under extreme conditions, and information relating to structure validation and publication, there is a good spread of relevant topics. Examples of this are the inclusion of chapters on sample preparation and data collection, and using chemical information and intuition in solving structures from powders. However, it is disappointing there are no contributions by G.S. Pawley and

Armel Le Bail, even if only in the form of reminiscences. It is their seminal contributions (Pawley in 1981 and Le Bail in 1988) that allowed solving structures from powder diffraction to start reaching escape velocity. Thanks also goes to Jeremy Cockcroft for observing that while crystallographers can now calculate the odds of solving structures from real space methods, they are not yet able to calculate the odds of the UK National Lottery (page 259): the real answer is $49!/(6!(49-6)!)$ [1 in 13,983,816]. The reviewer would also be interested to hear if there are IUCr or OUP publishing policies relating to where possible conflicts of interest by authors need to be declared up front: for example, two of the authors already have a "software patent" that seems related to some of the ideas and information in the text (see International patent WO9906824 titled "Method and apparatus for determining molecular crystal structures" - <http://l2.espacenet.com/espacenet/viewer?PN=WO9906824&CY=ep&LG=en&DB=EPD>). Overall, there is nothing in the text itself to stop this becoming a standard text on crystallographers' shelves for the foreseeable future.

What might be considered a minor problem to some, though a major issue to this reviewer, is that of the book's blurb and the publisher's promotional webpages which give the impression that it is appropriate for guiding novices (<http://www.oup-usa.org/isbn/0198500912.html> and <http://www.oup.co.uk/isbn/0-19-850091-2>). While appropriate and

useful for experts and those seriously involved in powder diffraction, this text is not appropriate for guiding novices. Using the "Crystal Structure Determination" book by W. Massa as a benchmark text for comparison, the SDPD book suffers from having separate chapters written by separate authors. The reviewer cannot think of any text where sets of authors writing separate chapters has made a good teaching text or guide to novices. The quantity and quality of "hints" and useful rules of thumb vary from chapter to chapter. There is also no "novice friendly" worked example as available in the Massa book.

Furthermore, given the importance of software programs in a crystallographic text of this type, many of the chapters give the impression of being quite insular in not referring to any real world software tools. Some of these unmentioned programs are highly conspicuous by their absence, which a novice reader may not realise. Some chapters concentrate on the attributes of a certain software package, while others seem oblivious to available software. The most striking example of this is in the chapter on Le Bail and Pawley extraction which concludes: "well-developed computer programs based upon the Le Bail and Pawley methods are available for extracting integrated intensities from powder diffraction data". Yet it does not name any such programs or provide a relevant software bibliography and Internet resource list. There is also no helpful technical comparison

between programs that novices would find helpful. The chapters on applying Patterson methods to extracted hkl data, while including references to SHELX, exclude any reference to DIRDIF (<http://www-xtal.sci.kun.nl/xtal/documents/software/dirdif.html>) and PATSEE (<http://www.org.chemie.uni-frankfurt.de/egert/html/patsee.html>). This is despite at least one publication (uncited in the book) showing PATSEE to be effective in this role (Acta Cryst. A56 (Supplement), s24, 2000). Direct references to some important real-space programs are missing. These include ESPOIR by A. Le Bail (<http://www.cristal.org/>); FOX by V. Favre-Nicolin and R. Cerny (<http://objcryst.sourceforge.net/>) and ZEFSAII by M. Deem et al (<http://www.mwdeem.rice.edu/zefsaII/>). This is further compounded by an appendix listing of computer programs that is very incomplete and strangely not Internet aware. Given that programs can date or change quickly, there are also no general guides or advice in the Software Bibliography to assist the reader on building up a modern, relevant software toolset (e.g., using the IUCr's Crystallography World Wide or the IUCr's Sincris facility). These omissions may not seem that significant to those experienced in the field, but would be significant to novice readers.

Again, none of the above is fatal to this book becoming a standard text in powder diffraction for the foreseeable future. It is, however, my opinion that at £70, the cost is excessive. The pricing goes against technological advances in

publishing that, in theory, should make this type of book cheaper, not priced in the stratosphere. To the young and impressionable, pricing of this type might in their minds justify the illegal use of a photocopier to make personal copies. An alternative for potential readers, institutes and libraries would be to make use of the Internet to find relevant up to date information on this topic. This Internet available information is plentiful (such as Armel Le Bail's website at <http://www.cristal.org>; the IUCr's Crystallography World Wide / Sincriis at <http://www.iucr.org>; and the Structure Determination by Powder Diffractometry (SDPD) mailing list via <http://www.yahogroups.com/list/sdpd/>). A revised price based in the reality of what is affordable to academics and students in both the developed and developing world might redeem this book and assist it in becoming a standard text in powder diffraction.

Lachlan M. D. Cranswick

Electron Microscopy & Analysis 2001, Proceedings of the IOP Electron Microscopy & Analysis Group Conference, Dundee 5-7 September 2001

M.Aindow and C.J.Kiely Editors
IOP Conference Series no. 168,
Institute of Physics Publishing,
2001.

Price £110 hardback
ISBN 07503 0812 5, 520 pages,
Author and Subject index

EMAG conferences are biennial events organised by the Electron Microscopy and Analysis Group of the Institute of Physics in the UK. This volume is a conference proceedings arising from such a meeting in Dundee in 2001. 'Not much here for the crystallographer', I can hear you say, and in one sense you would be right - the book is hardly awash with crystal structures (I counted one in the entire volume), and most of the work is involved with the analysis of high resolution electron microscopy images and related methods. But, and it is an important 'but', as crystallographers deal with ever smaller crystalline samples, it is useful to have a current window on the world of nano-crystallography and associated materials, even within all the expected limitations of a book of conference proceedings based on electron microscopy.

There are 128 contributions in 11 sections; each contribution takes 4 pages. The ones that may interest crystallographers most are those on HREM and Electron Crystallography; Ferrous Metals and Intermetallics; Carbons, Ceramics and Composites; Catalysts, Sensors and Environmental Materials and Semiconductors, Superconductors and Magnetic Materials. This is more than half the book, although it must be said that the crystallography is dominated by HREM. There is also lot of material on EELS spectroscopy, and elemental mapping. In this context, I especially enjoyed a paper by Pike et al. on 'A Microscopy Station for Mars'. What about an X-ray

diffractometer for Mars? - that would be exciting! Theory is not forgotten either: there are papers on image processing, image analysis, exit wave reconstructions in the electron microscope and tomography. Unlike many books of this sort, there is a uniformity of presentation that makes it easy to browse.

The crunch is: would I buy my own copy? The answer is 'no', but I might just persuade the university library to buy one.

Chris Gilmore

Valence Bond Methods – Theory and Applications

Gordon A. Gallup, University of Nebraska.

Cambridge University Press, 2002
Price: £65.00 (hardback)
ISBN 0-521-80392-6, xv + 238 pages .

Valence bond and *ab initio* molecular orbital theories were both developed in the 1920's, but as the former is not so amenable for calculation of large molecules, molecular orbital theory has come to dominate the field. There are several problems, however, such as bond breaking/making or interpretation of molecular orbital plots, where valence bond theory has been shown to be the more appropriate method. It is therefore important that researchers and students of computational chemistry are aware of this alternative method.

Gallup's book follows the tried

and tested format for computational chemistry texts: part I is devoted to a discussion of the basic theory, whilst part II focuses on case studies for sets of related molecules. In addition the text also advertises the freeware program CRUNCH, available from the author's website, from which most of the calculation results highlighted in the text were obtained.

The development of valence bond theory is comprehensively set out, starting with a general discussion on Schrodinger's equation, before moving on to the Heitler-London function and its subsequent extensions, and ending with the theory behind multi-configuration valence bond calculations. The hydrogen molecule is used as a simple two-electron illustration for many of the principles highlighted in the text. Special consideration is then paid to the treatment of three-electron doublet states, before an account of advanced methods, which are suitable for application to larger molecules, is presented. This section of the book also includes an extensive discussion on the symmetry grouping of wavefunctions. The author, however, does not give any indication of how large a 'large molecule' is or state how the calculations scale with e.g. basis set description or the number of electronic configurations included in the calculation. The reader is thus left a little in limbo to know how tractable this style of calculation will be for a particular application they may have in mind.

The case studies presented in part II begin with four simple three-electron systems: the allyl radical, $[\text{He}_2]^+$, the valence orbitals of BeH and the Li atom. The reader is guided through multi-configurational and other valence bond theory methods, and for each system a consideration of the accuracy of the calculation (in terms of dissociation energies, geometries, vibrational frequencies, dipole moments, and energies) is discussed. The next set of compounds presented are the homonuclear diatomic molecules of the second row of the periodic table, before considering a set of isoelectronic second row heteronuclear diatomics. The remainder of the book then focuses on organic examples, including small hydrocarbons, ring and aromatic compounds. Special consideration is given to the nature of resonance in benzene, which is perhaps the best known example of where valence bond theory (supporting the Kekule/Dewar model) rates higher than molecular orbital theory (supporting the delocalised model).

In short, this book provides a comprehensive introduction to valence bond methods, and the complexity of equations presented is not too daunting for the mathematically timid.

Carole Morrison

Education Posters For the BCA Annual Meeting in 2003

Education should be a lifelong experience, yet many people appear to think that it is confined to a few years of school and Institutions of Higher Education. The advent of the Open University has demonstrated that this is not the case. Members are invited to submit posters on any topic associated with education in crystallography at any level.

Read the report on the education sessions at the recent IUCr Congress held in Geneva in August to get some ideas. The Institute of Physics has a project to help school teachers by providing 'Resource CDs' on selected topics in physics. Your poster might suggest the essential topics for such a CD in 'condensed matter and materials'.

Alternatively, you might describe your own experiences, were you as a student expected to understand crystallographic topics with too little background knowledge? Tell BCA members about them, so that their courses may be modified.

Are lectures and textbooks old technology in these days of the Internet? Should introductory lectures be scrapped and students expected to learn the fundamentals from the Internet?

How would you explain the fundamentals of say biological structure determination to BCA members from other special interest groups? Whatever your educational topic, tell us about it in your Abstract and bring a Poster to the Annual meeting in 2003.

Kate Crennell

**CrystEngComm
Discussion 1 - Innovation
in Crystal Engineering
Bristol, UK
29 June – 1 July 2002**

The first CrystEngComm Discussion meeting was held in Clifton Hill House in Bristol at the end of June. The meeting took place over two and a half days and was an opportunity for discussions on various areas of research related to the field of crystal engineering. Topics discussed included intermolecular interactions (in particular hydrogen bonding), polymorphism, crystal growth and design, and the modelling and prediction of crystal structures. The meeting was divided into five sessions each starting with a plenary lecture and then followed by the short presentation of six papers and a discussion of each of these, lasting approximately fifteen minutes.

The opening lecture by Toda (Okayama, Japan) was entitled Crystal Engineering for Molecular Dynamics and reported the crystallisation of chiral molecules through the use of inclusion compounds. The second plenary lecture was by Davey (Manchester, UK) and looked at the importance of nucleation and pre-ordering in solution, in particular solute-solvent interactions, and how this relates to the crystallisation process and how this can be applied to crystal engineering. Coppens (Buffalo, USA) lecture was concerned with the use of solid state spectroscopy and time-resolved diffraction in particular to study calixarene based supramolecular solids. A

review of polymorph prediction and the future challenges for this field of research was given by Gavezzotti (Milan, Italy), in particular looking at the various energy terms which must be included within any prediction. The final plenary lecture was given by Yaghi (Michigan, USA) who reported on work in the area of metal-organic frameworks, the logical design of these materials and some of their applications and gave a very good overview of this area of research. The short presentations and discussions covered a wide range



of areas of research within the crystal engineering field. There was a paper from Price (London, UK) looking at the crystal structure of pyridine which has a Z' of 4. There were also papers covering hydrogen bonding research and intermolecular interactions including those by Pedireddi (Pune, India) and McKinnon (Armidale, Australia). The area of polymorphism was included in research presented by Steed (London, UK) and Grepioni (Sassari, Italy). Tedesco (Basel, Switzerland) reported on three case studies in which varying areas of crystal engineering research have been applied to problems that exist within the pharmaceutical industry. Harris (Birmingham, UK) gave an interesting presentation on the advances in the area of solving crystal structures from powder



diffraction data. Many papers reported research which used supramolecular synthons including Aakeroy (Kansas, USA) who reported on the oxime-oxime interaction and Podesta (Bristol, UK) who reported a new tecton nickel bis(dithiooxalate). Overall there were many interesting discussions throughout the meeting concerning crystal engineering as a field of research and in particular what directions the research should be taking in the future.

On the Sunday evening I had the opportunity to present my poster, Hydration in Molecular Crystals, which reported a Cambridge Structural Database study on the environments of water molecules within organic hydrates. My poster was well received and I obtained some valuable feedback on the research.

Of course on the Sunday afternoon there was a break to allow everyone to watch the World Cup final! The meeting finished on the Monday evening with a dinner on the SS Great Britain, the iron steamship designed by Isambard Kingdom Brunel.

Dr. A.L. Gillon
Research Associate

Diamond Developments

Progress with the planning and development of the new synchrotron facility, Diamond, at the Rutherford Appleton Laboratory, near Didcot, in Oxfordshire has been moving at an increasing pace during 2002. Diamond Light Source Ltd, the company that will commission and operate Diamond, was officially set up on the 27th March, and the outline architectural design for the Diamond building was published in July. Diamond should be up and running in 2006 when the first beamlines come into operation. Principal Beamline Scientists have been appointed for the Year-1 beamlines and include Dr Andrew Jephcoat (Beamline 1: Materials under extreme conditions), Dr Elizabeth Duke (Beamlines 8, 9, 10: Protein Crystallography), and Dr Andrew Dent (Beamline 13: Microfocus spectroscopy). More information on the progress of the project can be found on the diamond website, www.diamond.ac.uk.

The BCA has appreciated the importance and potential of this new facility, and at the Nottingham Spring Meeting, in March, a Special Interest Group (the Diamond SIG) was set up, with a steering group



The straw plan published by courtesy of Diamond Light Source Ltd.

representing the interests of the various subject groups. The SIG will be promoting the organisation of various meetings to discuss aspects of the Diamond project that will be of interest to BCA members, and will aim to stimulate action within the community to develop exciting new science that can take advantage of the Diamond facility. A SIG Meeting is scheduled at the York Spring Meeting, on 16th April. In addition, a meeting combining the interests of the SIG together with those of the SRS XRD Special User Group and the ISIS Crystallography User Group, entitled "Advanced Instrumentation for Crystallography (at UK Facilities)", is currently being planned. This will take at RAL in early April 2003, and details will be published as soon as they have been finalised.

Diffraction related beamlines form an integral part of the planning for Diamond, as can be seen from the straw plan that shows provisional positions for the Year-1, Year-2 and other possible beamlines. It should be stressed that this plan is provisional, and the Diamond Science Directors and the members of the Diamond Scientific Advisory Committee would welcome comments and suggestions from the general community. Crystallographers from the BCA are already contributing to the planning process. In November 2001, 16 beamline proposals were submitted to the Diamond SAC for consideration for development that would lead to them becoming operational in 2007. These included a high resolution powder diffraction beamline, a small molecule single crystal beamline, and a microfocus crystallography



A view of the Diamond buildings published with permission of JacobsGIBB Ltd / Crispin Wride Architectural Design Studio.

beamline for investigating the structure of large biological molecules. The powder diffraction beamline and the microfocus crystallography beamline both made it to the shortlist of six, and subsequently, with an X-ray spectroscopy beamline, were selected for development with the aim of going into operation in 2007. This is excellent news for the powder diffraction and protein crystallography communities as these beamlines will provide them with 'world beating' facilities for several decades to come.

The call for submissions for Year-3 beamlines, to become operational in 2008, with a submission date of 1st November, 2003, has appeared. Although the small molecule single crystal beamline did not make the shortlist last year it is being resubmitted with an even stronger case and a plethora of new science. Support from the whole community for this proposal would be much appreciated, and news as to how the proposal proceeds will be provided in the next Diamond SIG update that will appear in the next issue of Crystallography News.

Paul Raithby
Co-ordinator BCA Diamond SIG.

BCA Survey of the amount of crystallography in UK undergraduate courses.

More responses have been received since our request for information was publicised by the Mineralogical Society. A final report will be written for the next issue of 'Crystallography News' and discussed during the Annual meeting in York in 2003.

Kate Crennell

PANalytical Prize for Physical Crystallography

Since the purchase of Philips Analytical by Spectris PLC in September 2002 the company is trading under the name of PANalytical Limited. PANalytical have agreed to continue to sponsor the annual award for Physical Crystallography which will be renamed the "PANalytical Physical Crystallography Award". The award is presented for the best recently published work (say 2-3 papers in the last few years) by a relatively young person (usually 35 years of age or younger) working in the field of Physical Crystallography. The research represented by the published papers should be principally the work of the nominee and should be of a level to make a significant impact in his or her field. The 2003 award will be made during the Annual BCA Spring Meeting at the University of York and the recipient will be expected to give an oral presentation of his or her work

at that meeting. The committee of the Physical Crystallography Group (PCG, also known as the Structural Condensed Matter Group of the IoP) decide on the awardee and PANalytical sponsor the prize, which consists of a cash award of £500 plus expenses for attending the Spring Meeting to deliver the award lecture. The Award will be presented by a representative of PANalytical.

Nominations should include a brief CV of the nominee; copies of the papers on which the nomination is based (on which the main judgement is made); and a supporting statement from the nominator, including comments on the part the nominee has played in any research work published jointly with others. Optionally, a nomination form is available from the PCG Secretary (john.evans@durham.ac.uk) or on the web at <http://bca.cryst.bbk.ac.uk/bca/pcg/priz2003.htm>. Nominations of candidates from the same department as the nominator are not normally allowed.

Nominations for this award should be sent, not later than 31st January 2003, to the Chairman of the Physical Crystallography Group Committee:
Pam Thomas,
Department of Physics,
University of Warwick,
Coventry CV4 7AL, UK

Would you believe it?

Crystallography in the Press and elsewhere.

Sandy Blake reports evidence of undercover crystallographers in industry. One of his colleagues had proofs of a paper in *J. Chem. Phys* returned with a valuable correction. Whenever the firm SmithKlineBeecham was mentioned, the software had helpfully rendered it as *SmithklineBeecham*.

The summer edition of the Purdue University *Perspectives*, which the Editor still receives because he attended a summer course there in 1955, had an excellent centre-page spread on Michael Rossman. Surprisingly, though, they reported that his work on viruses was now enabling him to look at "tinier and tinier" structures! Who knows, he may attempt rock salt one day!

And something a little more useful: Howard Flack has discovered a minor breakthrough in typography. Scientists at the University of Mississippi have devised a new font, LinguistA, which enables a "bar" to be put over English characters and the most commonly used Greek characters in MS-Word documents. For

more information, go to <http://www.arxiv.org/abs/hep-ex/0208028>. The bad news is twofold – it only works for Apple-Macs, and it doesn't seem to work for digits, making it great for anti-matter but not much use for space groups. Does anyone have any solution that neither uses the equation editor nor puts an unwanted space in front of the symbol?

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But best of all, we have Kate Crennell to thank for spotting this in the 'Times' section T2 for 17 September 2002. The following paragraphs were printed as part of the review of David Attenborough's recently published biography. (more than they've had on crystallography for a while!)

Private Matters

In Madagascar, I heard of the wife of a long-established English resident. She was a White Russian by birth and was said to be a little eccentric, but everyone told us that she was a passionate animal lover. We were delighted when she sent us a formal invitation to dinner.

She proved to be small, somewhat withered, dressed in a number of voluminous cloak-like garments, one on top of the other, and given to large and dramatic gestures. "Welcome," she said huskily and waved us

into a huge living room. A wide shelf ran all the way round it. It was lined with a spectacular collection of crystals! Here was an obvious topic with which to break the conversational ice. I admired a double-ended quartz crystal, which pleased her, and moved on to a large pillar of a black mineral. Could this be a tourmaline? It was. I raked through my memories of mineralogy lectures at Cambridge and became bolder. Surely this wonderful specimen of mica, with its pinkish tinge, must be the rare variety known as lepidolite. For a moment I feared that I had over-done it, but she was greatly impressed.

"You are exactly the man I have been waiting to meet," she said. "People here are so ignorant. You know about these things."

I demurred, modestly. "Wait!" She turned on her heel, swept away into an adjoining room and returned within seconds, holding in front of her an object swathed in cotton wool. "You are the only person here who would realise how rare this is."

Fearing that the limits of my expertise were about to be exposed, I somewhat apprehensively unwrapped it. Inside, I found a long quartz crystal with two much smaller ones attached to its base. All three were covered with haematite, an iron-rich mineral with a smooth black surface that not uncommonly encrusts crystals of various kinds.

"You do know what it is, don't you?" she whispered.

"Well, yes," I said nervously, "It's three quartz crystals covered with mammiferous haematite." I sensed that this was not the right answer.

"You are wrong," she said firmly. "Those are the fossilised private parts of a pygmy. Why on earth would you think they are quartz crystals?"

"Well," I said nervously, "they are hexagonal. They have six sides and a pointed end."

She snatched the specimen away from me and wrapped it up again. "And how do you know," she said haughtily, "that a pygmy's private parts don't get six sides when they fossilise?"

To which question I failed to find an answer.



Diary Dates

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, bob@gould.ca

2-4 December 2002

Second International Conference on Structural Biology and Functional Genomics, National University of Singapore. [<http://www.dbs.nus.edu.sg/structbio/>]

5-6 December 2002

21st BESSY Users' Meeting, Germany. [<http://www.bessy.de/announcements/>]

6-8 December 2002

Automation for High-throughput Structure Determination, E.O. Lawrence Berkeley National Laboratory. [<http://bcsb.lbl.gov/Conference/ConferenceMain.htm>]

8-12 December 2002

The Second Pharmaceutical Powder X-ray Diffraction Symposium PPXRD-2, Concordville, Pennsylvania, U.S.A. [<http://www.icdd.com/ppxrd/>]

12-13 December 2002

The ninth workshop to discuss the neutron-beam instrumentation for Australia's Replacement Research Reactor, Lucas Heights, Australia. [<http://www.ansto.gov.au/ansto/neut/workshop8.html>]

12-14 December 2002

Magnetic Rietveld Workshop 2002, Abingdon, Oxon. [<http://bca.cryst.bbk.ac.uk/bca/pcg/magw2002.htm>]

12-14 December 2002

A workshop on the Perspectives in Single Crystal Neutron spectroscopy (SCNS), Institut Laue - Langevin, Grenoble, France. [<http://www.ill.fr/Events/ONSITE/SCNS/index.html>]

19-21 December 2002

3rd WSEAS International Conference on Mathematics And Computers in Biology and Chemistry (MCBC 2002), Puerto De La Cruz, Tenerife, Canary Islands, Spain. [<http://www.wseas.org/conferences/2002/tenerife/mcbc>]

3-4 January 2003

CCP4 Study Weekend "Experimental Phasing", University of York. <http://www.ccp4.ac.uk>

20-27 January 2003

International school on crystal growth of technologically important electronic materials (ISCGTIEM), Mysore, India. [<http://www.semiconductors.co.uk/iscg-tiem/>]

22-25 January 2003

2nd Workshop on Dynamics in Confinement. Institut Laue Langevin, Grenoble. [<http://www.ill.fr/Events/ONSITE/confit2003/confit.html>]

7-15 April 2003

9th BCA/CCG Intensive Course in X-ray Structure Analysis, Durham. [<http://bca.cryst.bbk.ac.uk/BCA/CCG/du03rg.pdf>]

9-11 April 2003

International workshop on hard synchrotron X-rays for texture and strain analysis, HASYLAB, Hamburg. [<http://www-hasyllab.desy.de/conferences/workshop/>]

14-17 April 2003

BCA Annual Meeting, University of York. [<http://bca.cryst.bbk.ac.uk/BCA/meets/BCAs.html>]

19-23 May 2003

Third National Crystal Chemical Conference, Crystal Chemical Section of the Scientific Council on Chemical Structure and Reactivity of the Russian Academy of Sciences, Moscow, Russia. [<http://www.icp.ac.ru/Conference/NC3/>]

25-30 May 2003

The Seventh International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors (M2S-HTSC-VII), Rio de Janeiro, Brazil.
[<http://www.m2srio.cbpf.br>]

4-15 June 2003

High Pressure Crystallography Erice, Italy.
[<http://www.geomin.unibo.it/orgv/erice/highpres.htm>]

22-25 June 2003

XIIth International Workshop on Quantum Atomic and Molecular Tunnelling in Solids, University of Florida in Gainesville.
[<http://www.clas.ufl.edu/QAMTS>]

22-27 June 2003.

The 12th International Conference on X-ray Absorption Fine Structure (XAFS 12), Malmö, Sweden.
[<http://xafs12.maxlab.lu.se/>]

29 June - 3 July 2003

11th Annual International Conference of Intelligent Systems for Molecular Biology, Brisbane, Australia.
[<http://www.iscb.org/ismb2003>]

20-24 July 2003

The Fifteenth American Conference on Crystal Growth and Epitaxy (ACCGE-15)". Keystone, CO, USA.
[<http://www.crystalgrowth.org/conferences/ACCGE15/index.html>]

26-31 July 2003

American Crystallographic Association Annual Meeting, ACA 2003, Cincinnati, Ohio, U.S.A.
[<http://www.hwi.buffalo.edu/ACA/ACA-A-Annual/futuremeetings.html>]

10-13 August 2003

Australian Crystallographic Association '03/Crystal-23, Cable Beach Club Resort, Broome, WA, Australia.
[<http://www.crystal.uwa.edu.au/CrystalsDownUnder/>]

14-15 August 2003

Workshop on Biological Structure, Cable Beach Club Resort, Broome, WA, Australia.
[<http://www.crystal.uwa.edu.au/CrystalsDownUnder/>]

14-19 August 2003

Sagamore Meeting (IUCr Commission on Charge, Spin and Momentum Densities), Cable Beach Club Resort, Broome, WA, Australia.
[<http://www.crystal.uwa.edu.au/CrystalsDownUnder/>]

24-30 August 2003

21st European Crystallographic Meeting, Durban, South Africa.
[<http://www.ecm21-africa.co.za/>]

2-6 September 2003

ECNS 2003 European Conference on Neutron Scattering, Montpellier, France.
[<http://www.sfn.asso.fr/>]

3-7 September 2003

Fifth International Conference On Molecular Structural Biology, Vienna, Austria.
[<http://pharmchem.kfunigraz.ac.at/icmsb2003/>]

8-13 September 2003

Aperiodic-2003, Belo Horizonte, Brazil.
[<http://www.fisica.ufmg.br/~ap2003/>]

14-19 September 2003

Structure Solution from Powder Diffraction Data, Stara Lesna, Slovak Republic.
[<http://www.sspd-03.sav.sk>]

10-21 June 2004

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

August 2005

XX Congress of the International Union of Crystallography, Florence, Italy.
[Carlo Mealli,
email: mealli@fi.cnr.it]

Final Accounts**BCA Spring Meeting 2002 University of Nottingham**

INCOME	Sponsorship	£7,510.00
	Registration	£45,221.68
	Exhibition	£9,050.00
	Bursary	£3,360.00
	Total	<u>£65,141.68</u>
EXPENDITURE	Accommodation & Meals	£26,433.30
	Facilities	£2,307.80
	Catering	£4,992.11
	Social Event	£1,753.20
	BCA Speakers Expense	£1,664.34
	Abstract Book	£2,958.00
	NN Fee	£8,953.50
	Administration	£3,225.31
	Stationery & copying	£300.00
	Bursaries	£5,400.00
	Total	<u>£57,987.56</u>
	TOTAL INCOME	<u>£65,141.68</u>
	TOTAL EXPENDITURE	<u>£57,987.56</u>
	MEETING SURPLUS (-DEFICIT)	<u>£7,154.12</u>

Dr A J Blake - The University of Nottingham

Mr D J Taylor - BCA Treasurer 15/10/2002

Note: These accounts include transactions made through the University of Nottingham, the BCA and BCA Group accounts. Expenses paid through Group accounts, which will appear in the restricted funds of the BCA, have been refunded from the BCA account.