Crystallography News

British Crystallographic Association

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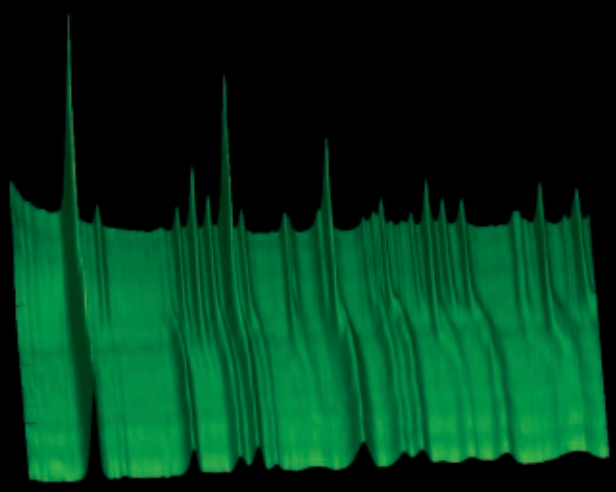

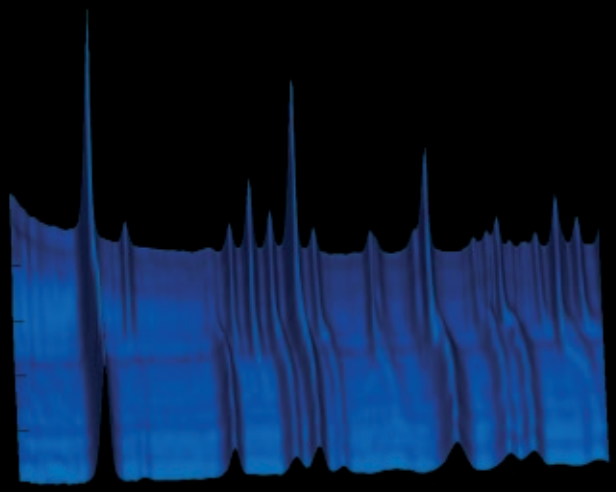

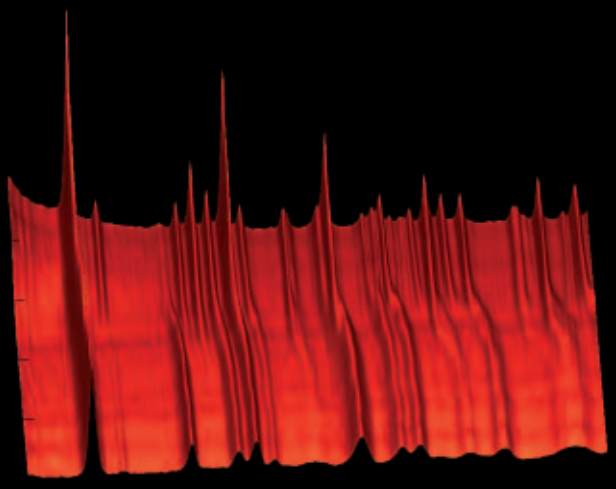

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association.

Text should preferably be sent electronically as MSword documents (any version - .doc, .rtf or .txt files) or else on a PC disk. 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 **September 2004** issue are sent to the Editor to arrive before **25th July 2004.**

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BCA News June 2004

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Foucault Pendulum at UMIST

This months cover:

Photographs are from prize-winning Poster BP-25 at the Spring Meeting, submitted by Rena Margiolaki of ESRF.

The main picture represents the temperature evolution of the diffraction pattern of Turkey egg-white lysozyme, and the refined conformation of the molecule is shown in the inset.

From the President

REFLECTING on the recent BCA Spring Meeting, the 22nd of our Annual Meetings, it is a pleasure to record that it was well attended, vibrant and successful.

A wide range of high quality talks was appreciated by good audiences, and the exhibition and poster sessions provided a well structured centre-piece for the meeting. Thanks are due to the indefatigable Paul Fewster, Programme Chair (of whom more later), to Northern Networking for their organisation, to the various sponsors and exhibitors for their support and of course to all participants for making it such an enjoyable meeting.

One innovation at this year's Spring meeting, of which there is more elsewhere in this issue of Crystallography News, was the Young Crystallographers' satellite. Organised by Charlie Broder, Andy Parkin and Julie Wilson, this attracted a large audience of between 70 and 90 for its various sessions. Although mostly an audience of young people, there were some elderly interlopers such as yours truly, who were of course made very welcome. The quality of the talks was quite outstanding and the YC meeting had a vibrancy and enthusiasm about it that bodes extremely well for the future of our subject. Thanks to all involved, and this meeting will be staged again, again organised by younger members of the community.

At the YC meeting, one of the undoubted highlights was Elspeth Garman's Kathleen Lonsdale lecture. This was one of three excellent named and prize lectures in Manchester, the others being the Bragg Lecture given by John Finney and the Dorothy Hodgkin Prize lecture delivered by George Sheldrick. We were fortunate indeed to have such an inspiring and diverse set of lecturers and topics at the meeting.

So then, who would have held sessions on the "Use of International Tables" and "Advanced Aspects of Symmetry" on the morning after the Conference Dinner (and starting at 8:30 moreover) and how could we possibly get an audience for it. Well, the BCA of course, and as a result of having an excellent set of lecturers/tutors, there were over 100 in session one and more than 60 in the advanced session. We are either keen or daft (I rather suspect the former). Either way it was great to see, and we will ensure such education-based sessions remain part of the Spring Meeting. Bill Clegg, Jeremy Cockcroft and Mike Glazer are to be thanked for taking this apparently tricky remit and making such a success of it.

The Spring meeting saw some changes on BCA Council, including changes in the group representations from Biological, Chemical and Industrial subject groups. We thank the outgoing council reps Andrea Hadfield, Harry Powell and Chris Frampton. I recorded in a previous column the departures of longstanding councillors Paul Barnes and Chris Gilmore, and Manchester also saw the retiral of our Vice-President Paul Fewster. The success of the science programmes at recent Spring Meetings have largely been down to Paul's hard work, and the degree of cooperation between our various subject groups in sessions at the SM has been enhanced during his tenure. All that hard work and only a Young Crystallographer's T-shirt as reward at the end of it! Well, that and the heartfelt thanks of all of us for his hard work and dedication to the cause. Paul is succeeded by John Finney, and Christine Cardin has succeeded herself as Secretary, taking on a second term in post. I once again take this opportunity to thank all the officers for their massive contributions to keeping our organisation on track.

Personally, the summer will see me, as well as attending ECM-22 in the beautiful city of Budapest in August, ending my co-location at CCLRC-RAL and Glasgow. Although I will be moving to a full-time post in Glasgow, I will retain strong links with many colleagues, collaborators and friends at RAL and will remain a committed user of the neutron facilities there. Plus ca change and all that, but it will be a wrench after 19 happy years at ISIS. On a practical note, all my usual email addresses should continue to reach me, and I welcome comments on the BCA and its workings.

Chick Wilson

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

From the Editor

FOLLOWING favourable comment on the last issue, we are continuing its style in Issue 89. The major item for reporting is, of course, the excellent Spring Meeting we have just had. As the President has noted, a major innovation this year was the Young Crystallographers Meeting.

Students obtaining bursaries are required to write reports, and this time we have organised the reporting of sessions to be almost entirely from student reports. I have done a little judicious(?) merging of these to cover sessions, but hope that I have retained the freshness of the authors' styles! To restrain the size of the issue, some of the reporting has been postponed to the next issue.

My thanks, as usual, to those who undertake book reviews, and particularly to those who do them quickly. This time, one of the reviews which modesty prevents me from mentioning, is of a book the reviewer collected at the Spring Meeting! Not all publishers think to send us copies; please do suggest books to be reviewed, both to us and to them.

A new feature this issue are a few "press releases" from our advertisers. In general, we hope to have about a page of these, and it is a condition of publication that an advertisement is taken out as well! We also wish to thank the exhibitors at UMIST for submitting to having their pictures taken for the centrespread!

I tried to take a good batch of pictures at UMIST. In fact, someone suggested that my trigger-happy picture taking in Bill Duax style might mean that I am keen to become president of the International Union. As usual, though, I do have to plead with people attending meetings on which they are going to report to take cameras with them. Meanwhile, I can promise you one issue free of tramcars and earth-shifting equipment!

Bob Gould

BCA Corporate Membership

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

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

The cost of this membership is **£600.00** per annum

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

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Rigaku MSC

News

Open-access charges waived for one year for UK FE staff publishing in IUCr journals

THE International Union of Crystallography (IUCr) is delighted to announce that it has been awarded funding from the Joint Information Systems Committee (JISC) to support open-access delivery of its journals, Acta Crystallographica Sections A-E, Journal of Applied Crystallography and Journal of Synchrotron Radiation, via its Crystallography Journals Online service.

The award will mean the waiving of open-access publication charges for UK higher education staff who publish in these journals for a one-year period from 1 March 2004. This will make UK research more visible worldwide, assisted by the international standing of IUCr journals.

JISC is a committee of all UK further and higher education funding bodies, and is responsible for supporting the innovative use of information and communication technology to support learning, teaching and research. In December 2003, publishers were invited to tender for open-access funding of £150,000, the first round in a three-year programme designed to encourage as much open-access delivery of research findings as possible. This initiative coincides with the IUCr's support of open standards as a means to promote its statutory objective of disseminating crystallographic information to the widest possible audience. From the beginning of 2004, authors publishing papers in IUCr journals have been given the opportunity to make their papers open access on Crystallography Journals Online, i.e. free of charge to all readers. Open-access papers will appear alongside standard subscriber-only papers for the foreseeable future.

The normal charge for making an article open access is £500. This charge is based on the average cost for the IUCr to produce the first copy of the article, excluding printing and distribution costs, and includes a contribution to the cost of the long-term preservation and access of the publication. Revenue generated from open-access payments will be used to keep subscription costs as low as possible. Open-access articles will be clearly marked in contents pages and search results, and because they are freely available, are likely to be cited more frequently.

The IUCr is one of four publishers to have made successful bids for this funding, the other three beneficiaries being the Public Library of Science (PLoS, for PLoS Biology), Institute of Physics Publishing (New Journal of Physics) and Lancaster University (Journal of Experimental Botany).

The IUCr journals, the first of which was established in 1948, appear consistently at the top of the ISI citation rankings for crystallography, and have a deserved reputation for high publication standards. They are published in conjunction with Blackwell Publishing.

For information about submitting articles, please visit **www.journals.iucr.org.** More information about the IUCr's open-access policy is available at **www.journals.iucr.org/services/openaccess.html.**

John Helliwell
Peter Strickland

Changes at Northern Networking/BCA Administrative Office

THE Spring Meeting in Manchester was effectively our last interaction with Jackie Sayers, who as Gill Moore's Assistant, has been our main contact at Northern Networking. Jackie is moving on and is succeeded by Matthew Hailey. We look forward to working with Matthew.

Europe Science and Technology Week

8 to 14 November 2004 will be Science Week Europe, a chance for national science week activities to be linked up and to showcase in particular how, on a day-to-day basis, science and technology can bring real improvements to our lives. This year, there will be more activities in European cities than ever before, to bring scientists and citizens closer together and enhance understanding.

Science Week is looking forward, not just in terms of the quest for knowledge but also in terms of the next generation of scientists and the future of science education. The week will include events at science museums, special lectures and exhibitions. While the Commission's European-level Science Week projects will have already been allocated funding, parallel activities organised subsequently may also participate under the same banner and have their event advertised on the Science Week website. The website has listings and links to current events and organisations.

http://www.cordis.lu/scienceweek/home.htm

SIENA 2005 - IUCr CompComm CRYSTALLOGRAPHIC COMPUTING SCHOOL

Certosa di Pontignano, of the University of Siena, Tuscany, Italy; 18th-23rd August, 2005

(just prior to the Florence IUCr 2005 congress)

COMPUTING schools have played in the past an important role in making crystallographic computing efforts known on a wider scale.

An excellent example is the 1969 school where a lot of least-squares and absorption correction code was presented in considerable detail and still in use to the present day.

Most of the people who attended this 1969 school are now retired or close to retirement. With the computing school to be held in Siena prior to the Florence IUCr2005 congress we hope to provide a similar experience for the next generation of software developers. This will be achieved by the use of an excellent (and full) program of lectures, workshops and projects. The tentative school program is viewable on the web.

Each day of the school is focussed on a different theme:

"principles & methods"
"joining things together"
"crystallographic implementations"
"selected topics in crystallography"
"special methods"

School Organisers:
Prof Anthony Spek (Utrecht)
Prof. Marcello Mellini (Siena)
Prof. Alessandro Gualtieri (Modena)
Dr Harry Powell (Cambridge)
Lachlan Cranswick (NRC Chalk River)

Consultants:
Dr David Watkin (Oxford)
Dr Simon Parsons (Edinburgh)

The Venue
The Certosa di Pontignano has its origins as a medieval 14th century monastery. It is now run by the University of Siena. Attractively placed on the top of a hill, it is surrounded by vineyards, with a direct view to the town of Siena, and a famous Chianti winery.

Registration information will be added to the Siena 2005 website when this is known. Thanks for the generous support of the University of Siena in providing the Certosa di Pontignano facilities. We are confident that we may be able to keep the entire costs for participants (including accommodation and meals) below 500 Euros. The major expense is accommodation and meals for the expected 15 to 16 speakers. We expect to further lower the registration costs with workshop sponsorship from crystallographic organisations and companies that also rely on crystallographic computing to have a productive future.

Lachlan M. D. Cranswick

A note from the IoP website

A GROUP from London Metropolitan University who have devised new ways to support women in science, engineering and technology (SET) in universities and colleges was rewarded today (Thursday 18 March) with a prize from the Institute of Physics.

The award, for the University's Scientific Women's Academic Network (SWAN), was made at the Royal Society's Athena Awards ceremony.

SWAN stands out from other networks for women in science as it brings together people from many different disciplines and professions, as well as from all areas of science. It has members from the social sciences and humanities, as well as members from professional and policy organisations. The network's aim is to raise awareness and to legitimise the introduction of gender and SET issues into the mainstream agenda in higher education institutions (HEIs).

Later this year, SWAN will launch a Charter that will allow HEIs formally to commit to addressing gender inequalities in their establishment. By signing the charter, HEIs will be starting an ongoing relationship with SWAN, who will give practical advice to institutions on how to make sure both women and men can thrive in their working environments.

Mary Wood, a member of the WIPG Committee, was able to represent WIPG at the Awards Ceremony held at the Royal Society.

IUCr Crystallographic Computing Commission (CompComm) Logo Competition (Submissions due by 2nd July 2004)

www.iucr.org/iucr-top/comm/ccom/logo_comp.html

THE IUCr Commission on Crystallographic Computing is holding a Logo competition and requests submissions to replace its current rather moribund and lame Newsletter logo, and very plain webpage banner (both created by this humble scribe).

Some might frown upon this emphasis on superficial eye candy, perhaps quoting John Lyly (1554-1606) *"The sun shineth upon the dunghill, and is not corrupted".* Nonetheless, it would be nice to have some graphics that the sun felt happy to irradiate. Potential contributors should feel empowered to use any graphics they feel to be relevant to historical and modern computing and crystallographic symbols: e.g.,

punch cards, digital circuits, mathematical equations, bits of source-code, computer valves, fourier maps, B-L strips, coffee-mug stains, discarded chip/crisp packets, empty softdrink/pop cans, etc,

There are three different images that are requested of crystallographic artists:

The IUCr Commission on Crystallographic Computing **Newsletter Logo** (currently a quickly drawn round thing with some text in it) www.iucr.org/iucr-top/comm/ccom/newsletters/

A **graphical banner logo** for its webpages at: www.iucr.org/iucr-top/comm/ccom/ (final version for web will most likely be 500 x 120 pixels)

A **web banner logo** for its 2005 Computing School being held before the Florence IUCr Congress at Siena (18th to 23rd August 2005) (see separate announcement)

The IUCr Commission on Powder Diffraction logo may give people an idea of what has been done in the past for IUCr based newsletters: **www.mpi-stuttgart.mpg.de/cpd/html/newsletter29.html.** Or such things as the Shelx homepage may serve as a guide for a banner logo: **shelx.uni-ac.gwdg.de/SHELX**

Submissions should be sent by 2nd July 2004 to Lachlan Cranswick at **lachlan.cranswick@nrc.gc.ca.** Preferably in a vector based format that is rescalable to small and large formats - and a JPG or GIF file representation. It would be nice if artists could contribute some explanatory text of the type given at the following "about the logo" pages. (a paragraph would be fine - and this is optional)
www.cins.ca/cpdw/logo.html
www.cins.ca/aca/ikaite.html

Artwork should be completely original and not use any copyright or trademarked material from other sources. All submissions become the property of the IUCr Computing Commission; and all submissions will be placed on its website for public view.

Lachlan Cranswick

Puzzle Corner

I'M delighted to report that this month's competition scored a bumper number of replies, many with ingenious solutions.

The substitution of one-letter for three letter codes quickly revealed that the first two pigs built their houses, as expected, from STRAW and STICKS. Various versions of the story have the third pig using STONES or BRICKS, both of which involve a letter not assigned to a unique code. Several readers pointed out that B is, in fact, allowable with the interpretation asx i.e. either asp or asn. Presumably such an uncertainty might lead to structural instability… **Carl Schwalbe** suggested gly-arg-ala-asn-ile-thr-glu, especially for Aberdeen pigs, and **Mark Roe** suggested ser-thr-glu-glu-leu gly-ile-arg-asp-glu-arg-ser, among other things.

The winner is **Steve Maginn,** whose entry arrived before my copy of Crystallography News! His solution was to leave the house building to trp-ile-met-pro-glu-tyr. Well, enough said about that!

This month, as we have a "book review" of a particularly good "Crystallographic Song", why not try your hand at another – or dig one up from somewhere in your past! Four lines or more, in any metre will do. Or how about a limerick? Here is a dreadful example to get you started:

Acta Cryst was once just A,B,C
Then biologists stretched it to D.
If you merit no print,
You're to E or F sent,
Just how long till we get Acta G?

The usual £10 book token for the best entry!

Editor

Foucault Pendulum at UMIST

BCA Spring Meeting

The BCA Spring Meeting – A Student View

AS usual, the BCA Spring Meeting was generally a success. It started with a day of "Young" Crystallographers, including "Not So Young" Crystallographers as an example, and "Younger" Crystallographers, showing what they can do.

On the whole both the invited speakers and the students were excellent, showing that crystallography has a very bright future. The one down side was the poster talks, which had been moved from its usual slot in the main BCA meeting. I, and many of my colleagues, felt that this was a retrograde step, as this is often the first opportunity that students get to speak in front of a professional audience. In previous years, the Great and the Good of British Crystallography have been there to watch, but moving the to the satellite meant that few "Older" Crystallographers were there. I felt this was a great shame, as I have always felt that this is an divide the BCA has always strived to avoid.

So, we move to the full BCA meeting, which as usual, was a fantastic mix of topics, including: Incommensurate Structures, Calibration, Catalysis, and Molecules in Medicine. Personally, while I am not averse to listening occasionally to people talking about areas of science other than my own, I felt I ended up listening to rather more biology than I would ordinarily have chosen to listen to. This was possibly exacerbated by the number of biological-based talks in YCM – I heard several people comment that they'd seen an awful lot of "ribbons and toilet rolls" this year.

So, ignoring the noisy late night trains, what were my personal highlights? Well, all the prize lectures were all interesting, particularly the Kathleen Lonsdale Lecture by **Elspeth Garman,** which was excellent, the PANalytical Lecture by **Andrew Wills,** who succeeded in casting light on magnetic structures and representational analysis for just about half an hour before it drifted back into fuzz, and the CCDC/CCG Prize Lecture by **Maryjane Tremayne,** who demonstrated that maybe structure solution from powder diffraction data will not be quite such a black art in the future.

Finally, ignoring the noisy late night trains once more, what was my favourite session? Well, to be honest, I didn't really have one, and as I have done for the last couple of BCA meetings, I frequently flitted from one session to another. One example where this approach really paid off was the second session on Wednesday morning, where I attended two excellent seminars in parallel sessions: **Kenneth Harris** on molecules running up and down urea straws (which gave an example that I could really understand of how incommensurate structures can happen) and **Bill David** on dehydration studies of paracetamol carried out at the ESRF (which despite his sore throat, was a beautifully clear presentation of powder diffraction data collected on phases

that exist for a very short time). Although there were other lectures that were very good, the other really outstanding seminar was given by **Mike Glazer,** on "Use of International Tables: Advanced Aspects" who, despite the complexity of his subject, that fact that it was the last day and a very short night's sleep (contributed to by the noisy late night trains), managed to keep my attention at 100% for almost the entire ninety minutes. The scheduling of the first International Tables Session was a master stroke, since those who like me should have known most of what was said, but were suffering overly could recover quietly while listening sufficiently to make notes of anything they had forgotten.

So, in conclusion, and ignoring the noisy late night trains, the BCA Spring Meeting lived up to its usual high standard. The seminars ranged from good to outstanding, the poster session was excellent as usual and most people got very little sleep throughout. The lunches were much better than last year (but to be honest, they couldn't have been much worse), and the one saving grace of the location of the train station was the close proximity of the associated shops. The service to our table at the conference dinner was very slow (another table had started their desserts before we got our main course!), but the wine (generously donated by Rigaku) was really quite good. The rooms were a little uncomfortable if you happen to get vertigo, but the view of, and sound effects from the railway were superb if you happened to be a train spotter!

Yes, we all really enjoyed the BCA - it was excellent, but I'm really glad next year will be on Loughborough campus, away from noisy trains!

Amber L. Thompson
Durham University

Young Crystallographers Meeting (5th-6th April 2004)

THIS year's BCA Spring Meeting featured the inaugural Young Crystallographers' Satellite Meeting, taking place the day before the start of the main meeting. The idea of this meeting was for post-graduate students and younger post-docs to get together, present their work and socialise in a more informal and relaxed environment than they might normally experience in the main meeting.

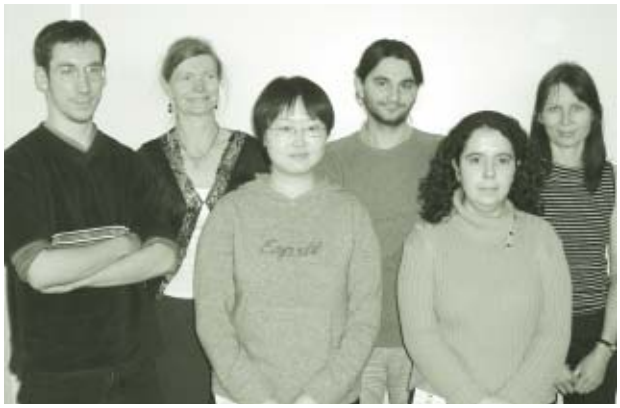
An impressive total of more than 60 young crystallographers thirsty for knowledge (both crystallographic, and of their fellow participants…) registered for the meeting, which featured a total of 13 short presentations from younger presenters supporting 3 longer talks from more established members of the community. Although the majority of the participants came from UK institutions, there were also a number of delegates from further afield.
The meeting consisted of three sessions, two on the

Colin Seaton, Beatrice Calmuschi, Sophie Dale, Simon Parsons, Cheryl Doherty and Charlie Broder.

Monday afternoon and one on the Tuesday morning. These sessions were planned to have as broad a remit as possible, and as such were broadly titled "Small molecules", "Larger molecules" and "Not molecules, and molecules under stress". After a welcome from "El Presidente", **Charlie Broder** (RAL) chaired the first session, which commenced with **Simon Parsons** (Edinburgh). He gave a wide-ranging and informative overview of work being carried out in various groups in the UK under the guise of small molecule crystallography, emphasising the strength and depth of this field in this country. This was amply demonstrated by the four short talks that followed. **Cheryl Doherty** of the University of Bath kicked things off with a talk describing her studies of the behaviour of hydrogen bonded radical adducts, and how they may be used as models for antioxidant action. **Beatrice Calmuschi** (Aachen) brought a European flavour to the session by discussing how chirality could potentially be used as a design tool in crystal engineering, before **Colin Seaton** (Bradford) gave an intriguing talk on ongoing work into the design of molecular interfaces in organic systems. The session closed with a description by **Sophie Dale** (Loughborough) of work towards the synthesis of supramolecular polygons and polyhedra containing the ruthenium-6-arene unit.

Session two, chaired by **Julie Wilson** (York), focussed principally on larger molecules, and contained short talks as an introduction to the **Kathleen Lonsdale** lecture, given by **Elspeth Garman** (Oxford). **Miguel Lombardia** (York) kicked off the session with a description of the highs and lows of terminase crystals, and he was followed by **Yu Gan** (Reading) who told us about the influence of metal ion coordination on the d(GCATGCT) quadruplex structure. **Paula Salgado** (Oxford) described how SAD experiments can provide useful structural information on Manganese containing proteins. Finally **Nick Hopcroft** (York) described some of his work on X-ray crystallographic studies of TRAP/RNA complexes.

This session was immediately followed by the 2-minute poster oral presentations that have become such a tradition at BCA Spring meetings, and this was hosted in inimitable fashion once again by **Bob Gould.** We were joined for this



Nick Hopcroft, Elspeth Garman, Yu Gan, Miguel Lombardia, Paula Salgado and Julie Wilson

and the Lonsdale lecture by a number of particpants in the main meeting, swelling the numbers considerably. The audience was treated to the usual entertaining mixture of snappy science, entertaining comments and loud gonging that has become such a feature of these sessions! After a 5-minute break, we were privileged to be able to host the Kathleen Lonsdale lecture.

This lecture, given by **Elspeth Garman,** was the most crowded and exciting of the Young Crystallographers' Meeting. She began by explaining what an admirable and amazing scientist Kathleen Londsdale was. Then, while talking about protein crystallography and the study of the HIV reverse transcriptase, she highlighted the use of birefringence as a way of selecting the best crystals for data collection, and some of the steps taken to overcome radical scavenging. She also gave some invaluable advice on keeping fingers warm when doing cryocrystallography. She also provided some delicious misquotations and other snippets from her encounters with the press. In short, Elspeth took us on a fabulous walk through her life as a scientist, and one that was enjoyed by all who heard her speak.

The president congratulates the Lonsdale Lecturer.

The evening's entertainment now kicked in, with the Young Crystallographers mixer being held in the open exhibition. This seemed to be greatly enjoyed (!) by the participants, who took to the supplied quiz (won jointly by groups from Durham and Edinburgh) with relish. Manchester hospitality was then allegedly sampled to the full, with the most important question on many lips was where they could find a good kebab at 3am…

Despite these distractions, the final session at 8.30 on Tuesday morning had a healthy, if slightly jaded, attendance. This final session, chaired by **Andy Parkin** (Glasgow), was brought to life early on by **John Evans** (Durham), with a very informative and wide-ranging discussion of powder diffraction as applied to molecules, lattices, and also incommensurate systems. **Gordon Barr** (Glasgow) followed this with a discussion of some of the problems of identifying powder patterns, and how they can be overcome, and **Robin Owen** (Oxford) then described the ongoing development of a system for identifying strongly diffracting protein crystals using optical microscopy. **Francesca Fabbiani** (Edinburgh) described initial work on crystallising compounds from solution at high pressure, and **Iain Oswald** (Edinburgh) described recent work showing that many predicted structures may well be high-pressure polymorphic forms of a compound. The final talk was given by **Neil Brooks** (Newcastle) and gave a general overview of how to deal with twinning in a practical context.

Andy Parkin, Iain Oswald, Francesca Fabbiani, Gordon Barr, John Evans, Robin Owen and Neil Brooks.

The general feedback from this inaugural Young Crystallographers' meeting has been very positive. The quality of the talks was particularly noteworthy, with many of the speakers able to teach those at the main meeting a thing or two! Many participants commented on the broad base of the science being presented, with people attending talks they found interesting and meeting colleagues that they might otherwise not have, had these sessions been part of the main meeting. Overall the meeting seemed to be enjoyed by the vast majority of participants, with in particular the breadth of the subject matter being very highly regarded by the participants. Many thanks are due from the organisers to the speakers, and particular thanks are due to **Julie Wilson** for her "Fatal Diffraction" t-shirt design. Feedback from any participants would be particularly welcome – please send your comments to .

Andy Parkin
with a little help from his friends

Incommensurate Structures

THE Incommensurate Structures session gave an overview of the variety of materials which exhibit aperiodic structures and the formalism which is required to model them. This ranged from the high pressure forms of group I, II, IV, and V elements, through to the organic structures of urea inclusion compounds. Some of the computer programs that can be used to deal with these materials were also introduced.

Gervais Chapuis started the session with The Strange World of Aperiodic Crystals. An aperiodic crystal is defined in reciprocal space and not in real space. Defining an aperiodic crystal in real space is not straight forward but a working definition was suggested as a crystalline structure with a long range order which is different from its periodicity. With a periodic crystal it is possible to describe every point in reciprocal space by the reciprocal lattice vectors but a non-periodic crystal has satellites around the unit cell and these require an additional vector to enable definition. Aperiodic crystals occur in all types of crystalline materials and many structures previously reported as disordered structures actually have well ordered aperiodic structures. Incommensurate phases may also appear during phase transitions, for example there is an incommensurate phase of quartz. $La_2Co_{1.7}$ has hexagonal satellites where the periodicity of the Co is different to that of La.

The extra vector and associated index needed to describe incommensurate structures leads to the construction of a superspace with a supercell replacing the unit cell. Superspace axes may not be interconverted with one another and so this leads to 775 inequivalent superspace groups.

Vaclav Petricek gave a talk on Some Practical Aspects of Modulated and Composite Crystals. Taking the assumption that all satellite peaks are clearly separated, the structure solution may proceed in two parts. First the average structure is solved taking only the main peaks and using a standard technique to gain a solution. Strongly modulated atoms in this solution will have large ADPs which may appear split and it is these badly modelled atoms which are used as the starting point for the modulated structure. Where there are weak modulations (<1 Å) it can be modelled by considering small randomly chosen displacements of known atoms in the structure. Where there are strong modulations (>1 Å), the problem is more complex and must be tackled by using specific programs such as DIMS which is equivalent to direct methods or JANA2000 which is equivalent to Patterson methods. The presence of modulation of atoms also means that the ADPs must also be modulated. Fourier difference maps may be used to get a starting model for this modulation.

JANA2000 also allows refinement of selected groups as rigid bodies. This can allow the shape of the group to be fixed, the use of the same rigid group at different positions and a TLS approximation to the temperature parameters. A workshop was also run on the JANA2000 software. This

Gervais Chapuis, Pam Thomas, Rob Hooft, Clivia Hejny, Ken Harris, Ivana Radosavljevic-Evans and Vaclav Petricek.

gave an introduction to solving and refining a modulated structure from single crystal data.

Kenneth Harris gave a talk on Fundamental and Applied Aspects of Incommensurate Urea Inclusion Compounds. Urea can adopt a host structure with one-dimensional tunnels of diameter 5.5-5.8 Å in which guest molecules which have a compatible size and shape to the host may be included.

The diffraction pattern arising from urea inclusion compounds consists of both Bragg and diffuse scattering giving sheets in reciprocal space due to the presence of order along the tunnel but disorder between tunnels. The diffraction patterns arising from the host and guest structures are overlaid. In an incommensurate structure the guest molecules are free to slide up and down the tunnel whereas in commensurate structures the guest molecules have anchored positions. The three-dimensional structure of the material is defined by the correlation between the guest molecules in neighbouring tunnels with different families of guest molecules having different arrangements between tunnels. This is described in terms of how the end groups interact with one another between tunnels. The structure can effectively be described by the overlap of two structures with different periodicity.

The dynamic properties of the material in the form of translations and rotations of the guest molecules can be investigated using incoherent quasielastic neutron scattering and solid state NMR. Phase transitions where there is an abrupt change in motional freedom of the guest molecules can be observed as a function of temperature. This is not usually an incommensurate to commensurate phase transition.
The guest molecules cannot be located by diffraction and so other methods must be deployed. The interaction between guest molecules can be investigated using EXAFS, NMR and computer simulations and the conformation of the guest molecules is explored by EXAFS and Raman spectroscopy.

Urea inclusion compounds may have practical applications. Control of the alignment of asymmetric guest molecules will have applications in non-linear optics and they also provide an environment which may allow control of crystal morphology or shape. Transport of guest molecules may be

possible in the form of molecular capillaries. An empty urea compound is unstable but it is possible to carry out guest exchange experiments by applying a chemical potential across the ends of the tunnel for example using dibromoalkane and pentane.

Clivia Hejny delivered a talk on Incommensurate Structures in Elements at High Pressure. The high pressure phases Ba-IV, Sr-V, Rb-IV, As-III, Bi-III, and Sb-II are found to exhibit a self-hosting structure with a body-centred tetragonal host framework and a chain-like guest structure. The *a* and *b* axes are commensurate in each case but the *c*-axis is incommensurate. Powder and single-crystal diffraction have been combined with synchrotron radiation to investigate these high pressure structures. Ba-IV exists between 12 and 45 GPa and contains three different guest structures: monoclinic C-centred which undergoes a phase transition after 12.5 GPa; tetragonal C-centred; and a diffuse structure. To study Bi-III (6.8 GPa), the superspace approach is required to account for the satellite peaks in the powder pattern. Rb-IV (16-20GPa) has only very few peaks attributed to the guest structure and releasing the pressure leads to a blurring of the pattern equivalent to melting. Increasing the pressure causes recrystallisation.

Te has been reported to have many high pressure phases; monoclinic Te-II; orthorhombic, Te-III; rhombohedral Te-IV; and body-centred cubic, Te V. It is also a pressure-induced superconductor. Discrepancies between the space group determined by powder and single-crystal experiments respectively led to the inclusion an additional vector to allow for a modulated structure. Te-II was found to be triclinic not monoclinic, Te-III is a modulated monoclinic structure and Te-IV does not exist – the single-crystal data suffers from twinning effects.

The Ba-IV incommensurate structure exists because of a difference in the electronic structure of the host and guest atoms. For As-III, Sb-II, and Bi-III there is a balance between band energy and electrostatic energy.
The structure of iodine under pressure also showed an incommensurate phase between two commensurate phases. Between 19 and 25 GPa the iodine exists as molecules in an orthorhombic structure. Above 25 GPa the structure is modulated and incommensurate in nature. At higher pressures the iodine packs as single atoms. The incommensurate phase exists due to a transformation between molecular and aromatic structure.

Rob Hooft gave a demonstration of a Hexagonal Monster. The demonstration showed the capability of the "dirax" refinement program. In the straightforward structure solution of the hexagonal diffraction pattern, some peaks were left unfitted. A structure solution using only the strongest half of the peaks found a small volume unit cell. To include the remaining peaks a further 4 incommensurate vectors were included using "evalccd" which created a 7-index *hkl* file. The structure remains unsolved!

Lynne Thomas
Cambridge University

Bragg Lecture

by Professor John Finney

John Finney receiving the prize from John Helliwell.

PROFESSOR FINNEY covered the early years of crystallographic work undertaken by Lawrence Bragg in Manchester including the solution of pyrites which was then a breakthrough with 11 parameters.

The development of powder methods, understanding of the coercive force of permanent magnets and the rationalisation of silicate structures by the Manchester School was also covered. The work by Zachariasen and Warren on silica glasses led to many conceptual developments in the analysis of non-crystalline structures. Professor Finney explained how his supervisor **J. Desmond Bernal** had believed that understanding liquids was essential to understanding function of biological molecules.

Professor Finney outlined how the radial distribution function (rdf) obtained by solution scattering studies can be used to describe a disordered crystalline system and how mixed systems can be analysed most effectively by the use of neutron scattering. The remainder of Professor Finney's lecture was concerned with the hydrophobic effect which his team has analysed by neutron scattering studies of isotopically labelled tertiary butanol. He explained how they had essentially taken a leaf from the protein crystallographer's book to analyse the neutron data by performing simulations which were constrained by the experimental neutron data. Professor Finney outlined how the spatial distribution function obtained from these refinements could be used to study the congregation of the solute in 3D and to revise the currently available potential functions used in molecular dynamics simulations. Professor Finney's work suggests that the first shell of water molecules surrounding a hydrophobic group is unperturbed by the presence of the solute - a concept somewhat at odds with the simplistic text-book notion of the hydrophobic effect. However, some differences are apparent in the second shell of water molecules which appear to be more ordered.

Gordon Beaven
University of Southampton

Methods in macromolecular crystallography

DR JOHN TATE (EBI, Cambridge) spoke about software developments by the molecular structure database (MSD) group at EBI including tools (MSDlite, MSDchem) for searching the protein database, not just for specific proteins but also for structures with homology to a specific sequence and structures containing certain types of ligand.

John summarized recent developments to the AutoDep web interface for structure deposition including improved validation of the electron density and the detection of biologically significant quaternary interactions that might have been overlooked during model building. Other programs, including MSDfold which searches for structures with similar tertiary structure and MSDsite which searches for structures with similar ligand-binding environments, were also described.

Paul Emsley, Tony Savill, Jon Hadden, Elspeth Garman, Mark McAlister and Martin Walsh

Dr Jon Hadden (Leeds) described a number of interesting techniques for optimizing conventional crystallization conditions, including the use of a 'temperature ramp', slow cooling to obtain better ordered crystals and the use of streak-seeding to obtain crystals of a selenomethionine-substituted enzyme. Jon reported on the successful use of low-molecular weight silicone oils for preventing evaporation during the pipetting of small nanolitre droplets. This was found to be essential when using a crystallization robot since evaporation during the slow pipetting stages, even with more modern machines, is very significant.

Dr Martin Walsh (ESRF, Grenoble) gave a summary of the changes in data collection and processing that have taken place during the last 15 years, including the development of cryoprotection allowing MAD experiments to be undertaken, the phasing out of the use of films, as well as improvements to the methods by which crystals may be transported to synchrotron facilities. He stated the previously-problematic synchrotron was now user-friendly, with much less dependence on technicians. Dr Walsh also laid out the challenges presented by the onset of high-throughput methods. He reported on the remarkable success of the sulphur SAD method in determining a number of structures using the BM14 beamline at ESRF, with 20-30 structures already having been solved at the ESRF via this technique. The collection of highly redundant data appeared to be a key requirement for these experiments and the use of a kappa goniometer to aid the collection of datasets with improved redundancy was planned in the near future.

The final BSG session started with a talk by **Dr Mark McAlister** (AstraZeneca) who outlined strategies for protein engineering in structure-based drug design. Mark gave an interesting industrial perspective on parallel high-throughput protein engineering and expression methods for the crystallization of proteins that would otherwise be difficult or impossible to work on. This was followed by a lively demonstration by **Dr Paul Emsley** (York) of a number of new programs including the automated fitting program Buccaneer and Coot, a molecular graphics viewer which has many powerful features for display and interpretation of electron density maps. Finally, **Tony Savill** (Molecular Dimensions) presented a new etched mylar loop with a number of advantages (particularly for very small crystals) over conventional loops used for crystal freezing.

Gordon Beaven
University of Southampton

Diamond Special Interest Group

THE Diamond SIG gave an overview of the wide-ranging science that will be accessible on both the physical science and macromolecular science instruments at Diamond.

Professor John Evans (Southampton, Diamond) gave an introduction to the Diamond Light Source, the new 3rd generation synchrotron facility currently under construction in Oxfordshire. He showed prospective applications in materials, engineering, processing, environmental and physical sciences. An update was given on the current state of building – the shell is currently being constructed with the LINAC due to be installed in November. Scheduled to open for users in 2007, the facility should, if the construction work goes to plan, make 7 beamlines available in its first year. The facility will have a better brightness than the SRS providing high flux at high energies. Phase I instruments will include instruments for extreme conditions, materials diffraction, macromolecular crystallography, microfocus spectroscopy, and soft x-ray nanostructures. This will be followed by the installation of a test beam line and instruments for non-crystalline diffraction, powder diffraction, microfocus macromolecular crystallography, and small molecule crystallography in phase II. As part of the second phase of construction, a further 5 beamlines are promised for year 2. In total, phase 2 should give rise to 15 additional beamlines, and is scheduled for completion in 2011.

John Evans, Liz Duke and Paul Raithby

Professor Evans spoke of the pledged attributes of Diamond, the fact that it is a tunable source, the user friendliness of it (including its layout, particularly with respect to laboratory location, and the easy-to-use computer technology). He also spoke extensively on its brilliance, with comparisons to the SRS (Daresbury) and ESRF (Grenoble). Diamond will make possible a whole range of experiments including the use of small samples, one example given being supercritical CO_2, and spatial and/or time resolution, allowing picosecond crystallography and *in situ* catalysis experiments.

The facility will be optimised to allow tenability, polarisation, and brightness whilst remaining user friendly. The brilliance of the source will allow small samples, imaging techniques, high resolution and time resolution experiments to be studied and will also have high sensitivity and coherence. This will facilitate small and dilute samples, small sample environments (particularly for experiments under extreme conditions), high-throughput materials including *in situ* structure-function monitoring, picosecond crystallography, laser excitation, spatial phase mapping, coherence imaging and x-ray circular dichroism.

Liz Duke (RAL) introduced the plans for macromolecular beamlines on Diamond. The instruments will operate in the energy range 0.5-2.5 Å but will be optimised for 1Å. The instruments will allow non-experts to access the machines whilst also catering for more complex problems. Automation will be maximised but still ensure stability of the beam and sample position. There will be one beamline which will have category 3 biological containment and there will be robotic sample changers. These will work at negative pressure allowing both frozen and room temperature measurements to be recorded. Future instruments will include a fully tuneable microfocus beamline in phase II and a side station in Phase III which will be for high throughput. A proposal for a long-wavelength optimised instrument has also been submitted.

In discussion the idea of bringing the implementation of the test beamline forward was mentioned since the ESRF test beamline has been one of the best. This would be dependant on funding but in the event that this became available it was more likely that one of the other instruments would be brought forward instead. The implementation of a "top-up" approach to maintaining the beam causes concerns as to whether this would be compatible with time-resolved experiments. However, the Swiss light source already uses this method and no distortion to the beam has been observed. There is some money available for complimentary techniques although it would be impossible to provide everything. The users will be responsible for providing anything extra but there will be a general lab available to all users. Each beamline has the responsibility for deciding on how best to automate themselves but all beamlines are working together to achieve this. Consultation is taking place between Soleil and Diamond. It was also announced that Simon Teat would be moving to Diamond in the summer.

Lynne Thomas
Cambridge University

Gordon Beaven
University of Southampton

International Tables

THE day after the conference dinner kicked off with a sharp exit from our accommodation. No lie-ins for us which was just as well otherwise we would have missed the lectures on International Tables!

Thursday was Symmetry Day. A review of the simpler aspects of Volume A was given by **Bill Clegg** and **Jeremy Cockcroft** first thing. For those who had been on the intensive X-ray crystallography course in Durham the year before, a few of the slides may have looked familiar (for which Bill apologised), however the session was very worthwhile with lots of examples.

Those looking forward to some more hardcore symmetry were not disappointed as this discussion was continued by **Mike Glazer** who introduced us all to the parts of International Tables that we never look at but really should, the subgroups and supergroups in the afternoon session on advanced aspects of symmetry. As crystallographers interested in phase transitions, we found this talk very worthwhile and relevant, showing how to interpret this section, and how it can give much needed insight into how certain phase transitions can occur.

Iain Oswald and Stephen Moggach
Edinburgh University

Mike Glazer, Jeremy Cockcroft and Bill Clegg

Non-Bonded Interactions

THE study of the hydrogen bond has become one of the most challenging topics since the 1950's. The hydrogen bond is very important in the solid state, in organic, biological and inorganic molecules. Several computational tools have been developed in order to achieve a good understanding of its chemistry and properties. This was amply illustrated by the talks given by Robin Taylor and M. Madan Babu.

Madan Badu, Vanessa Hoy, Andy Parkin and Lourdes Infantes.

Robin Taylor (CCDC) presented on the programs designed by the CCDC for the investigation of non-bonded interactions using data held in the Cambridge Structural Database (CSD) and the Protein DataBank (PDB). The program Isostar is an intermolecular interactions database, providing an experimental distribution of interactions around a central functional group, thus helping to identify the directional preferences of non-bonded contacts. This can be of use in selecting suitable ligands for interaction with certain protein residues. When there are a lot of data to look at, it is possible to create density maps, with the density surface contoured on the number of contact groups in that area. The program Superstar provides an overlay of an Isostar interaction plot onto a molecule being considered for, e.g. binding to a protein site.

Madan Badu (MRC, Cambridge) highlighted the use of the online server NCI for the identification of non-canonical interactions within protein structures, including C-H...O interactions, for example. It is possible to provide geometric constraints for the non-canonical interactions that NCI searches for, *e.g.* limits may be applied to contact distances (C...O, H...O) and contact angles (C-H...O). He spoke about the strength of different types of non-canonical interactions in terms of bond distance, angle and energy, for interactions (N-H…, C-H…, (S, O)-H… and C-H…O). To our benefit, this talk was full of good literature references which covered some important aspects of the non-canonical interactions.

Andy Parkin (Glasgow) presented his work on multi-temperature diffraction aimed at locating the hydrogen atom within acid-base hydrogen bonds. Andy showed that as the temperature of the study is increased, the ellipsoid of the hydrogen atoms also increases in size, resulting in a disordered model for the hydrogen atom position. The examples given for this type of research were Urea Phosphoric Acid (UPA) and Carboxylic Acid dimers. Temperature has an important effect in the degree of hydrogen-bond disorder. For example, he showed how UPA presents disorder around the position of a hydrogen atom, which is closer to urea than to phosphoric acid at 150K, but shifts its position to be in between both molecules at 350K. Thus, the movement of the hydrogen atom could be followed by changing the temperature and collection of diffraction data at different steps. At poor resolution, he showed that the minor disorder position is sometimes lost in the noise of the structure and that care should be taken to consider the position of the X-ray Fourier peak as well as the refined O-H bond length when discussing the position of the electron density in the hydrogen bond.

Lourdes Infantes (CCDC) talked about Hydrates and the water interactions in their crystal structures. An analysis using the Cambridge Structural Database (CSD) was done in order to obtain the frequency of hydrates and donors/acceptors involved in the hydrogen bond interactions and to determine the possible arrangements of molecules in the different structures (discrete chains, discrete rings, infinite chains…).

Finally, **Jordi Bella** (Manchester) dealt with the weak hydrogen bonds in proteins, protein folding and protein-protein interactions. The importance of these types of interactions might by underestimated since they are weak interactions. Jordi Bella explained how these weak interactions play an important role in the macromolecular structure of proteins and in their functions (macromolecular recognition). As Jordi Bella said: *" The functional roles of these weak hydrogen bonds support the notion that these interactions should be examined in detail in the structures of macromolecules with biomedical or biotechnological interest, and their potential should not be neglected in rational drug design approaches".*

Sophie Dale
Loughborough University

Patricia Lozano-Casal
Edinburgh University

Exhibitors

BCA Spring Meeting

Many thanks to our exhibitors, without whom our meeting would be much poorer in at least two senses!

Here they are, caught in the act!

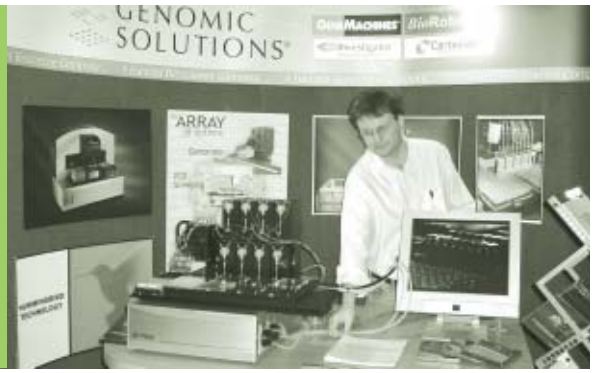
BMMU

Bruker

Douglas

Fluidigm

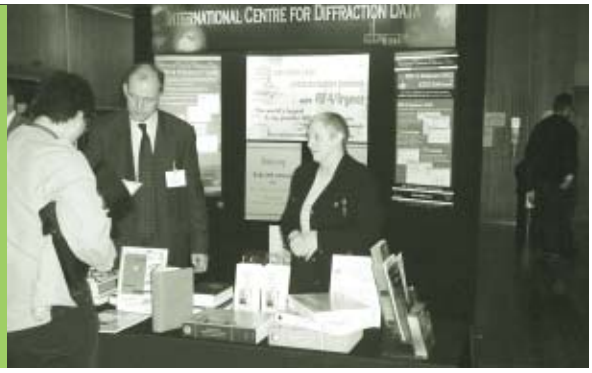
Genomic



Hamilton

HiltonBrooks

ICDD



IUCR

Moldim

Nextal

Oxford Cryosytems

Oxford Diffraction

Oxford University Press

Perkin

Rigaku

Xpert

Molecules and Biomolecules in Medicine

Professor Malcolm Walkinshaw (Edinburgh) described the use of a high-throughput data mining program (LIDAEUS) for finding potential ligands to proteins based on their known 3D structures with specific reference to the development of drugs capable of binding to cyclophilins.

The talk covered work that Professor Walkinshaw's group has done on determining the binding constants of ligands based on their refined occupancies in crystal. He then described work that his group has done on cyclin-dependent kinases - enzymes that play an important role in cancer. The LIDAEUS program was used to find a ligand that was subsequently derivatised, eventually leading to inhibitors with nano-Molar affinity that were effective at inducing apoptosis in cultured tumor cells.

Gary Parkinson, Christine Cardin and Malcolm Walkinshaw

Dr Gary Parkinson (London) outlined the current understanding of the structure of telomeric DNA - the overhanging 3' regions of chromosomes which consist of a repeated G-rich sequence that forms a DNA quadruplex. Shortening of the telomere is associated with senescence and therefore inhibitors of the enzyme telomerase, unregulated in 85% of cancers and responsible for the regeneration of the 3'-end of the chromosome, could be useful in cancer therapy. As yet there is no determined structure of the telomerase enzyme. Dr Parkinson described the design and structure analysis of ligands that bind to DNA quadruplexes. Several were found to be effective at inhibiting cancer cell growth in tissue culture. He also described the results of FRET (fluorescence energy resonance transfer) and ITC (isothermal titration calorimetry) studies, rapid screening techniques used to investigate the interactions of drugs binding to quadruplexes.

Neil Feeder (Pfizer) gave an informative talk on the careful selection of the best possible solid form of a drug for development into the final drug product. The selection process involves a number of stages ranging from full characterisation of the parent compound to the screening of

Nuria Verdaguer, Andrea Hadfield and Jeremy Derrick

salts produced with pharmaceutically accepted counterions and polymorph and hydrate screening. Automation of the salt, polymorph and hydrate screening speeds up the process, with multiple analysis carried out for self-consistency. It is important to automate both the sample generation and the analysis methods to eliminate bottlenecks in the process: even the comparison of powder patterns is becoming automated (PolySNAP). Neil used the example of Ritonavir, an HIV protease inhibitor, to demonstrate the financially damaging outcome of the marketing of drugs that have not been fully screened in the solid form.

Carl Schwalbe (Aston) spoke about the development of amidrazone derivatives as antimycobacterial drugs. The solid state conformations of drugs, and the comparison of these conformations to the binding site of the relevant enzymes provides information for further development of the optimum drug.

Bill David (ISIS) highlighted the use of XRPD in the analysis of both stable and metastable pharmaceutical compounds, aiding the need to analyse all possible polymorphs of a given compound before the drug can reach the market. Dehydration of the drugs paracetamol and Zopiclone and taking XRPD patterns after each temperature increase has led to new hydrated and anhydrous forms of these drugs being found.

Dr Jeremy Derrick (UMIST) described the work in his laboratory to analyse the outer membrane proteins produced by the organism *Neisseria meningitides,* the UK's principal cause of the diseases meningococcal meningitis and septicaemia. The aim is to develop improved vaccines against this pathogen. Crystals of the adhesin OpcA, an outer-membrane protein and potent antigen, were obtained from protein expressed in E. coli and refolded from solubilised inclusion bodies by rapid dilution in detergent. Phases were extracted using xenon and platinum derivatives. The resulting structure consists of a 10-stranded -barrel with long external loops that bind various carbohydrate molecules terminating with sialic acid. Dr Derrick then described his work on the pilQ protein, a 765 residue protein related to the secretin super-family which forms part of the bacterial pili that are associated with cell

motility. Structure analysis by cryo-negative staining EM using pilQ purified from the native pathogen suggests that the protein forms a hollow aggregate which may become filled by other proteins during pilus assembly and disassembly.

Dr Nuria Verdaguer (Barcelona) gave an account of research to determine the structure of domains from the VLDL receptor which are recognised by rhinoviruses. Recombinant minireceptors were expressed containing the domains of interest and these were shown by EM to bind to the 5-fold vertices of the virus, instead of the canyon which is the usual place of receptor attachment in rhinoviruses. Co-crystallisation of the minireceptors with human rhinovirus was successful but data collection on one crystal form required the use of 315 crystals! The structure solution yielded electron density for one receptor module repeated around the 5-fold vertex. A model was proposed in which binding to the receptor at this vertex aids the release of RNA from the viral capsid during infection of the host cell.

Gordon Beaven
University of Southampton

Sophie Dale
Loughborough University

Catalysis, from Metals to Macromolecules

THE main program for the meeting started on Tuesday morning with the opening plenary session on Catalysis: Following a welcome by Paul Fewster, the first speaker was James Naismith from St Andrews University on the subject of F substitution for H in drug compounds and the activation of inorganic fluorides in macromolecular systems, and in particular enzymes that were able to incorporate fluorine into organic molecules.

This was followed by an extremely interesting lecture from **Guy Orpen** of Bristol University. He was outlining the use of structural studies to design phosphine ligands for homogeneous catalysis. He explained how the Cambridge Structural Database was extensively used in this research of phosphine metal complexes. This session was divided over a lunch which was welcome as it had already been a long day for the young crystallographers!!!

After lunch, **James Kaduk** from B.P Chemicals in the USA talked about zeolite Y (faujasite) that is used in catalytic processes. Using crystallography has enabled the accurate characterisation of cation and water positions in the zeolite framework. He noted that most of the zeolites have a different structure at reaction temperatures than at ambient temperature. He characterised numerous zeolites with varying cations at both ambient and high temperatures and found that they all behaved differently to one another. The session closed with a talk by **Philip Woodruff** of Warwick and Berlin on surface crystallography and catalysis.

Cheryl Doherty
Bath University

Iain Oswald
Edinburgh University

Philip Woodruff, Paul Fewster, James Kaduk, Jim Naismith and Guy Orpen.

PANalytical Prize for Physical Crystallography 2004

THE PANalytical Prize for Physical Crystallography for 2004 has been awarded to Dr Andrew Wills of the Chemistry Department, University College, London.

The prize was awarded by the committee of the Physical Crystallography Group of the BCA (and the Structural Condensed Matter Group of the Institute of Physics) for the best recent publications by a younger scientist in the broad area of crystallography in Physics. Dr Wills won the prize for his publications[1-3] concerning the solution of magnetic structure from neutron powder patterns and, in particular, the application of group representations to structure analysis as implemented in his programme SARAh.

Andrew Wills receives his prize from Reg Nicholls of PANalytical.

Andrew accepted his prize at the BCA Spring Meeting in April and gave an excellent lecture – clear, concise, authoritative and elegant – outlining his prize-winning work. After an introduction explaining the concepts of magnetic structures and their description through colour symmetry, Andrew explained the principles of the group representational approach to structure refinement. In this generalized approach, the restrictions of the 230 crystallographic space groups are initially dispensed with in favour of the group representations governing the wave-vectors. The methodology is elegant, versatile and exact and has been tested by Andrew on magnetic pyrochlore systems such as $ErTi_2O_7$, in which the there are disordered magnetic structural units with different arrangements and orientations of magnetic moments. The power of the method in solving for the correct magnetic structure was clearly demonstrated. As Andrew explained, the approach can be generalized to all sorts of structural problems to include incommensurate and aperiodic structures that currently require a super-space approach within the usual confines of crystallographic refinement. These comments were particularly apposite when set alongside the CCG/PCG symposium on incommensurate structures and the highly enjoyable workshop on the use of the JANA program.

The large audience present for the lecture clearly appreciated the high standard of Andrew Wills' work and was fully convinced that he was a very worthy winner of what is the last of these prizes to be sponsored by PANAlytical. We would like to take the opportunity here of thanking PANalytical for sponsoring the prize both as themselves in the last two years and before that, as Philips Analytical X-ray for the preceding eleven years. The relationship has been a happy one throughout and I am sure that many of the past recipients have benefited considerably in their scientific careers after earning this early encouragement (see the next issue of Crystallography News for an article about the previous winners). The PCG would like to reassure readers that the Physical Crystallography Prize will continue to be awarded under the auspices of the group. Further details of the new procedure will be given in a later issue.

(1) Wills AS; Lappas A: "The use of symmetry in the search for canted ferromagnetism, its application to the molecular magnets $Mn[N(CN)_2]_2$ and $Fe[N(CN)_2]_2$" JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS 2004, Vol 65, Iss 1, pp 65-71

(2) Wills AS "Long-range ordering and representational analysis of the jarosites" PHYSICAL REVIEW B 2001, Vol 6305, Iss 6, art. no. 064430

(3) Wills AS "A new protocol for the determination of magnetic structures using simulated annealing and representational analysis (SARAh)": PHYSICA B-CONDENSED MATTER 2000, Vol 276, pp 680-681

Pam Thomas

Books

No Time to be Brief – A Scientific Biography of Wolfgang Pauli

Charles P. Enz, University of Geneva
Oxford University Press, 2002

Price: £35.00 (hardback)
ISBN 0198564791
573 + vi pages

WITH reference to a particularly difficult proof in QED that he and Werner Heisenberg had published in 1929, Wolfgang Pauli used to say "I warn the curious!" The same deterrent could be applied to this book.

The title says it all. With 573 pages, it is certainly not brief, and it definitely is a scientific biography. Do not embark upon reading this book if you are not interested in Pauli's science, and approach it warily if you derive little enjoyment from quantum mechanics. A smattering of German will also be helpful, as the early chapters are irritatingly peppered (gespickt) with German terms (deutschen Ausdrücken) from which the English has been translated (übersetzt), these being useful only insofar as they reveal occasional mistranslations. Another annoying habit of the author's is to keep breaking the flow of the narrative with incidental remarks, details and directions to the reader (e.g. see page 159) which by right belong in a footnote or in the notes at the end of each chapter. The text reads rather like a Ph.D. thesis, and in common with young Wolfgang's first publication – "it puts some strain on the reader's goodwill."

However, it cannot be denied that this is a monumental opus. Appearing in print two years after the centenary of his birth, it is the first biography of this Nobel Prize winner to be published, and it is written by someone who knew him personally and worked with him. Charles Enz was Pauli's last assistant, at the ETH Zürich. He has analysed a vast body of source material to produce a comprehensive and detailed account of Pauli's life and work, which places the man and his science into the historical context of twentieth century physics. The contents are arranged chronologically, beginning with Pauli's ancestry, moving through his life and career in Europe, in the USA during World War II and then back in Europe again, and ending with the management of his scientific estate on his demise. The reader is spared no detail of his theoretical physics, so brush up on your spinor calculus. Also included are interesting brief biographies of Pauli's colleagues, acquaintances and contemporary scientists.

Pauli's contributions to physics are well known, but less famous is his contribution to psychology. Pauli first went to see Carl Jung in 1932 during a personal crisis. Part of his therapy was for him to record his dreams. Pauli went on to send Jung detailed accounts of some 1,300 of his dreams, from which both his mental health and the science of psychology benefited. For a quarter of a century, Pauli and Jung corresponded and exchanged ideas, and even jointly published essays. No doubt it was this contact which led to the development of Pauli's interest in the philosophy of science, the history of ideas, and the relationship between natural science and religion.

Most people reading this review will be familiar with Pauli's Exclusion Principle, but fewer, I imagine, will have heard of the "Pauli Effect". Examples of this pop up from time to in the book and explain why colleagues were anxious to keep Pauli out of their labs and well away from their experiments. It is known that Wolfgang Pauli's contemporaries admired his wit, but this aspect of his character does not come across very well in Charles Enz's account of his life. The often clumsy translation of Pauli's German does not help.

It will interest the crystallographer to learn that in 1933 Pauli posed Heisenberg the "arbitrarily stupid question": Why should the nucleus be built in analogy to the liquid drop and not to the crystalline state? Heisenberg's reason why is given on page 324. However, the subsequent discovery of quarks and neutron stars has since led to an FCC lattice model of the nucleus being proposed (see e.g. Cook, N. & Dallacasa, V., New Scientist 117 no.1606, 31 March 1988, 44-46). Maybe Pauli's question was not so stupid after all – and there are crystals in atoms as well as atoms in crystals.

Stephen Clackson

High Resolution Electron Microscopy

John C.H. Spence, Arizona State University
Oxford University Press,
Third edition, 2003

Price: £69.95 (hardback)
ISBN 0198509154
401+ xxi pages

JCH SPENCE is well known to be an original and innovative physicist and a prolific publisher, not only in premier scientific journals, but also of highly regarded texts.

Spence was one of the key figures in the translation of the capabilities of High Resolution Electron Microscopy (HREM) from the domain of experimental and theoretical

physics into the hands of materials, biological and other scientists investigating the nanoscale universe. His first edition of this book in 1980 accompanied a period of rapid advances in instrumentation and of HREM applications. Since activity in this field has slowed little, if at all, since 1980, the significantly updated 2002 edition has been eagerly anticipated.

In reviewing this new edition, I decided to make comments in the framework of three somewhat different perspectives:-

Firstly, what does this new book offer the scientist contemplating HREM for the first time? Be warned - this book certainly takes nothing of an "HREM for Dummies" approach. While it is skilfully written throughout and is clear, concise and engaging, the book is uncompromising in its rigour and allows the reader little room for taking short cuts in their understanding of the physics involved. It will clearly be of highest value to those with the need to go deeply into HREM. Of the several alternative texts available for the HREM student, this is the most comprehensive in its co-ordinated and thorough discussion of the fundamentals of optics, of image formation and interpretation, and of practical limitations. In my opinion, it is the reference book for practical, fundamental HREM and will be the text preferred for extended graduate courses in the field. In contrast, it is unlikely to be favoured by those seeking a short course in HREM, that is unless they already have a very firm grounding in the physics of optics, interaction of waves with matter, etc.

Secondly, what does this 2002 edition offer the microscopist familiar with the 1980 edition? (I make no comparisons to the second, 1988 edition). Spence does not comment about removing the word "Experimental" from the title but his extensive revision deals with many practical issues, including scanning transmission (STEM) advances, technical developments in electron sources, in aberration and astigmatism corrections, and in signal detection, and selected examples of recent successes in imaging defects. These are all valuable additions to the book, with Spence adroitly matching important information about fundamental, technical and applications perspectives. Fundamental and self-contained material from the first edition, with minor updates, has been transferred to and makes up about half of the new edition. The remainder of the book is largely new. Spence understandably points to the literature in HREM having become so vast that it represents a serious challenge even to refer to and to summarise other excellent reviews. As a result, the newest material is different in style, being much less self-contained and requiring the student to consult many other sources. While this is perhaps unfortunate, it is impossible to do better in four hundred, already concisely written, pages. I selected one of the new topics, HREM in biology, for closer inspection as a non-specialist and came away with a much improved general knowledge about developments in the field (even though I read none of the many references made to other literature). Nevertheless, I doubt that this material alone would convince many life scientists to rush out to buy the new, improved edition. However, if my overall impression as a practising electron microscopist is any guide, most readers will be impressed favourably by the 2002 edition, will gain new insight into a remarkable range of HREM-related topics, and will be stimulated by the sense of vitality and excitement embedded in the book.

Thirdly, what does this book offer the reader of Crystallography News? Two state-of-the-art topics, reviewed by Spence in some detail, will attract attention - namely super-resolution schemes, and the value of the electron microscope for extracting information about atoms in crystals. Spence emerges, unsurprisingly, as an enthusiast for application of modern electron techniques. At the same time, he is adamant that HREM images in isolation, appealing as they are, and notwithstanding the sub-angstrom resolution that is now achievable, cannot yet be interrogated to yield unknown structures. Even in combination with image simulations and electron-diffraction-intensity measurements, insufficient knowledge of basic specimen parameters like thickness continues to stand in the way of unconstrained structure solution using electrons. Perhaps not everyone will agree with Spence about this, but his arguments are well made.

I am impressed by the user-friendliness of this book. The variety of information is logically and excellently laid out. Material is cross referenced carefully and extensively, and is indexed reasonably thoroughly. I searched particularly carefully through material which has been transported from the first edition and found very few errors in the renumbered cross references and the new index - an impressive achievement in itself. Illustrations in general clearly bring home the messages from the text. If I can be critical about presentation, the quality of reproduction of black-and-white images has deteriorated since 1980 - line diagrams are fine but some of the images appear muddy and with inappropriate contrast. For example, the 2002 reproduction of the pair of images in the book's Figure 6.16, intended to illustrate graininess, is now worthless since reproduction has obliterated its intended message. How ironic, considering this is a text directed at maximising image information!

Finally, like thousands of other scientists around the world, today I am able to carry my specimen off to a modern TEM and be confident of returning to my office carrying some high magnification images of lattices and nanostructures. But are they high resolution images, and are they interpretable? John Spence's new book is one that I will repeatedly consult in my search for the answers, not only in analysing the image detail, but also in better planning how my next experiment can be improved.

John Fitz Gerald
Australian National University

Crystal Structure Determination

Werner Massa, University of Marburg
(English translation Robert Gould)
Springer Verlag, Second edition, 2004

Price £34.50 (hardback)
ISBN 3540206442
210 + xi pages

"Crystal Structure Determination" gives a concise introduction to the subject, with particular emphasis placed on the manner in which contemporary analysis actually occurs. The second edition has been completely updated, most notably the chapter describing experimental methods where description of area-detector techniques has replaced much of the material on "classic" methods. The book is aimed principally at students of chemistry who wish to undertake their own structure determinations or to interpret more effectively crystallographic results, encouraging them to "take a look inside the black box". The author takes the view that it is important to attain a broad appreciation of the basic principles as they apply in the crystallographic arena and treats the fundamentals as briefly and intuitively as possible. The resulting text is relatively short – ca. 200 pages – with a distinctly "matter-of-fact" attitude; the information content is high and there is no unnecessary "padding".

The text follows a logical path through the subject, starting from a description of the crystalline state and the nature of X-ray diffraction, continuing with experimental techniques, structure solution and structure refinement, and arriving at two chapters describing errors and the interpretation of results. The overwhelming feel of the discussion is one of brevity. In places this leads to beautifully lucid descriptions, for example in the introduction of the reciprocal lattice. In other parts, however, the discussion is perhaps a little too brief to stand entirely in isolation and reference to more detailed texts might be beneficial. As an example, direction vectors [111], [210], etc. are quite naturally employed within a description of symmetry in the crystal systems, but prior definition of the notation is overlooked. While the discussion remains quite clear – often admirably so – to the more experienced reader, such anomalies might be frustrating to the genuine novice.

The chapter concerning experimental techniques constitutes the major revision from the 1st Edition and warrants particular mention. The focus on area-detector methods makes for one of the most up-to-date discussions currently available in a textbook of this kind. Some description of film methods and serial diffractometers remains, giving a well-balanced chapter that is a most welcome addition. This chapter also contains one light-hearted highpoint of the book, namely the author's valiant attempt to describe the ever-changing face of instrument manufacturers: "Diffractometers operating in this way are manufactured by … Bruker-AXS (formerly Bruker, formerly Siemens, formerly Nicolet, formerly Syntex, formerly Scintag)".

Several notable features appear towards the end of the book. There is a brief but up-to-date description of crystallographic databases and the final chapter describes a worked example of a structure determination. As is the case throughout the book, the focus is placed on the SHELX suite of programs. Some references to other programs are made through the text, and there is a relatively comprehensive appendix, but the author's particular program preference is clear. That possible restriction aside, the annotation of the various input and output files from the SHELX programs are genuinely informative and offer welcome insight into the perceived "black box". Admittedly, the tutorial follows a somewhat similar line to the examples presented in the SHELX manual, but it is well placed within the context of the preceding text and thereby perhaps a little more accessible. It should certainly prove to be a useful exercise for new SHELX users.

The strengths of this book are numerous. The presentation is excellent: the diagrams are plentiful and often impressive, and the formatting of the text is very pleasing to the eye. Particularly appealing is the "swashbuckling" depiction of the character theta, bringing a lively flourish to each sentence in which it appears. The book constitutes an excellent concise reference, with a resoundingly up-to-date and relevant feel. It contains many helpful tips and practical insights that help to distinguish it from other books of this type. As a first introduction to the subject, it is perhaps a little overwhelming. The brevity of the discussion, in particular the early treatment of the fundamentals, gives a somewhat intimidating feel in places. For the author's target audience, however – the research chemist with a desire to appreciate more fully a technique that they are likely to use with increasing frequency – the book should be a helpful companion.

Andrew Bond

A Bravo to Bravais - The Bravais Lattices Song

Walter Fox Smith, Haverford College, PA, USA
Internet, 2002

BEING a thespian patron of the scientific art, it is perhaps not surprising that the mischievous muses, the Muse of Music and the Muse of Crystallinity, have their debauchful way with me, often at unexpected and inconvenient moments.

Recently, while trawling through the Internet morass, a site that gained my attention was the "The Bravais Lattices Song" by Walter Fox Smith; sung to the tune of "I Am the Very Model of a Modern Major General" by William Gilbert and Arthur Sullivan. PDF and word files are downloadable with the lyrics, and MP3 and Real Audio files of the song being played and sung by Bruce Morrison, Marian McKenzie, Michael K. McCutchan and Faith H. McKenzie. It starts with a quartet of obvious universal appeal, even to the most amorphous heart.

"If you have to fill a volume with a structure that's repetitive,
Just keep your wits about you, you don't need to take a sedative!
Don't freeze with indecision, there's no need for you to bust a seam!
Although the options may seem endless, really there are just fourteen!"

Even with the misaligned voices of the chorus, and levels of noise indicating an ignorance of counting statistics and

signal to background ratios, tears well up in the eyes with such lyrics as:

"The cubic is the most important one in my 'experience', It comes in simple and in face- and body-centered variants."

So true, so true.

And thus the lyrics continue, educating not only the two dimensional heart, but the three dimensional mind about the 7 crystal systems and the fourteen Bravais lattices.

Some, with "modern" views of education may be concerned that a song like this could challenge delicate young minds the "wrong way". That symmetry-song lovers should be strongly cautioned and parental advisories issued. These are the minds and opinions of the merohedrally twinned! Give the young good crystallographic nectar to drink and symmetric oceans to swim in at as early an age as possible. Get them comfortable thinking in three dimensions; seeing mirrors, centres of inversion, rotation, translations, glides and screws; not just splashing around, drowning in an ocean of GUI diffraction, that claims to completely sample everything, but by itself leads to an understanding of nothing. What be it if the school and university youth of today are not all destined to enter the Elysium basements of crystallography. Songs like this can only give an appreciation of the undervalued and undertaught arts of crystallographic symmetry. While one might fear the havoc an unethical monster with a karaoke machine could inflict, Walter Fox Smith's efforts are a laudable effort to be praised and congratulated.

Paderewski Dolding-Beadle

PRESS RELEASES

Oxford Cryosystems launch Cobra - the new non-liquid Cryostream

Oxford, UK - Oxford Cryosystems, the manufacturer of low temperature systems for x-ray diffraction have just launched the Cobra non-liquid Cryostream.

The Cobra offers:
- Temp range 80-500K
- Fast cooldown time (30 mins to 100K!)
- Stability of 0.1K
- One-switch start function

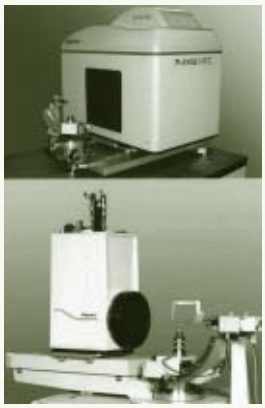
The Cobra can be supplied with or without a nitrogen gas generator, so you can use your lab nitrogen gas supply if available. The Cobra has been designed to combine all the features expected from the Oxford Cryosystems Cryostream, with the benefits associated with a non-liquid system.

Further details are available at **www.oxfordcryosystems.com** or by contacting **kate@oxfordcryosystems.co.uk**

Kate Pope
Sales & Marketing Manager

Performance Comparison of Imaging Plate vs. CCD Detector Systems for Macromolecular Crystallography

The Woodlands, TX - May 3, 2004. Rigaku/MSC, Inc. today announced the publication of a new Application Note that compares and contrasts the performance of new high-throughput imaging plate (IF) technology with that of a high-performance Charge Coupled Device (CCD) detector system. While both detectors provide excellent performance, CCD's are optimal for data collection of well diffracting crystals as well as rapid screening of crystals prior to a synchrotron trip. IP's, on the other hand, afford maximum experimental flexibility - allowing about anything that can be done with a CCD (albeit not as fast) but also the collection of very long exposures on poorly diffracting crystals.



Titled "CCD/IP detector performance comparison: Saturn 92 vs. R-AXIS HTC," the two page document describes the result of an experiment in which the performance of Rigaku's new 3-plate (R-AXIS HTC) imaging plate (shown above) detector is compared to the state-of-the-art Saturn 92 CCD detector (shown below) for data collection on a proprietary protein crystal. Every effort was made to ensure the number of variables was minimized so that the comparison would be both accurate and unbiased. Results indicated that short exposures favored the CCD, but longer exposure times (due to limited flux or poorly diffracting crystals) favored the IP technology.

ICDD Announces New Officers and Directors for 2004

Newtown Square, PA–April 5, 2004

Chairman - James Kaduk
Vice Chairman - Paolo Scardi
Treasurer - Julian Messick
Corporate Secretary - Theresa Maguire
Executive Director - Timothy Fawcett
Chairman, Technical Committee - Raymond Goehner
Directors-at-Large, Board of Directors
Evgeny Antipov, Thomas Blanton, Herbert Goebel, Ting Huang, Daniel Louër.
Past Chairman - Camden Hubbard

Helen M. McDonnell

Group News

Biological Structure Group

Annual General Meetings: The annual general meeting was moved to the Winter Meeting last year to ensure that a maximum number of BSG members are present at the AGM. This raised a difficulty with the BSG accounts. They have to be ratified after the end of the calendar year and before the BCA AGM because they are part of the BCA accounts which have to be audited each year to conform with the increasingly complex rules for a charity organisation. We have therefore agreed to keep the AGM at the winter meeting and present preliminary accounts at that meeting, and deal with all other business at that time, but to adjourn the AGM at the end until the Spring meeting to deal with the final item, ratifying the final accounts. All business that has been discussed and voted on during the Winter meeting will be effective immediately.

The composition of the current BSG committee is as follows:
Chairman: Richard Pauptit (2000-2006)
Vice Chairman: Vacant
Secretary/Treasurer: Andrea Hadfield (2000-2006)
Webmaster: Jon Cooper (1998-2004)

Committee:
Dr. Nick Keep (2001-2004)
Dr. Harry Powell (2001-2004)
Dr. Vilmos Fulop (2001-2004)
Dr. Katy Brown (2001-2004)
Dr. Sheila Gover (2003-2006)
Dr Steve Prince
(co-opted, joint Local Organiser, Spring meeting 2004)
Dr. Jim Spencer
(co-opted: Organiser, Winter meeting 2004, Bristol)
Prof. Jim Naismith (co-opted: Local organiser, Spring 2005, Loughborough)

BSG Winter Meeting:
This will be held at the University of Bristol on Friday 17th December. The provisional title is 'Structural Enzymology'. Watch the BSG Webpage for further announcements. Comments and suggestions to the Organiser Dr. Jim Spencer Jim.Spencer@bristol.ac.uk and Co-organiser Dr. Andrea Hadfield a.t.hadfield@bris.ac.uk.

Andrea Hadfield

AGM of the Physical Crystallography Group

SCMP @ IoP PCG PCG @ BCA

The PCG AGM was held on 7th April 2004 at UMIST. Full minutes will be published on the web. The chairman reported that the group had an active and successful year in 2003-4 with activities including a successful winter meeting on "Probing Structure at the Nanoscale" at Cosener's house, the joint spring meeting session on incommensurate structures with the CCG, and the teaching session on symmetry.

Retiring members of the committee (Jon Goff, David Allan and Steve Collins) were thanked for their efforts over the years. Mina Golshon, Andrew Wills and Jonathan Wright were voted onto the committee. Current committee members are given in the table below.

Title	Name	Grade	Since
Dr	Pam Thomas	Chairman	2002
Prof	Paolo Radaelli	Vice Chairman	2002
Dr	John Evans	Honorary Secretary/Treasurer	2002
Dr	Jeremy Cockcroft	Ordinary Member	1999
Dr	Jon Wasse	Ordinary Member	2002
Dr	Jon Loveday	Ordinary Member	2003
Dr	Tom Lyford	Ordinary Member	2003
Dr	Mina Golshon	Ordinary Member	2004
Dr	Andrew Wills	Ordinary Member	2004
Dr	Jonathan Wright	Ordinary Member	2004

PANalytical Thesis Prize for Physical Crystallography – First Announcement

The Physical Crystallography Group is pleased to announce the inauguration of a Thesis Prize to be awarded for the first time in 2005. The prize will be for the best use of techniques or methods of Physical Crystallography in a successfully-examined thesis submitted in the period from September 1st 2003 to December 31st 2004. Methods and techniques of Physical Crystallography will be

interpreted in a broad fashion, for example, to include x-ray and neutron diffraction or scattering, Rietveld analysis and structure refinement, structure-property relationships, development of structure-solution techniques, crystallography under non-ambient conditions, use of complementary techniques to diffraction (e.g. optical studies, NMR), computational crystallography and modelling, electron diffraction, diffuse scattering, applications of physical crystallography in biology. In order for a thesis to be eligible for the award, the Physical Crystallography element must be central to the work of the thesis, which must also demonstrate a context over and above structural work for its own sake.

Nominations for the prize must be submitted to the Chair of the Physical Crystallography Group by January 31st 2005 and the prize will be awarded at the 2005 BCA Spring Meeting in Loughborough 2005. The nomination procedure, which is currently under review, will be published in the next issue of Crystallography News. The amount of the prize, which will be sponsored by PANAlytical Ltd, will be £500.

Pam Thomas

Chemical Crystallography Group: the new Committee:

Seated: Sandy Blake, Simon Parsons and Georgina Rosair. Standing: Catherine Bowes, Michaele Hardie, Andy Parkin, Andrew Bond, Richard Cooper, Simon Teat and Mary Mahon

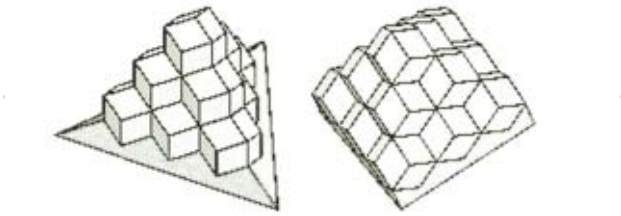
Education

THE following articles illustrate some of the goodies put on the website by Kate Crennell, our indefatigable Education Officer. Lots more is to be found there – and, of course, in full colour!

Editor

Kid's stuff! *A young crystallographer explores packing at RAL*

At a computer show in February we were demonstrating how rhombic dodecahedra can be packed together to build model crystals when the small visitor shown in Fig.1 above (image stored in 2004.Mar02.02.jpg taken at 13.02) came up to try his hand at this. His father was busy discussing programming paying little attention to his son who was having a fine time cuddling as many polyhedra as he could hold and reluctantly giving them up one at a time to build a stack of them. The boy was clearly fascinated because an hour later he escaped from his father who was busy at another stand and toddled back to our stand to have another go at this exciting puzzle. He was building up towers like these.



Instructions for making this toy for your students (or grandchildren) can be found on the BCA website at **bca.cryst.bbk.ac.uk/bca/ed/rhombi.htm**

Kate Crennell

County Science Fair at CCLRC Rutherford Appleton Laboratory - Friday 6 February 2004

THIS event was hosted jointly by the CCLRC Rutherford Appleton Laboratory, Diamond Light Source Ltd, the Oxfordshire County Science Advisory Team (OCC) and the Oxford Trust.

About 20 Local Education Authority secondary schools in Oxfordshire sent a teacher and a team of 6 students from Key Stage 3.

The day began with an egg race and quiz provided and run by the OCC team, followed by essential refreshments, drinks and doughnuts all round. At 11am the students were split into two groups for 5 science activities each lasting about 15 minutes.
The 2 most closely relevant to crystallography were:
• a 'bright light' activity with crystal models
• model building (a practical application using 'molymod' atoms which clip together.

Each team began the 'bright light' activity with a set of card models and worksheets showing projections of the shapes on to a flat surface and photographs of minerals which crystallise in that shape. For example a shadow of a hexagon might be formed by a cube, a hexagonal prism, a regular dodecahedron or a rhombic dodecahedron.

Worksheet and card models: *Instructions for making the models are on the BCA web site.*

The rest of the 'bright light' activity was designed by scientists at the Daresbury Laboratory who have organised similar schools activities. They showed how to model a 'diffractometer' using a desk lamp, an empty 'Pringles' tube, a mounting pin and some shapes to make a shadow of the object on a sheet of greaseproof paper stretched tightly across the end of the tube.

Liquorice Allsorts made good objects which were precut to different shapes before the session began. The students draw the shape of the shadow, then ask the 'technician' to rotate the object to another direction, draw that shape, and continue until they can work out the 3D shape from the 2D shadows it casts.

The mounting pin is a 'hat pin' which can be rotated to cast different shaped shadows of the object on the screen. A typical worksheet is seen on the table.

This activity was held in R18 adjacent to the model of a diamond beam line so that students could see the resemblance between their 'diffractometer' and the ones to be built for diamond. Students and teachers were also show images of proteins and encouraged to ask questions about the diamond light source. Teachers were given instruction and information sheets to enable them to recreate this activity for other students in their schools.

Kate Crennell

Nominations for the BCA Prize Lecture

Nominations are sought for the BCA Prize Lecture. The system is a little unusual but works as follows:

1. It is called the "BCA Prize Lecture" and can be awarded to any crystallographer in the world, but is named in honour of a prominent British crystallographer; this name would change with each award. So we would have, for example, "The BCA Prize Lecture in honour of XXX".

2. The crystallographer in whose honour it is given would attend the BCA Meeting and present the prize. Their expenses would be paid for by the BCA. There should be some link between the work of the two people involved.

3. The recipient would receive full travel costs, and would give a lecture at the BCA Meeting.

4. Nominations for this award, to be presented at the Loughborough BCA Spring Meeting in April 2005, are now sought.

I will be happy to have informal discussions with any of you about possible nominations, as there must be two names involved. A formal proposal can follow later, but please start thinking about ideas now. The deadline will be 31st December.

Christine Cardin

Other Meetings

The 2nd BCA/PCG Rietveld Workshop

THE course, run from 14th-15th March 2004 at Birkbeck College, was aimed at crystallographers wishing to get a kick-start in powder refinement. In attendance were postgrads and postdocs from across the crystallographic spectrum, from earth scientists to physicists, all hoping to gain more insight to the practical aspects of the Rietveld method.

The course was structured around practical exercises guided by the course tutors; **Jeremy Cockcroft, John Evans, Ivana Evans** and **Kevin Knight.** These exercises were supported by formal lectures covering a host of aspects of powder refinement experiments. During the first day the lectures and examples were focussed on data from angle-dispersive techniques and covered topics from data collection to constraints. Both extended and molecular systems were covered, keeping the wide range of crystallographers happy.

After an evening spent by many being entertained by the delights of London, the attendees emerged eager for yet more powder refinement. Building on the previous day's work, we were introduced to time-of-flight diffraction techniques and multiphase analysis. More time was allowed to complete further exercises, and the students given the opportunity to seek help from the tutors with their own data. With a Q&A session to address any specific concerns, the course was drawn to a close.

Stephen Crawford

Specialist User Group Meeting on Applications of Recent Advances in Synchrotron Radiation Diffraction - Weston Building, UMIST, 4th-5th April 2004

IN recent years attendance at X-ray Diffraction Specialist User Group meetings has declined and it had been suggested that, as with other SUGs, the meetings could be held at different university sites rather than at Daresbury Laboratory which might at least encourage interest from the local area each time.

In line with this, for the first time, the XRD SUG meeting was arranged as a satellite to the BCA Spring Meeting. The theme chosen highlighted recent advances in diffraction instrumentation and methodology and the combination of techniques and measurements used to explore structures, processes, properties and other phenomena.

The west coast rail timetable confounded the attempt made by the SUG Chairman, **Paul Raithby** (University of Bath) to reach Manchester on time, so attendees were welcomed to the meeting by the organisers from Daresbury. The first session concentrated on instrumentation and technique developments with the first talk being presented by **David Laundy** (Daresbury) who described how bent Laue monochromators are being developed to focus X-rays on a number of SRS stations. The diffracted intensity is enhanced not only by focusing a beam into small sample cross sections, but also because the resulting increased band pass and divergence of the incident radiation are a better match to the reflecting range of the samples. Close to two orders of magnitude gain has been demonstrated in trials of a prototype apparatus. Applications include improving performance of high pressure experiments using diamond anvil cells, particularly for weakly diffracting materials, and to optimise conditions when combining with laser heating experiments to be developed on Station 9.5. Early tests also show that focusing 60keV X-rays is possible which will benefit strain measurements in engineering materials on Station 16.3. This concept will be extended to Station 16.4 where high penetrating power is necessary to obtain higher resolution data than energy-dispersive powder diffraction (EDPD) methods allow when solving and refining the structure of new phases synthesised at high pressure and temperature in the large volume press.

Regrettably, a speaker from Paul McMillan's team (University College London) was unavoidably unable to attend, so the anticipated presentation on recent results of *in situ* high PT studies of new materials had to be substituted. In this late change to the programme, **Chiu Tang** (Daresbury) described instead results from the first experiments completed on the new multipole wiggler beamline at the SRS, Station 6.2. Combining the focusing of mirrors (vertically) and a sagittal monochromator (horizontally) with fast wide and small angle X-ray detectors has resulted in a powerful instrument for *in situ* materials processing studies. Chiu demonstrated this by showing results of phase transitions as a function of temperature for minerals, ceramics and phases found in meteors. The RAPID2 detector electronics has a cycle time of 10s but so far this has not been challenged by the reaction times investigated by users.

Alistair Lennie (Daresbury) demonstrated the benefits of combining high pressure and low temperature data on ikaite to shed light on the role played by oceanic carbonates thought to be implicated in volcanic processes following subduction at tectonic plate boundaries. He showed how the hydrogen bonded network undergoes distortions consistent with those reported in other carbonate systems

which allowed him to explain variations in compressibility along different crystallographic axes. Single crystal studies are also planned.

Phil Withers (Manchester Materials Science Centre) kept the audience spell bound with some amazing images which easily convinced them of the benefits of 3rd generation SR sources. He described work undertaken on ID19 at the ESRF on the microstructure of interfacial regions in Ti:SiC continuous fibre composite materials. Switching rapidly between diffraction and imaging detectors was essential to map and identify defect formation and propagation and the stress-strain relationship both within the fibres and in the surrounding matrix. The technique is already making an enormous contribution to understanding how the strength of composite materials can be retained even when individual fibres have cracked, leading engineers to use them with confidence in critical applications such as for aeroengine components.

That evening, the attendees did their best to consume the sumptuous buffet and plentiful supply of wine but had to admit defeat as yet more dishes were produced in the Weston Conference Centre. This clearly set them up for the following morning when a larger audience joined them for the second session which **Paul Raithby** opened by inviting **Paul Barnes** (Birkbeck College) to give his presentation. Paul cited examples of a wide range of problems he has successfully investigated using SR at the SRS and ESRF as well as with neutrons at ILL and ISIS. Combining EDPD and HRPD diffraction data with X-ray spectroscopy results and other measurements has allowed a complete understanding of many industrially important processes such as the hardening of cements during oil exploration. Combining results from a variety of techniques has served to realise a vision initiated by J D Bernal many years ago at Birkbeck College which inspired Paul to pursue it through his own research. He went on to outline current plans for developing Tomographic Energy Dispersive Diffraction Imaging (TEDDI).

Gopinathan Sankar (Royal Institution of Great Britain) gave a talk on catalytic framework materials, many of which have been synthesised at the Davy-Faraday Research Laboratory. He showed how it was possible to create different cage geometries from various compositions and explained the methods he had used to locate the positions of charge compensating cations and reaction sites for molecules able to be included in the pores. Once again, a wide variety of techniques had been employed over a number of years at the SRS and ESRF, with diffraction and spectroscopy data exploiting the full range of SR X-ray wavelengths.

The final speaker was **Tony Bell** (University of Manchester) who described progress on elucidating the structural phase diagram of transition metal sulphides using EDPD. Focusing on cinnabar, he presented recently obtained data and postulated that formation of the illusive high temperature phase was dependent on sample 'history' and may have a very narrow stability range. A further series of experiments are planned using a newly developed sample cell aimed at more closely confining the sample under the conditions necessary to mimic the naturally occurring process.

As the attendance at this meeting was again low considering the potential audience from this community, the concluding discussion session sought to explore how better to attract participants to future SUG meetings. There was a general consensus that this approach should be attempted again but with better integration with the main meeting programme. Several helpful suggestions will be followed up for the BCA Spring Meeting in Loughborough next year, and the Chairman and organisers would welcome further ideas for improvement. Suggestions for themes, whether complementary to that of the related BCA subject groups or in distinct contrast, are also invited.

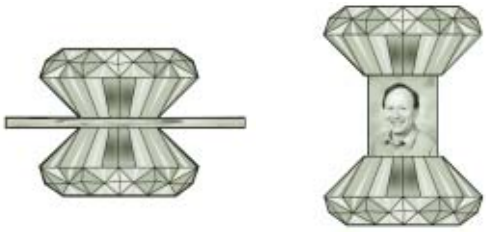
Graham Bushnell-Wye

Centre for Science at Extreme Conditions opens in Edinburgh

ON April 30, Lord Sainsbury, Parliamentary Under-Secretary of State for Science and Innovation, opened the new Centre for Science at Extreme Conditions (CSEC) on the King's Buildings site in Edinburgh.

Thiis £7m facility was funded by the Office of Science and Technology through the EPSRC, and is concerned with materials, living and inanimate, at extremes of temperature and pressure, and in high electromagnetic fields. Its scope will range from life on the ocean floor to the interiors of other planets. It is the first Centre of its kind in the UK, and brings together scientists from many backgrounds. Crystallography is understandably very well represented by an across-the-board selection of members of the BCA.

In their press release, CSEC director **Andrew Harrison** said: "There's a real buzz of excitement surrounding the opening of the Centre. The quality and scope of the work carried out in extreme conditions science at Edinburgh is widely recognised. Now we hope that CSEC will develop that reputation further and become a focal point for researchers who are approaching this emerging field from different directions." CSEC chairman **Richard Nelmes** added: "It is all about fostering a collaborative approach, which it is hoped will lead to significant and groundbreaking advances in knowledge."



In a lighter vein, Andrew noted that "You wait weeks for a diffractometer, and then four arrive at once!" The day was concluded by a talk on planetary interiors by **Sandro Scandolo** of the University of Trieste, who illustrated the flexibility of the diamond anvil cell with an animated strip of which we show two clips!

Bob Gould

BCA Accounts 2003

Examining Accountant: R A Young, BSc. FCA.
The Young Company, Lakeview Court,
Ermine Business Park, Huntingdon PE29 6XR

These are consolidated accounts and include the BCA, BSG, CCG and IG funds and are expressed in pounds sterling (£).

INCOMING RESOURCES:	**2003**	**2002**
Grants and sponsorship	6,240	(328)
Donations	553	2,240
Annual conference	62,623	65,142
Meetings of groups	2,252	2,988
Newsletter	22,978	27,231
Membership subscriptions	19,704	16,022
Course fees	14,198	-
Net income from trading	-	(2,369)
Investment income	5,627	6,097
Interest received	2,358	1,498
IUCr Bursary	22,242	-
Sundry income	1,410	-
TOTAL INCOME	**160,185**	**118,521**

EXPENSES:	**2003**	**2002**
Direct charitable expenditure[1]	116,508	97,093
Management and administration[2]	20,994	19,380
TOTAL EXPENDITURE	**137,502**	**116,473**

	2003	**2002**
NET INCOME	22,683	2,048
Unrealised gains (losses) of investment assets	2,422	(6,144)
NET MOVEMENT IN FUNDS	**25,105**	**(4,096)**
Balances brought forward at 1 January 2002	190,125	194,221
Balances carried forward at 31 December 2002	215,230	190,125

ASSETS:

Fixed Assets	**2003**	**2002**
Tangible assets	702	1,037
Investments	92,963	91,210
	93,665	92,247
Current Assets		
Stocks	743	743
Debtors	1,722	5,691
Cash at bank	124,868	102,252
	127,333	**108,686**
LIABILITIES: amounts falling due within one year	(3,543)	(8,970)
LIABILITIES: amounts falling due after more than one year	(2,225)	(1,838)
NET ASSETS	**215,230**	**190,125**

INCOME FUNDS:	**2003**	**2002**
Restricted funds (3)	89,305	63,849
Unrestricted funds (3)	125,925	126,276
	215,230	**190,125**

NOTES TO THE SUMMARY FINANCIAL STATEMENTS:

1. DIRECT CHARITABLE EXPENDITURE

	2003	**2002**
Previous year conferences	-	8
Subscription to International bodies	3,903	3,492
Annual conference	58,853	57,988
Meetings of groups	2,460	331
Newsletters	27,040	29,147
Course fees and accommodation	16,000	-
Grants and sponsorship	800	500
Prizes	364	627
Crystallography Reviews	4,428	-
Arnold Beevers Bursary Fund	2,660	4,000
Bursaries from restricted funds	-	1,000
	116,508	**97,093**

2. MANAGEMENT AND ADMINISTRATION

General expenses		
Depreciation	335	340
Administration fee	14,626	13,187
Accounting fee	3,298	2,262
Insurance	368	368
Bank and security charges	222	190
Spring Meeting Planning	796	34
Special Interest Group administration	481	546
Council members' expenses	128	924
Officers	378	636
Other Council expenditure	362	893
Total	**20,994**	**19,380**

ACCOUNTING POLICIES

These summary financial statements are based on financial statements which have been prepared under the historical cost convention, with the exception of investments which are included at market value. The financial statements have been prepared in accordance with the Statement of Recommended Practice, "Accounting and Reporting by Charities" published in October 2000 and applicable accounting standards.

All incoming resources are included in the Statement of Financial Activities when the charity is legally entitled to the income and the amount can be quantified with reasonable accuracy. All expenditure is accounted for on an accruals basis and has been included under expense categories that aggregate all costs for allocation to activities. Investments are stated at market value at the balance sheet date.

Tangible fixed assets are stated at cost less depreciation. Depreciation is provided at rates calculated to write off the cost of fixed assets, less their estimated residual value, over their expected useful lives. Stocks are valued at the lower of cost and net realisable value after making due allowance for obsolete and slowmoving stocks.

3. STATEMENT OF FUNDS

	Brought Forward	Incoming Resources	Resources Expended	Gains/ (Losses)	Carried Forward
UNRESTRICTED FUNDS					
General fund	**126,276**	**112,204**	**114,977**	**2,422**	**125,925**
RESTRICTED FUNDS					
IUCr bursary fund	-	22,242	-	-	22,242
Arnold Beevers bursary fund	17,707	1,927	2,660	-	16,974
Dorothy Hodgkin prize fund	6,691	594	-	-	7,285
Chemical group teaching school	8,315	19,833	16,346	-	11,802
Chemical group fund	4,218	1,309	-	-	5,527
Industrial group fund	6,240	1,921	2,508	-	5,653
Biological structure group fund	20,678	155	1,011	-	19,822
Subtotal	**63,849**	**47,981**	**22,525**	**-**	**89,305**
Total of Funds	**190,125**	**160,185**	**137,502**	**2,422**	**215,230**

Treasurers Report 2003

The Association had a surplus of £25,105 during the year ended 31 December 2003 and has no material commitments or guarantees which could affect its future solvency. The major contribution to the reported surplus was the return of £22,242 from the IUCr bursary loan to Geneva. The shortfall from the original £25,000 was a result of exchange rate differences with the US dollar used for the meetings transactions. The residual funds have now been offered to the organisers for the 2005 IUCr congress in Florence. Other contributions came from investments still producing a healthy £5,627 of income. With total incoming resources of £160,185 and operating expenses of £137,502 we maintain a positive cash flow. However, the unrestricted funds show a small deficit of £2,773 over the year before revaluations. A revaluation of investment assets of £2,422 gives the unrestricted funds an overall deficit of £351.

Council members have conducted a review of the reserves that the Association requires for sustaining its objectives. The major considerations are with regard to the long term funding of meetings, bursaries and funding projected deficits from reduced investment income. Existing investments of £92,963 are considered adequate to meet these needs. A review of the major risks to which the Association is exposed has been conducted. The only consideration is with regard to its investments and to mitigate those risks the Association has all its investments placed with an independent professional management company.

The Chemical Crystallography Group closed a Bank Account and took out an account with the Charities Aid Foundation paying better interest. The Associations agreement with Taylor & Francis to publish highlights of the Spring Meeting proceedings in "Crystallography Reviews" resulted in every member receiving a copy with the June 2003 edition of Crystallography News at a cost of £4,428.

Thirteen bursaries totalling £2,660 were taken up this year. The Neutron Summer School received sponsorship of £800. The York Spring Meeting awarded bursary funding of £4,960 to benefit 31 students with 6 being commercially sponsored. The Spring Meeting made a surplus of £3,770.

Crystallography News made a deficit of £3,502 this year on a turnover of £22,978. Increases in postal costs due to a Revenue decision to impose VAT on postage carried out on our behalf by Northern Networking and the additional costs incurred for the inclusion of Crystallography Reviews had a major impact on the deficit. The BCA owes a debt of gratitude to its advertisers and sponsors who generously support our activities.

Subscriptions to International bodies (IUCr & ECA) have increased by £411 due to currency variations. Administration costs are a little higher this year at £20,994, up by £1,614 mainly due to an increase in the administration fee following Northern Networking's contract renewal.

Membership income is up by £3,682 with thirteen organisations paying Corporate Membership dues in 2003. We did benefit by sending out renewal notices early and some of the increase is for subscriptions paid in December for 2004 renewal. Donations totalling £553 were received, down from £2,240 last year. Many of our members have signed Gift Aid declarations and a refund of £1,146 from the Inland Revenue further boosted the Arnold Beevers Bursary Fund.

Meetings of interest

Further information may be obtained from the website given. If you have news of any meetings to add to list please send them to the BCA Web Master cockcroft@img.cryst.bbk.ac.uk or to the Editor. The help of Dr Simon Parsons and the IUCr listing is gratefully acknowledged.

1-4 June 2004
PNCMI, The fifth international workshop on Polarized Neutrons in Condensed Matter Investigations Washington DC USA.
www.sns.gov/pncmi2004

2-4 June 2004
13th Annual CCP13/Fibre Diffraction & Non Crystalline Diffraction Workshop, ILL/ESRF, Grenoble, France.
www.ccp13.ac.uk

4-5 June 2004
Neutrons and Energy for the Future: workshop, Washington DC, USA
www.sns.gov/jins/nmi3

6-10 June 2004
American Conference on Neutron Scattering, College Park MD, USA.
www.ncnr.nist.gov/acns

6,10-12 June 2004
Summer School on Neutron Small-Angle Scattering and Reflectometry from Submicron Structures, Gaithersburg, MD USA
www.ncnr.nist.gov/summerschool/information/index.html

7-11 June 2004
Fundamentals of X-ray Powder Diffraction, ICDD, Newtown Square PA, USA
www.icdd.com/education

8-13 June 2004
VII International School And Symposium On Synchrotron Radiation In Natural Science, Zakopane Poland
www.issrns04.us.edu.pl

9-20 June 2004
Electron Crystallography: Novel Approaches to Structure Determination of Nanosized Materials, Erice, Italy
www.crystalerice.org/2004/ElCryst2004.htm

9-20 June 2004
Polymorphism: Solvates and Phase Relationships. Erice, Italy
www.geomin.unibo.it/orgv/erice/bernstei.html

10-11 June 2004
Gaseous Neutron Detector Workshop, Penn State University, USA
www.sokol.phys.psu.edu/gdw

13-17 June 2004
Conference on Experimental and Computing Methods in High Resolution Diffraction Applied for Structure Characterization of Modern Materials (HREDAMM), Zakopane, Poland
www.info.ifpan.edu.pl/cepheus/HREDAMM2004

14-18 June 2004
Advanced Methods in X-ray Powder Diffraction, ICDD, Newtown Square PA, USA
www.icdd.com/education

16-20 June 2004
The Joint Slovenian Croatian Crystallographic Meeting, Trenta, Bovec, Slovenia
www.uni-lj.si/%7Efn01leban/slkr13

20-25 June 2004
8th Canadian summer school on neutron scattering techniques and applications, Chalk River, ON, Canada
www.neutron.nrc.gc.ca/school01.html

27-30 June 2004
Asian Crystallographic Association Meeting, Hong Kong, China
www.ust.hk/asca04

28 June-2 July 2004
The 8th International Conference on Surface X-ray & Neutron Scattering - 8SXNS, Physikzentrum Bad Honnef, Germany
www.8sxns.de/

29-30 June 2004
Neutron And Muon User's Meeting (NMUM 2004), Warwick
www.cclrc.ac.uk/Activity/NeutronsAndMuons

1-10 July 2004
XVI International School on the Physics and Chemistry of Condensed Matter: Structural Aspects of Solids, Bialowieza, Poland
www.alpha.uwb.edu.pl/schoolXVI

4-6 July 2004
Probing Dynamics at Interfaces - Options for Inelastic Neutron Reflectometry, Paul Scherrer Institut, Switzerland
www.sinq.web.psi.ch/sinq/ws/workshop.html

5-9 July 2004
EPAC'04 - 9th European Particle Accelerator Conference. Lucerne, Switzerland
www.epac04.ch

7-9 July 2004
Polymorphism in Liquid and Amorphous Matter, ESRF Grenoble (France)
www.esrf.fr/Conferences/Polimat

11-16 July 2004
Gordon Research Conference on Diffraction Methods in Structural Biology, Maine, USA.
www.grc.org/

11-17 July 2004
LAM12: Twelfth International Conference on Liquid and Amorphous Metals. Metz, France.
www.lam12.sciences.univ-metz.fr

17-22 July 2004
Americal Crystallographic Association Meeting, Chicago, IL, USA
www.hwi.buffalo.edu/ACA/index.html

18-21 July 2004
VIIIth European Conference on Surface Crystallography and Dynamics (ECSCD-8), Segovia, Spain
www.phantomsnet.com/ECSCD8

19-23 July 2004
20th General Conference of the Condensed Matter Division, European Physical Society, Prague, Czech Republic
www.cmd.karlov.mff.cuni.cz/CMD

21-23 July 2004
4th European Workshop on Piezoelectric Materials (4th EWPM), Montpellier, France
www.lpmc.univ-montp2.fr/~4ewpm

2-6 August 2004
53rd Annual Denver X-ray Conference, Steamboat Springs, CO, USA
www.dxcicdd.com

7-14 August 2004
PHASE TRANSITIONS: 3rd Summer School on Condensed Matter Research, Lyceum Alpinum, Zuoz, Switzerland
www.num.web.psi.ch/zuoz2004

9-13 August 2004.
14th International Conference on Crystal Growth (ICCG-14). Grenoble, France
www.iccg14.inpg.fr

15-29 August 2004
Sixth United States National School on Neutron and X-ray Scattering, Argonne National Laboratory IL USA
www.dep.anl.gov/nx

18-21 August 2004
High Pressure Commission Workshop: 'Crystallography at High Pressure', Saskatoon SK Canada
www.lightsource.ca/enews/iucr2004.php

18-21 August 2004
Algorithms for Macromolecular Modelling, Leicester
www.am-3.org

20-28 August 2004
32nd International Geological Congress, Florence, Italy
www.32igc.org

22-24 August 2004
Satellite meeting on "Mathematical and Symmetry Aspects" (ECM-22). Budapest, Hungary
www.lcm3b.unancy.fr/mathcryst/satellite.htm

23-25 August 2004
SRMS-4: 4th Conference on Synchrotron Radiation in Materials Science. Grenoble, France
www.esrf.fr/Conferences/SRMS-4

24-26 August 2004
Satellite meeting on "Mathematical and Symmetry Aspects" on occasion of ECM-22. Budapest, Hungary
www.lcm3b.uhp-nancy.fr/mathcryst/satellite.htm

24-27 August 2004
8th International Symposium on Ferroic Domain (ISFD-8), National Institute for Materials Science (NIMS), Tsukuba, Japan
www.sntt.or.jp/isfd-8

26-31 August 2004
22nd European Crystallographic Meeting, Budapest, Hungary
www.ecm22.mtesz.hu

29 August-3 September 2004
26th International Free-Electron Laser Conference and 11th FEL User-Workshop. Trieste, Italy
www.elettra.trieste.it/fel2004

30 August-8 September 2004
6th EMU School on Spectroscopic Methods in Mineralogy, Vienna, Austria
www.univie.ac.at/Mineralogie/EMU_School

31 August-2 September 2004
Size-Strain IV workshop, satellite to EPDIC, Prague, Czech Republic
www.xray.cz/s-s4

31 August – 10 September 2004
The Synchrotron Radiation Summer School 2004, Chester College and Daresbury Laboratory.
www.srs.ac.uk/summer-school/index.htm

1 - 4 September 2004
The Seventh International Conference on Quasi-Elastic Neutron Scattering, QENS2004, Arcachon near Bordeaux (France)
www.qens2004.org

1-4 September 2004
42nd EHPRG Meeting 2004 on High Pressure Research, Lausanne, Switzerland
www.icmb.epfl.ch/ehprg42

2-5 September 2004
EPDIC-IX, European Powder Diffraction Conference, Prague, Czech Republic
www.xray.cz/epdic

4-8 September 2004
5th European Conference on Mineralogy and Spectroscopy (ECMS 2004), Vienna, Austria
www.univie.ac.at/Mineralogie/ECMS_2004

5-7 September 2004
Annual Conference Of The British Association For Crystal Growth, Leeds
www.leeds.ac.uk/chemeng

5-10 September 2004
3rd International and 28th European Peptides Symposium - Prague, Czech Republic
www.kenes.com/28eps

5-10 September 2004
Molecular Self-Assembly: Biomimetics as a Route to Novel Products and Processes, Cambridge,
www.nano.org.uk

6-10 September 2004
E-MRS Fall Meeting, Warsaw, "Applications of Linear and Area Detectors for X-ray and Neutron Diffraction and Spectroscopy (ALADINUS)", Warsaw, Poland
www.e-mrs.org/fall2004

7-10 September 2004
X-TOP 2004 - 7th Biennial Conference on High Resolution X-Ray Diffraction and Imaging, Pruhonice (near Prague), Czech Republic
www.xray.cz/xtop

12-17 September 2004
Solid State Chemistry 2004, Prague
www.ssc2004.cz

14 September 2004
Second Neutrons and Numerical Modelling Workshop: Student School, Institut Laue-Langevin, Grenoble, France
www.ill.fr/Events/N2M2

15-18 September 2004
Second Neutrons and Numerical Methods Workshop, Institut Laue Langevin, Grenoble, France
www.ill.fr/Events/N2M2

15-18 September 2004
Structural Biology at Crossroads: From Biological Molecules to Biological Systems, EMBL (DESY) Hamburg Germany
www.embl-hamburg.de

20-25 September 2004
XV Symposium of the Spanish Group of Crystallography and the II Reunion of the Spanish Society of Neutron Techniques, Tenerife, Spain,
www.webpages.ull.es/users/matmol/congreso

21 September - 2 October 2004
VII School of Neutron Scattering: Small and ultra-small angle neutron scattering: structural and dynamical studies, Capra, Palau (SS), Italy
www.fis.uniroma3.it/sns_fpr

1-8 October 2004
FEBS advanced course: Advanced methods in protein crystallization. Nove Hrady (Czech Republic)
www.img.cas.cz/igm/cc

4-7 October, 2004
Analysis of Functionally Graded Materials (1st SOTAMA-FGM) Krakow, Poland.
www.imim-pan.krakow.pl

18-20, October 2004
NOBUGS 2004 Conference - New Opportunities for Better User Groups Software, PSI, Switzerland
www.lns00.psich/nobugs2004

21-22 October 2004
SSRL 31st Annual Users' Meeting. Stanford, CA, USA
www-ssrl.slac.stanford.edu/users/user_admin/news.html

10-13 November, 2004
EMBO Conference on Structures in Biology. Heidelberg, Germany
www.embl-heidelberg.de/conferences/StructBiol04/

16-17 November 2004
CrSJ 2004 Annual Meeting, Osaka, Japan
www.soc.nii.ac.jp/crsj/index-e.html

19-26 November 2004
Biocrys 2004: Fundamentals of Modern Methods in Biocrystallography, Instituto de Tecnologia Química e Biológica, Oeiras, Portugal
www.biocrys.itqb.unl.pt

17-21 November 2004
SGO International Conference on Structural Genomics 2004 (ICSG 2004), Washington Hilton & Towers Hotel, Washington, DC, USA
No website yet given

27 November - 2 December 2004
Recent Advances in X-Ray Powder Diffraction, Assiut, Egypt
www.geocities.com/egyptiansca

6-7 December 2004
Micro- and Mesoporous Mineral Phases: Mineralogical, Crystallographic and Technological aspects, Accademia Nazionale dei Lincei - Rome, Italy
www.lcm3b.uhp-nancy.fr/cims/micromesoporous.htm

19-29 May 2005
Evolving Methods in Macromolecular Crystallography, Ettore Majorana Centre, Erice, Italy
www.crystalerice.org/futuremeet.htm

28 May-2 June 2005
ACA Annual Meeting, Walt Disney World, Florida, USA
www.hwi.buffalo.edu/ACA

20-24 June 2005
International School on Mathematical and Theoretical Crystallography, Nancy (France)
www.lcm3b.uhp-nancy.fr/mathcryst/nancy2005.htm

18-23 August 2005
IUCr Compcomm Crystallographic Computing School, Siena, Italy,
www.iucr.org/iucr-top/comm/ccom/siena2005

23-31 August 2005
XX Congress of the International Union of Crystallography, Florence, Italy
www.iucr2005.it

28 November-2 December 2005
2005 International Conference on Neutron Scattering (ICNS 2005), Sydney, Australia
www.st.gu.edu.au/icns2005/announce.html

9-18 June 2006
The Structure Biology of Large Molecular Assemblies, Ettore Majorana Centre, Erice, Italy
www.crystalerice.org/futuremeet.htm

7-17 June 2007
Engineering of Crystalline Materials Properties: State-of-the-Art in Modeling, Design, and Applications, Ettore Majorana Centre, Erice, Italy
www.crystalerice.org/futuremeet.htm