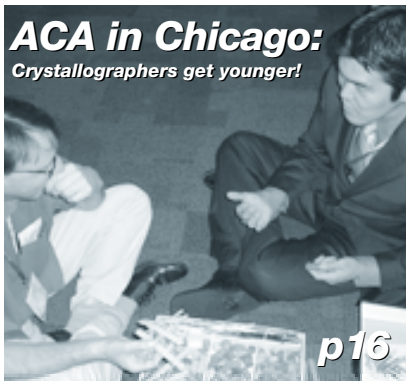
BCA News September 2004

Contents



This months cover:

David Blow, amazingly, only has his name appear once in the CSD! We salute him here with a representation of that structure, D-(methyl-1,2-dihydro-naphtho(2,1-B) furan-2-carboxylate), from P.S. Rogers, L.C.G. Goaman and D.M. Blow, J.Amer. Chem.Soc. 98, 6690 (1976).

BCA Administrative Office,
Northern Networking Ltd,
1 Tennant Avenue,
College Milton South,
East Kilbride, Glasgow G74 5NA
Scotland, UK
Tel: + 44 1355 244966
Fax: + 44 1355 249959
e-mail: bca@glasconf.demon.co.uk

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 **December 2004** issue are sent to the Editor to arrive before **25th October 2004.**

Bob Gould
33 Charterhall Road
EDINBURGH EH9 3HS
Tel: 0131 667 7230
E-mail: gould@ed.ac.uk

From the President

AS MEMBERS will already know, it is with great regret that we record the passing of Professor David Blow FRS, President of the BCA from 1984-1988, and Dr Sam Small, BCA Secretary from 1985-1987. An obituary for David appears in this issue, and one for Sam will be in the December issue of Crystallography News.

The summer is often an odd time to write a column, and this is also true in the BCA. After our major event of the year as an Association, the Annual Spring Meeting, there is something of a quiet period while we regroup, and the conference and vacation season being very much upon us reinforces this feeling. However, since it is conference season, instead of ranging more widely, I would like to focus here on the Spring Meeting, partly since it is absolutely true that work on this never ends. Indeed, planning for the 2005 Loughborough meeting started before the 2004 meeting was held, and the Programme Committee chaired by BCA Vice-President John Finney has now met. The initial outcomes of this meeting are summarised elsewhere in this issue, and I believe an exciting programme will once again be on offer.

The plenary/review theme for the 2005 meeting is related to the study of structures under change, or *"in situ"* crystallography to use a common phrase. This is for sure a hot topic, and one close to my own heart since John Helliwell and I organised an RSC Faraday Discussion on "Time-Resolved Chemistry" in 2002. The subtitle of that meeting - "From Structure to Function" - stressed the high relevance of this topic in a crystallographic context, and this relevance is emphasised by the fact that not only is the 2005 Annual Spring Meeting theme in this area, but this year's CCG Autumn meeting is also exploring a closely related topic. It is important that the BCA maintains a dual approach to its meetings, combining a focus on hot topics such as this with an appropriate high degree of coverage of more traditional but still highly relevant, exciting and interesting areas of our science. I believe we continue to do so.

We are also continuing to work to open up the participation base in the BCA, and it is a pleasure to note that in Loughborough 2005 we will be joined by the X-ray Fluorescence community, and also by the RSC Solid State Chemistry group. While these links are informal, they are underpinned by lively strands within the programme, and one hopes that this brings more people along to sample the vibrant atmosphere of the BCA Annual Meeting and encourages them to return. The Programme Committee has also recognised that until now the "invitation-only" nature of many of the sessions at the Spring Meeting can discourage participation from younger members of our community. To correct that, session organisers for Loughborough are being encouraged to leave slots open for contributed talks. In support of this intention, this year the Abstracts Web-site will be open for business considerably earlier than previously and a call for contributed papers issued.

But I still believe that our planning for the Spring meeting, the annual unifying focus for our community, can evolve further to make it more relevant and appropriate to modern practice and expectations. To this end, for the first time as far as I am aware, the 2006 Programme Committee will be constituted and have an initial meeting before the 2005 meeting takes place. The aim of this is to allow initial plans for 2006 to be drawn up in time to allow them to be presented and publicised to the community a full year in advance. This allows for better planning in our increasingly busy schedules, allows ideas to be trawled in focused discussions in the formal and informal meetings taking place in Loughborough, and to allow a "call for papers" as discussed above to be issued in plenty of time to encourage submissions. In addition, it has been my opinion for some time that it is asking too much of a BCA Vice-President to organise the Spring Meeting programme three years in succession, and it is a pleasure to note that we have a volunteer (!) to Chair the 2006 Programme Committee. We look forward to working with Paul Raithby on this.

Chick Wilson

Council Members
2004-05

COUNCIL MEMBERS

President (2006)
Prof. Chick Wilson
Department of Chemistry
University of Glasgow
GLASGOW G12 8QQ
Tel: 0141 330 8552
chick@chem.gla.ac.uk

Vice President (2007)
Prof. John L Finney
Dept. of Physics and Astronomy
University College
Gower Street
London WC1E 6BT
Tel: 020 7679 7850
j.finney@ucl.ac.uk

Secretary (2007)
Dr. Christine Cardin
University of Reading
Dept of Chemistry
Whiteknights
READING RG6 6AD
Tel: 0118 9318215
c.j.cardin@reading.ac.uk

Treasurer (2006)
Mr. David J. Taylor
35 Birchley Road,
Billinge
WIGAN WN5 7QJ
Tel: 01744 893108
djtaylor@lineone.net

ORDINARY MEMBERS

Dr Alexander J. Blake (2006)
School of Chemistry,
University of Nottingham
University Park
NOTTINGHAM NG7 2RD
Tel: 0115 9513488
a.j.blake@nottingham.ac.uk

Dr Elspeth F. Garman (2006)
Laboratory of Molecular Biophysics
Rex Richards Building
University of Oxford
South Parks Road
OXFORD OX1 3QU
Tel: 01865 275398
elspeth@biop.ox.ac.uk

Dr Peter C.E. Moody (2006)
Department of Biochemistry
Adrian Building
University of Leicester
University Road
LEICESTER LE1 7RH
Tel: 0116 2523366
pcem1@leicester.ac.uk

GROUP REPRESENTATIVES

Biological Structures
Dr Sheila Gover,
Laboratory of Molecular Biophysics,
Rex Richards Building,
South Parks Road,
Oxford, OX1 3QU
Tel: 01865 275392
Fax:01865 510454
sheila@biop.ox.ac.uk

Chemical Crystallography
Dr Georgina Rosair
School of EPS - Chemistry
Perkin Building
Heriot-Watt University
EDINBURGH, EH14 4AS
Tel: 0131 451 8036/4241
Fax. 0131 451 3180
g.m.rosair@hw.ac.uk

Industrial
Dr Jeremy K Cockcroft
School of Crystallography
Birkbeck College
Malet Street
London WC1E 7HX
Tel: 020 7632 6853
cockcroft@img.cryst.bbk.ac.uk

Physical Crystallography
Dr John Evans
Department of Chemistry
University of Durham
DURHAM DH1 3LE
Tel: 0191 334 2093 / 2052 (lab)
Fax: 0191 384 1297
john.evans@durham.ac.uk

CO-OPTED MEMBERS

Professor John Helliwell
Department of Chemistry
University of Manchester
MANCHESTER M13 9PL
Tel: 0161 2754686
john.helliwell@man.ac.uk

EX-OFFICIO MEMBERS

Editor "Crystallography News"
Dr Robert Gould
33 Charterhall Road
EDINBURGH EH9 3HS
Tel: 0131 667 7230
gould@ed.ac.uk

Education Officer
Mrs K.M.Crennell
'Fortran Friends'
P.O.Box 64
DIDCOT OX11 0TH
Tel: 01235 834 357
bca@isise.rl.ac.uk

Webmaster
Dr Jeremy K Cockcroft
School of Crystallography
Birkbeck College
Malet Street
London WC1E 7HX
Tel: 020 7632 6853
cockcroft@img.cryst.bbk.ac.uk

GROUP CHAIRMEN

Biological Structures Group
Dr. Richard Pauptit
Protein Structure Lab
AstraZeneca
Mereside, Alderley Park
MACCLESFIELD SK10 4TG
Tel: 01625-516135
richard.pauptit@astrazeneca.com

Chemical Crystallography Group
Dr Alexander J. Blake
School of Chemistry,
University of Nottingham
University Park
NOTTINGHAM NG7 2RD
Tel: 0115 9513488
a.j.blake@nottingham.ac.uk

Industrial Group
Dr Jeremy K Cockcroft
School of Crystallography
Birkbeck College
Malet Street
London WC1E 7HX
Tel: 020 7632 6853
cockcroft@img.cryst.bbk.ac.uk

Physical Crystallography Group
Dr P. A. Thomas
Department of Physics
University of Warwick
COVENTRY CV4 7AL
Tel: 0113 233 2538
p.a.thomas@warwick.ac.uk

Full committee details on the BCA website
www.crystallography.co.uk

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

SINCE our spring issue, we have been saddened by the deaths of David Blow and Sam Small. Both of them were supporters of the BCA from its foundation. I am very grateful to Eleanor Dodson for her appreciation of David which is included in this issue. One for Sam will appear in the December issue. David was always a great supporter of Crystallography News, and even won the first puzzle competition after I became editor. During his last illness, he worked with Steven Wallwork on a history of the founding of the BCA (see Eleanor's article) and we hope to be able to reproduce part of it in a future issue.

As many of you will have been noticing, recent editions of the IUCr Newsletter have featured Crystallography in various countries, large and small. Council has been asked to produce a British Issue, and I have agreed to co-ordinate this. As the country with the strongest claim to be the hometown, if not exactly the birthplace, of crystallography, it is essential that we do a good job, getting the right balance among history, geography and subject matter. The style and content will be discussed at the September Council Meeting, but it is important to get all views on what should be done here, so please e-mail anyone on council with views you have.

This issue is always difficult to predict. Many summer meetings are not over in time to get a report, and the late spring is a quiet time for reportable activities. I hope, however, that you will like what you find here. The remaining sessions from the Manchester meeting are covered, as are a variety of other meetings in which some of our members have taken part. Principal among these is the ACA, which was in Chicago this year. It was one of the highest attendances ever, although the number of participants form Europe (yes, that does include us!) was lower than usual. Three sessions are covered here – I make no apology, they were ones that appealed to me.

Other matters serious and less serious are here too. International Tables are burgeoning. The long-awaited Volume D is reviewed here, and we hope to have Volume A1 reviewed for the next issue. While the egregious Professor Dolding-Beedle has held his peace this time, a lively letter from Tony North might stir up some discussion. I wonder whether people actually like to have a chance to turn away from their audience – you know, the way pop stars insist on having quite unnecessary microphones? Meantime, the industrious Kate Crennell has turned up some fascinating crystallography-after-death which warrants comment and discussion!

One eminent member of the BCA who needs no introduction and who did get to Chicago remarked at the reception that people were commenting that she had appeared three times in the last issue of Crystallography News. Just as I was sending off this issue to the printer, the following photograph appeared in my mail, and I thought I ought to include it showing just how good a meeting it was!

Bob Gould

Letter to the Editor

From Professor A.C.T. North

Dear Bob
Some time ago, we corresponded re bars over variables in Word. Now for something completely different!

It is now becoming almost universal for people to use Powerpoint for illustrating talks. A major advantage (beyond the immediately obvious) is that the lecturer can face his (or her) audience (given a suitably-placed console or laptop) without having to turn round in order to check that the correct slide has appeared. But there is one great snag - the lecturer does have to turn and face the screen if he wants to point to any feature on the slide. Many lecturers do not realise that they then have to speak up - and many have the maddening habit of waving a laser pointer around so that the audience cannot follow what is being pointed at.

Surely it should be possible for the lecturer to use the computer mouse to point to the required feature, but unless I am mistaken, (1) it is not possible to enlarge the mouse arrow to a sensible size (2) the mouse arrow switches itself off if it is not moved from time to time. It is possible to change the usual arrow into a silly little pencil (I have done it, but have now forgotten how!), but that is no better. What is needed is the facility to have a nice fat pointer of chosen shape, colour etc. that is under mouse control and will stay switched on. Do you know if this can be done? I feel it ought to be possible quite readily. Could the great weight of the BCA (or perhaps IUCr) persuade Microsoft that such a thing would be helpful?

Best regards
Tony

Puzzle Corner

Well, shame on you all – not a single line of poetry submitted for this issue, although I must admit that a single line might have been a bit difficult to identify as poetry! So here's another educational exercise for you to ignore.

At the BCA in April, a quiz submitted to young crystallographers included some photographs to identify of eminent crystallographers. I was saddened at how few forms I saw had many names on them. The best known ones appeared to be Karle and Hauptman, and in that case the identities were reversed more often than not. So here, in an attempt to widen knowledge of our past (and present!) I present a simple "hidden word" problem.

The surnames of seven eminent crystallographers – some of them living – of the past century are given. Your job is to supply the first names – or more exactly the calling names of those people. If you get it right, the first letters of your names will spell a highly significant word.

1. Taylor	**2. Franklin**	**3. LePage**	**4. Hall**
5. Powell	**6. Beevers**	**7. Patterson**	

There is a little ambiguity, and, sorry, the first one is not Dave, our esteemed Treasurer! But try your luck and let me know how it goes. A ten-pound book token awaits someone!

Editor

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:

BCA Administrative Office
Northern Networking Ltd
1 Tennant Avenue, College Milton South
East Kilbride G74 5NA
Phone 01355 244966 Fax 01355 249959
e-mail bca@glasconf.demon.co.uk

Corporate Members

Anachem Ltd
Astex Technology
bede plc
Bruker/Nonius
Chemical Computing Group
Cambridge Crystallographic Data Centre
deCODE genetics (Emerald Biostructures)
Fluidigm Europe/EMEA
Hampton Research
International Centre for Diffraction Data
Oxford Cryosystems
Oxford Diffraction
PANalytical
Rigaku MSC

BCA 2005 Spring Meeting

NEXT year's meeting will take place at Loughborough University from Tuesday 12th to Thursday 14th April. As in recent years, the meeting will run from 11.00 on the Tuesday to the Thursday afternoon. As this is not the week immediately before Easter, and recent meetings have generated internal pressure to increase the time available for both sessions and informal contacts, there is a possibility we may run later run a little later on the Thursday than in recent years (what do you think? – let me know!). Timings will be similar to previous years with sessions being made up generally of one or more 1.5 hour slots.

Loughborough, home of the carillon!

The review theme and plenary sessions

The overall theme to be addressed in four linked plenary talks is "*In situ* and Non-ambient Crystallography", which will include discussion of following structures under change. This is a very hot area at present and promises some really neat new ideas and results. Details remain to be fully confirmed, but the session will include a talk from **Phil Coppens,** State University of New York at Buffalo, entitled "X,Y,Z and Time: Introducing the Time Dimension in Crystallographic Research", and one on Process control in the cement industry using both X-ray fluorescence and X-ray diffraction. The two remaining plenaries are still under discussion, ideas being followed up including aspects of phase transitions, pressure induced chemical change, photochemistry, and the trapping of intermediates in macromolecular crystallography. With this particular review theme, it seems natural to follow the plenary talks with a plenary session in which manufacturers of equipment for non-ambient experiments will be offered a platform to present the kit they have available.

Scientific sessions

Much of the rest of the meeting will be built up of parallel sessions, of which the following have so far been agreed.

- *In situ diffraction.* This session will probably take place on the Wednesday, and will likely include processing of inorganic materials and opportunities for non-ambient and *in situ* crystallographic work at central facilities including DIAMOND.

- On the Thursday, **Pam Thomas** will lead a session on *phase transitions.* Following on from the successful teaching session at UMIST on using International Tables, this session will start with an introductory teaching session (Do you really know what a phase transition is? How can you characterise one? Is there really such a thing as a second order phase transition?).

- *Photocrystallography.* This session will be chaired by **Paul Raithby** (Bath).

- *Modern techniques for crystal structure refinement.* This session should be of interest to all crystallographers, as many of us – biologists, physicists, chemists, geologists – have similar problems and can learn from how others get round them. **Bill Hunter** and **Simon Parsons** will chair this session.

- As Chick mentions in his piece in this issue, next year we will be joined by the **X-ray fluorescence community,** who will run a parallel session throughout the meeting that is likely to be of interest to many of us. It will be organised jointly by BCA Treasurer **Dave Taylor** and **David Beveridge** of Ilford Ltd. Sessions will include presentations on state-of-the-art equipment and consumables, working with liquid and awkward samples (aren't all liquids difficult samples?….), standards and calibration, and light element analysis.

- Other sessions currently being put together address non-ambient aspects of pharmaceuticals, crystallography in industry, membrane proteins, high throughput methodologies in macromolecular crystallography and *in situ* drug discovery. More on these later.

BCA 2005 Spring Meeting

Workshops

By popular request (yes, really!) we will continue to include a number of workshop sessions in the programme. For 2005, there will be, in addition to the workshop aspect of the *Phase Transition* session, a *Crystals* workshop organised by **David Watkin** and **Richard Cooper** from Oxford, and *Industrial Crystallography* and *WinGX* workshops. Other possible workshop sessions are still under discussion. We are also examining the possibility of a one day 'satellite' white beam workshop on the Monday preceding the meeting.

We are also examining the possibility of building on last year's experience of holding one or two facility user meetings just before or after the main meeting.

Offer a talk!

Two final points

Although the Young Crystallographers session at UMIST was thought to be a great success, we want this year to improve integration! I heard many of the Young Crystallographers' talks and felt strongly that it was a great pity they weren't seen and heard by a wider audience. So next year, we are purposely not filling all the 'slots' in the scientific sessions with invited speakers. Rather, we are calling for offers of talks from everyone in the community, a procedure I have seen work very well in other meetings. Details of how to bid for one of these slots through submitting an abstract will be publicised later when the overall programme is finalised. But do begin to think now about either submitting an abstract for an oral presentation, or encourage your students and postdocs to do so. There will of course be poster sessions as well, and we are working to improve the integration of the posters with the rest of the meeting.

And in addition, check your diary now and make sure that you have "BCA meeting" blanking out everything else for 12-14 April 2005. It promises to be an excellent and exciting three days. If you have any queries or suggestions about the programme – perhaps there's a really exciting development that we haven't included? – please get in touch with me. If you have suggestions concerning the individual sessions, please also contact either me or the session organiser.

John Finney
j.finney@ucl.ac.uk

News from the Groups

Biological Structures Group Sessions at BCA Spring Meeting

THIS year the Spring meeting was once again organised around a condensed format, to keep delegate costs down and to take up less of the Easter holiday with one day registration for the central day, the main focus of the BSG sessions. Thanks in particular to Steve Prince (UMIST) assisted by Jordi Bella (University of Manchester) and Jon Read (Astrazeneca) for their efforts in organising an excellent meeting.

Biological Structure Group AGM

The first BSG Winter AGM took place at the meeting at Birkbeck in London, 2003. It was very well received and enabled a lot more BSG members to participate than have done in recent years at the Spring meeting. Financially the BSG remains healthy, whilst it is walking a fine line between profit and loss each year for its two meetings. It was agreed that the BSG would transfer bank interest accrued during year to the Arnold Beevers Memorial Bursary fund administered by the BCA, where it is accessible to BSG members to support travel to scientific meetings. One organisational issue had to be resolved: the acceptance of final accounts by the BSG after the end of the financial year, but before the presentation of the BCA accounts at the Spring meeting. It was resolved by presenting the provisional accounts and dealing with all other business at the Winter meeting, adjourning the AGM, with all decisions made there taking effect immediately, and reconvening at the Spring meeting just in order to accept the final accounts. This procedure will be followed in future years. The AGM will be therefore be held at the winter meeting again in 2004.

Elections to be held at AGM, 2004

The position of Vice Chairman remains vacant. The current secretary/treasurer has announced her intention to stand down from that position. It has been proposed that the roles of treasurer and secretary should in future be kept separate. Nominations are therefore sought for the positions of Vice-Chairman, Treasurer and Secretary. A number of committee members reach the end of their three year term in 2004 so nominations are also sought for the position of committee member. Nominations, with details of a proposer and seconder, should be sent to the secretary, **Andrea Hadfield,** details below. Anyone interested in standing should get in touch - we can always help to organise a proposer and seconder if necessary!

The current committee is composed as follows:

Chairman
Dr. Richard Pauptit (2000-2006)

Vice-Chairman
Vacant

Secretary/Treasurer
Dr. Andrea Hadfield (2000-2004)

Committee
Dr. Nick Keep (2001-2004)
Dr. Harry Powell (2001-2004)
Dr. Jon Cooper (2001-2004)
Dr. Katy Brown (2001-2004)
Dr. Vilmos Fulop (2001-2004)
Dr. Peter Moody (2003-2006)
Dr. Sheila Gover (2003-2006)

Biological Structures Group Winter Meeting 2003

The BSG winter meeting will be held on 17th December this year at Imperial College London as a Memorial to Professor David Blow. Details will follow.

Andrea Hadfield
a.t.hadfield@bris.ac.uk
Dept. of Biochemistry,
School of Medical Sciences,
Bristol University,
University Walk, Bristol BS8 1T

Autumn/Winter Meeting of the PCG

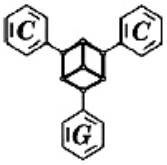
THE PCG Winter meeting will be held on Monday 13 and Tuesday 14 December, 2004 at Cosener's House, Abingdon, Oxon. This year's theme is "Neutron Scattering from Biological Systems".

We aim to give a broad overview of the contribution of neutrons to biology, with particular emphasis on neutron protein crystallography, protein dynamics, neutron fibre diffraction, small-angle scattering and reflectometry from

systems such as enzymes, amyloids, membranes, proteins absorbed on surfaces, drug delivery vehicles, biosensors and many more. These topics will be introduced by a series of invited and contributing speakers and by a poster session, but there will also be ample time for an open discussion about the present and future of neutron techniques and facilities. Keynote speaker will include **Peter Timmins** (ILL) and **Bob Thomas** (Oxford).

In particular, we will explore the opportunities for neutron scattering experiments in biology at existing and future neutron sources, such as the ISIS Second Target Station. We expect a stimulating discussion on these topics to continue over our traditional Christmas Dinner. The level of the presentations will be suitable for beginners and experts alike. For those interested in this meeting, which is co-sponsored by the ISIS-TS-II project and the SCMP group of the IOP, further information will be available on the PCG and ISIS websites.

Organising committee: Paolo Radaelli, John Helliwell, Jeff Penfold, Pam Thomas, John Evans



Chemical Crystallography Group

Summary of the Chemical Crystallography Group AGM

The Chairman, **Dr. Sandy Blake,** spoke of the highlight of the past year, the very successful Autumn Meeting entitled "After Refinement - What comes next?" It was hosted by Accelrys in Cambridge and there were over 80 participants. He thanked MSC Rigaku and Accelrys for sponsoring the meeting, Pfizer for sponsoring student registration and Vanessa Hoy for excellent local organisation.

He also thanked Oxford Diffraction for sponsoring the CCG poster prize at this Spring meeting and Simon Parsons for organising the scientific sessions at this meeting.
He announced the winner of the CCDC Chemical Crystallography Prize for Younger Scientists as **Dr Maryjane Tremayne** of the University of Birmingham.

He thanked the retiring members of the CCG committee for their hard work and support, namely **Dr Simon Coles** who retires as an ordinary member and **Dr Harry Powell** who has served two terms as Secretary/Treasurer and has done an excellent job throughout.

The Intensive Course in Durham will be held 4 -11 April 2005, just before the BCA Spring meeting in Loughborough. Dr Blake proposed that one unit of sponsorship (£700) be available to anyone who could not afford to come otherwise.

Dr Harry Powell presented the Group's financial statement for 2003. The healthy position of the group's finances was greatly helped by the generous sponsorship of the Autumn Meeting by MSC Rigaku and Accelrys.

Elections

Secretary/Treasurer

Dr Georgina Rosair (Heriot Watt University), period of office 2004 – 2008.

Member of Committee:

Dr Andy Parkin (Glasgow University) 2004 – 2007.

Member of Committee:

Dr Andrew Bond (University of Southern Denmark) 2004 – 2007.

Autumn Meeting 2004

Sponsored by Bruker-AXS

The CCG Autumn meeting 2004 will take place at Aston University on Wednesday November 17, 2004 with the following programme:

In situ crystallography

10.25-10.30	**Welcome**
10.30-11.15	**Dermot O'Hare** (University of Oxford) Studying Solid State Reactions using Time-Resolved X-Ray and Neutron Diffraction
11.15-12.00	**Richard Ibberson** (ISIS) Molecular crystal structures by neutron powder diffraction - the highs and lows of parametric studies.
12.00-1.30	**Lunch**
1.30-2.00	**John Warren** (SRS) Single crystal, powder, liquid, volcano, spotty rings, star wars: *in situ* diffraction at the SRS
2.00-2.30	**Andrew Bond** (University of Southern Denmark) *In situ* crystallisation and co-crystallisation.
2.30-3.00	**David Allan** (University of Edinburgh) Crystal growth from the melt or from solution at high pressure: generating new small-molecule polymorphs.
3.00-3.20	**Tea**
3.20-3.40	**Katherine Bowes** (University of Cambridge) Structure: Determination of Excited States, using single crystal X-ray crystallography
3.40-4.00	(Short contribution from postgraduate or postdoc.)
4.00	**Close.**

The local organizer is **Dr Carl Schwalbe,** School of Life and Health Sciences, Aston University, Birmingham:
Tel: +44 (0) 121 359 3611 ext 4201;
Fax: +44 (0) 121 359 0733
Email: c.h.schwalbe@aston.ac.uk.

A registration form is included with the September edition of Crystallography News and on the CCG pages of the BCA website.

There is room for one 20 minute presentation. Offers of short presentations (particularly by post-graduates and post-doctoral workers) at the meeting should be sent to the scientific session organizer: **Dr Simon Parsons,** School of Chemistry, Joseph Black Building, West Mains Road, Edinburgh, EH9 3JJ. Tel: +44 131 650 5804,
Fax: +44 131 650 4743, E-mail: s.parsons@ed.ac.uk

Please send completed registration forms with cheques made payable to "Chemical Crystallography Group" to: **Dr Georgina Rosair,** William Perkin Building, School of Engineering & Physical Sciences, Heriot Watt University, Edinburgh EH14 4AS

Georgina Rosair, CCG Secretary/Treasurer

Industrial Group Committee

Autumn meetings of the Industrial Group

5th October 2004 Pharmaceutical SIG, AstraZeneca, Alderley Park.
MORE DETAILS SOON!
This follows the same format of previous SIG's with a mix of topical presentations at the fore front of the technique.

4th November 2004 Autumn Meeting "DIY Crystallography", Birkbeck College, London.
MORE DETAILS SOON!
The morning theme will be "Heath Robinson Hardware" and the afternoon devoted to public domain software.

Industrial Group Committee

Following the AGM at Manchester, the Committee of the Industrial Group is:

Chairman
Dr Jeremy Cockcroft, Birkbeck College London
Email: cockcroft@img.cryst.bbk.ac.uk

Vice Chairman & Newsletter Editor
Dr Phil Holdway, QinetiQ Ltd, Farnborough
Email: pholdway@QinetiQ.com

Secretary/Treasurer
Ms Judith Shackleton, Manchester Materials Science Centre
Email: judith.shackleton@man.ac.uk

Committee Members
Dr David Beveridge, Ilford Ltd, Knutsford, Cheshire.
Email: david.beveridge@ilford.com

Mr Mark Farnworth,
Pilkington European Technical Centre, Ormskirk, Lancs.
Email: Mark.Farnworth@pilkington.com

Mr Richard Morris, Huntsman Surface Sciences UK, Oldbury, West Midlands. Email: Richard_Morris@huntsman.co.uk

Dr Anne Kavanagh, PAR&D AstraZeneca, Macclesfield, Cheshire.
Email: anne.kavanagh@astrazeneca.com

Mr Martin Gill, Mineralogy, Natural History Museum, London.
Email: m.gill@nhm.ac.uk

Co-opted:
Dr. Steve Norval, ICI plc, Measurement Science Group, Redcar
Email: steve_norval@ici.com

ICDD Representative (Ex officio) & IG Webmaster
Mr. DaveTaylor, 35, Birchley Rd, Wigan.
Email: djtaylor@lineone.net

Books & CDs

International Tables for Crystallography

Volume D: Physical Properties of Crystals

André Authier, Editor
Published for the International Union of Crystallography by Kluwer Academic Publishers: Dordrecht/Boston/London, 2003
Price: £135, €205, $220 (institutions/libraries) – half-price for personal use.
ISBN 1-4020-0714-0
522 + xii pages + CD-ROM

CRYSTALS are anisotropic media and each one possesses a certain structural symmetry. The physical properties of crystals are therefore described by tensors, the elements of which are determined by the particular symmetry. Crystals may also transform from one structural phase to another, grow as twins or have domain structures. The vibrations of their constituent atoms (phonons) and the behaviour of electrons in crystals are also subject to the effects of crystal symmetry. All these important topics, and their useful applications, are treated in this new and weighty volume, in the world-renowned series published for the International Union of Crystallography.

As the series title implies, the volumes contain many useful tables, but they also comprise comprehensive explanatory chapters. The present tome brings together the widest ranging and latest crystallographic information, distilled by 28 international experts (from 9 different countries). Terry Willis originally proposed the idea for this volume and André Authier has skilfully orchestrated the whole project. The high standard of the IUCr has been maintained: the book is beautifully produced, together with fine illustrations, some in colour, and numerous references to the extensive literature; and it is supported by a CD-ROM with a further 140 pages of explanation (including, amongst other things, algebraic details of groups and subgroups) as well as useful software. The latter contains calculations involving tensors, irreducible group representations and structural phase transformations: (for example, the changes in tensor properties of physical quantities during ferroic phase transitions).

The volume is divided into three parts, of which Part 1 is the largest, comprising half the book. This describes the tensorial aspects of physical properties and sets up the necessary mathematics. Tensors of rank 2, 3 and 4 are treated, together with all the intricacies that the effects of crystal symmetry have upon their constituent elements. Strain and stress tensors are described, together with the geometrical interpretation of their coefficients; and some nice pictures of the representation surfaces of the inverse of Young's modulus for several simple crystals are shown. Experiments for the determination of elastic constants and of thermal expansion are described. Various types of magnetism, disordered and ordered, are discussed; and many diagrams of magnetic lattices are displayed. The detailed theories of linear and non-linear crystal optics are given, as well as much helpful practical advice on the use of the polarizing microscope.

As is well known, light and matter interact through their electric fields, inducing a dipole. Electric polarization is a vector, which is related to the applied electric field via the dielectric susceptibility tensor. The latter is tabulated here for all crystallographic point groups. Transport properties – the flow of electricity or of heat through crystals – are also described. The site symmetry places restrictions on the tensor coefficients of atomic displacement parameters, either from thermal motion or positional disorder. There are informative tables on these, as well as colourful graphical representations of density modulations. Superspace groups and tensors in higher-dimensional space are introduced to describe quasiperiodic structures – incommensurate or modulated structures, or quasicrystals.

Symmetry aspects of excitations are discussed in Part 2. The collective motion of atomic displacements, small compared with interatomic distances, are described by phonons. Here again, symmetry plays a key rôle and matrices are used for the calculations. Several examples are given of phonon dispersion. The electron energy band structure in crystals is described with the aid of group theory, Brillouin zones and Bloch functions. The electric field gradient tensor is introduced and, as an example, the various oxygen sites in the high-temperature superconductor $YBa_2Cu_3O_7$ are discussed. Phonons give rise to Raman scattering and tables provide the details of the Raman tensor in each of the 32 crystal classes. The longitudinal and transverse modes of Brillouin scattering are also tabulated in the various Laue classes.

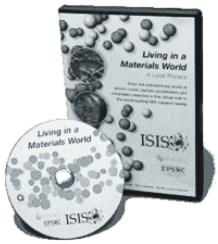
The many different types of ferroelectric, ferroelastic and ferroic structural phase transitions are examined in Part 3, together with their symmetries and thermodynamics. There are tables giving detailed information on the lowering of point group symmetry associated with irreducible representations and there are many examples and diagrams of particular crystals. The subject of twinning usually occupies only a short section of textbooks on crystallography, and usually only one aspect is given,

whether it be growth twinning, transformation twinning or mechanical twinning. Here the fascinating early history of twinning is outlined, together with all the necessary lattice aspects and group-theoretical mathematics needed for understanding twinning and domain structures. Many examples of twins, twin boundaries and fault vectors are given, beautifully illustrated with diagrams of the various crystal structures and atomic-resolution transmission electron micrographs. Domain structures are examined in detail and a large table of group-subgroup symmetry descents is provided. Domain pairs, domain twin laws and domain walls are all comprehensively discussed.

Crystallographers, materials scientists, mineralogists and solid-state physicists will all welcome this up-to-date, handsome and most distinguished reference book. Our grateful thanks go to the editor, André Authier, to all the authors and to the IUCr technical editors, Nicola Ashcroft and Amanda Berry, for all their painstaking work.

Moreton Moore

Living in a Materials World



Published by CCLRC,
Rutherford Appleton Laboratory

THIS CD is freely available to secondary schools; it was published in 2003, funded by EPSRC and supported by the ISIS department of the CCLRC Rutherford Appleton Laboratory (RAL) in southern Oxfordshire. It was developed in a collaboration between RAL scientists and local teachers to match the A-level physics course specifications.

The CD is stored in a DVD sized box and comes with a note giving the password for the teacher. This allows access to the model answers to the questions as well as further web links, a curriculum audit and the text in an easily printed format.

Visits to ISIS, the spallation neutron source used to study materials, can easily be arranged for local schools where students can see the accelerator and its facilities for themselves. Students who live further away can get a very good idea of what ISIS looks like using the Virtual tour provided on this CD. There are sections on how particle accelerators work, as well as descriptions of the current research in physics, earth science, chemistry, engineering, biology and archaeology. There is also an introduction to interference, with animations illustrating constructive and destructive interference. This section goes on to explain Bragg's law. Hyperlinks to a glossary of terms are provided to define unfamiliar concepts and terms.

Another section, 'People at work', has video clips of ISIS employees talking about their work and the qualifications and experience needed to get their jobs. The people have a range of skills, they are mostly research scientists but technicians and secretarial staff are also included.

A historical section has photographs of early research workers in the field and a description of their discoveries. I noticed particularly that their clothing was very different from that of today's workers as seen in the video clips. Perhaps it was merely that the photographs were monochrome in the 1930s, certainly the people were more formally dressed, no jeans and Tee shirts in the lab then.

More information about the CD is available on the ISIS web site at **www.isis.rl.ac.uk/materialsworld** where you can order a copy of the CD-ROM as well as see much of the Teacher Resources information on the CD itself, such as videos and animations from the Research Section, the people at Work video, the questions and answers for the sections and the full text from the CD-ROM in an easily printable format.

Since so much of the information is on the web already, I wondered why the authors did not make the CD using HTML rather than using this very similar screen display seen in the image above. Each screen has a header describing the section at the top. On the right hand side of the screen three clickable icons give access to the glossary, the questions on this section and 'sound'. This is independent of the sound in the video clips of people talking about their work. Initially it is turned on, producing a synthetic drumming noise which personally I found irritating; luckily it is easily turned off. At the bottom of the screen four icons allow navigation through the CD, 'menu' allows you to jump to a different section, 'back', 'next' and 'quit CD' are self explanatory. The central area is divided into three, with two small regions on the left, the upper where the video clips are shown, the lower with 'postage stamp' sized versions of possible images for you to click on to see them in the upper area. The larger area on the right has descriptive text.

Further Information

No site licence is required to run multiple copies on a school network. For more information about the ISIS facility or the CD-ROM please contact Dr Martyn Bull or Dr Christopher Frost, ISIS Facility, CCLRC Rutherford Appleton laboratory, Chilton, Didcot, Oxon OX11 0QX. Tel: (01235) 445805

Computing Technicalities

This CD was reviewed using a PC clone laptop, a Dell Inspiron 7500, with Windows 98, a 500MHz Pentium III processor with 64Mbytes memory, and an LCD screen size 1024 x 768. I loaded and ran the CD with few problems, but it does need some familiarity with PCs and their packages. There is a brief introductory screen, but I should have liked to see a little more explanation; for example, how to distinguish whether an underlined phrase links to the glossary or to the Internet, and that the 'questions' icon was only active when it changed to showing question marks.

The recommended minimum system requirements are a PC with a Pentium II 300MHz, Microsoft Windows 95,98,NT, 2000 or XP, 43MB (64 recommended) 32xCD ROM drive, 16 bit colour display, 800 x 600 screen. A copy of QuickTime 5 is provided on the CD which will be loaded automatically unless you already have one.

They did not mention that the word processing package Microsoft Word is needed for the text of the questions and answers. Presumably any school with a PC will also have Word, but PCs for personal use can be bought just for games or with other, cheaper, word processing packages.

They did not explain that to access the external links you also needed a live Internet connection and a Web browser. In these days of virus infections and spam many people only switch on their modem when they want to use the Internet. Schools may not allow their students unrestricted Internet access.

My laptop has a larger screen size than that suggested, so I saw the display surrounded by a white frame about 200 pixels wide, with a rather small area used for the video clips. If the authors had used HTML rather than this proprietory display package with a fixed screen size, the Web browser would have a display which filled the screen. The CD would have not only looked better but would have been accessible to any computer system not just PCs.

Conclusions

This CD is a very useful resource for schools, with easily accessible resources for teachers as well as showing students the wide range of research done at ISIS and a little particle physics. I particularly liked the way that the examples in the engineering section showed broken bicycle parts which students might have encountered. This would make them realize the importance of strain testing much better than showing them turbine blades.

Kate Crennell

Diamond Memorials?

THIS is a summary of a remarkable article which appeared in The Times magazine for 19 June 2004 on page 57.

The British tradition is to commemorate the life of a loved one by erecting a lasting memorial. Queen Victoria created perhaps the most well known example for her beloved husband, the Albert Memorial in Hyde Park. After less than 200 years this has just been expensively restored to its former glittering splendour. Less exalted folk erect gravestones of varying hardness, with inscriptions which are eroded with time and become illegible after about four hundred years. It is reported that a significantly longer lasting memorial can now be made of diamond.

A newly formed company, 'LifeGem' will take a small amount (about 200gm or approximately 15% of the ashes of an average sized adult) of your loved one's cremated remains and turn them into a diamond. The exact process is a commercial secret; the colour cannot be guaranteed, most turn out to be yellow and some have flaws. Security precautions are taken to ensure your diamond is not made from the ashes of some one else's beloved. Each order has a security code assigned to the ashes which goes with them at each stage and is laser-etched on the resulting diamond, together with more text of your choice. The process can also be done with the remains of your pets; the ashes can be mixed together allowing the creation of a diamond made, for example, from the ashes of mad Aunt Sybil and all her favorite pussies.

Further details and prices can be found on the web site www.lifegem-uk.com

There is a link to the parent company website in the U.S.A, which has further links to pages of explanation of the crystallography of diamond.

I would be interested in comments from members of the BCA about this process. I understood that cremation converts all the carbon in the body into carbon dioxide, how much is left to be made into diamond?

Kate Crennell

Obituary

David Blow 1931-2004

PROFESSOR David Blow, a founding father and Past President of the BCA, died on June 8th, 2004. He will be sorely missed.

David was trained as a physicist who became a pioneer of protein crystallography, a gifted and inspiring teacher, and an able administrator who made great contributions to both the British and European scientific communities.

He studied physics at Cambridge, then did his PhD with Max Perutz working towards the crystal structure of haemoglobin in the old annex to the Cavendish laboratory which housed the structural biology group. At that time no structure with more than 150 atoms had been solved; haemoglobin had more than 2500 atoms, and many people thought the task of phasing such a large crystal was hopeless. However with the insight that "isomorphous replacement", the technique of adding extra heavy atoms to a crystal without disturbing the rest of the structure, could provide some phase information, Perutz's team set out to develop these methods, to derive the phases and assess their quality, and to find ways of interpreting the low resolution electron density they yielded, using the pre-existing knowledge of protein structure, the presence of α-helices, solvent volumes and so on. It was a wonderful time to be a research student, and David with his physicist background, and the adaptability to acquire new skills, made many fundamental contributions. The paper he wrote with Crick in 1959 "The treatment of error in the Isomorphous Replacement Method" must be one of the most widely cited in the field.

After obtaining his PhD he spent two years in the USA, then returned to the newly rehoused Laboratory for Molecular Biology (LMB) – by this time Perutz and Kendrew had been awarded the Nobel Prize, and conditions were much better, although success soon brought the familiar overcrowding. He joined Michael Rossmann, and together they developed the basis of "molecular replacement", the technique which uses information from duplicate copies of the same molecule, either within the same crystal or in a different crystal form to derive or refine phases. Thus David is a principal author of two sets of ground-breaking papers on fundamental methods for finding phases for crystals of large molecules.

However, both David and Michael were most interested in applying their methodology to the solution of new structures and using the knowledge of the 3-dimensional organisation of the molecules to give biological insights. David began to work on the crystal structure of the enzyme chymotrypsin, whose mechanism was already under investigation down the corridor by his biochemist colleague, Brian Hartley. The structure was solved by 1967, the fourth protein structure to be determined, and they were able to describe the first catalytic triad, a pattern of residues we now know is exploited to facilitate many biochemical processes. (The project had the added bonus that there were two copies of the molecule in the crystal asymmetric unit, allowing him to exploit his molecular replacement methods.).Achieving this level of collaboration between biochemist and physicist is still the ideal for structural biology research groups.

In 1977 David left the research orientated environment of the LMB to set up the Biophysics group in the Physics department at Imperial College. This presented him with new challenges familiar to academics, how to reconcile maintaining a research profile with the demands of teaching, and the inevitable administrative responsibilities, here made more difficult by the need to maintain inter-disciplinary and inter-departmental collaborations. He succeeded in the juggling act; many students remember his lucid, rigorous and entertaining lectures, and his graduate students and those others he interacted with remember his inspiring approach, enthusiastic, rigorous, perceptive and sympathetic. He has written an outstanding text book built on his teaching experience; "An Outline of Crystallography for Biologists", reviewed in the September 2002 issue of Crystallography News. He took on many tasks for Imperial College, serving as Dean of Science and as Head of Department, and helped to establish and maintain its scientific excellence.

The environment at Imperial persuaded him of the need to provide a forum where chemists, physicists and biologists could discuss crystallographic problems. At that time there was a Chemical Crystallography Group as part of the Royal Society of Chemistry, and the Institute of Physics had a Special Interest Group in crystallography, each organising their own meetings. It was agreed that these should merge to form the British Crystallographic Association. Typically, having recognised the need, he brought his persuasive and organisational skills to the task of setting up the committee, and encouraging a wide membership. By 1982 the BCA was well established and on a reasonable financial basis. He and Steven Wallwork have written a record of this, which could well be used as a model for any aspiring network. It was published by the Royal Society shortly before David's death (Notes Rec. R. Soc. London 58,177-186 (2004)). His achievement in establishing this cross-disciplinary group has helped the whole British scientific community, fostering contacts not just between physicists and chemists, but also biologists, computer scientists and engineers. He will be sadly missed at BCA meetings, which he continued to attend regularly till last year where he chaired the Max Perutz Memorial lecture.

His influence will continue, carried on by his students and colleagues, many of them now leading their own research groups, by his friends, and by new generations who are introduced to the subject by his excellent book.

Biographical Outline

- **David Mervyn Blow; born Birmingham 27 June 1931;**
- **Staff, MRC Unit for Study of Molecular Biological Systems, Cambridge, 1959-62;**
- **Laboratory of Molecular Biology Cambridge 1962-77;**
- **Fellow Trinity College. 1969-77;**
- **FRS 1972;**
- **Professor of Biophysics, Imperial College, London 1977-1994;**
- **Senior Research Fellow, 1994-2004;**
- **Dean, Royal College of Science 1981-84;**
- **Head of Physics Department, 1991-94;.**
- **President British Crystallographic Association 1984-87;**
- **Married Mavis Sears 1955 (one son, one daughter);**
- **Died Appledore Devon 8 June 2004.**

Eleanor Dodson

Obituaries which have appeared in the press include: 23rd June 2004 The Independent, by Richard Henderson (this one is now, by permission, on the BCA webpages. On 25th June 2004 there were tributes in The Guardian from Michael Rossman and Guy Dodson. On 1st July 2004 The Times published an anonymous obituary.

Royal Society 2004 Rosalind Franklin Award

ON 12 May 2004 the Royal Society issued a Press Release announcing that an expert in protein interactions has won the second annual Royal Society Rosalind Franklin Award. Professor Carol Robinson, of the University of Cambridge's Chemistry Department, is a world leader in the field of mass spectrometry, a technique traditionally used for measuring the mass of individual molecules. Professor Robinson's research has applied the process to study interactions of proteins.

As the winner, Professor Robinson receives £30,000 and will also deliver a lecture at the Royal Society later this year. She will use part of the prize money to fund a mentoring project to support women in careers in science, engineering and technology (SET).

The Royal Society Rosalind Franklin Award was set up in 2003, at the suggestion of Patricia Hewitt, Secretary of State for Trade and Industry, to address the issue of under-representation of women in SET and is open to mid-career scientists who have developed an area of science with which they are identified. Nominees must propose a project that will raise the profile of women in SET in either their host institution or field of expertise. The award is funded by the Government's Office of Science and Technology as part of its efforts to promote women in SET.

During a career that has seen her rise from lab technician at Pfizer, to world leader in biological mass spectrometry, Professor Robinson has carried out pioneering work to understand how chains of amino acids form folded proteins and subsequently interact with other molecules. More recently, becoming frustrated with the limits of what mass spectrometry could achieve, she was instrumental in extending the abilities of the equipment to study much larger groups of proteins.

Professor Julia Higgins, Vice-President of the Royal Society and chair of the Rosalind Franklin Award Committee, said: "The work of Professor Robinson speaks for itself. She is an outstanding winner and excellent role model for younger women scientists. It is pleasing to note that the Royal Society was able to support her at an earlier stage in her career through our University Research Fellowship scheme."

Further details can be found on The Royal Society website at www.royalsoc.ac.uk/franklin or on the BCA website at www.bca.cryst.bbk.ac.uk/BCA/Obits/CVS/RF.htm

Kate Crennell

American Crystallographic Association

Chicago, July 17-22 2004

The ACA in Chicago was, as usual, a good and varied meeting. Full details will, of course, be available in the ACA Newsletter. Three special reports, written for Crystallography News, appear below.

Teaching Advanced Crystallography

This session, organised and chaired by **Dr. Peter Müller** under the auspices of the Service Crystallography SIG, was very well attended with standing room only for some talks. The session addressed the difficulties in teaching crystallography to those without a large amount of prior knowledge or training; "advanced" generally meant that the intended audience had at least some knowledge of what a crystal was.

Left to Right: *Peter Müller, Bob Gould, Larry Falvello, Michael Sawaya, Bill Clegg, Jenny Glusker, George Sheldrick.*

The first talk in the symposium was given by **Professor Jenny Glusker** (Institute for Cancer Research, Philadelphia) outlining her methods for teaching biologists about crystallography. A biologist typically looks to crystallography to definitively answer "What is the structure of my protein?": it is the job of the crystallographer to provide the biologist with the tools for intelligent interpretation of the crystallographic results. Use of relevant examples is crucial; biologists know about DNA so examples drawn from the work of Franklin are useful, or a simple example of the use of the Patterson function to solve the structure of copper sulfate can be linked to the solution of the heavy atom sites in vitamin B12.

Jenny's suggestion that diffraction gratings can be made from paper gave rise to some interesting suggestions from the floor; apparently sieves can be used as DIY diffraction gratings. Fabrics are also useful but shop assistants tend to look oddly at customers shining lasers through their wares.

Dr. Bernard Rupp (University of California, LLNL) continued the theme of teaching crystallography to people with a biological background. He advocated a "less is more" approach to the teaching of the fundamentals; many students now lack the mathematical background to fully understand detailed crystallographic theory. At the same time, the unsupervised or naïve use of software is a high risk factor for bad science. Too much stress on space groups at the expense of critical appraisal of structure quality is to be avoided.

The difficulties in teaching a specialized subject not covered in widely available crystallographic texts were described by **Dr. Michael Sawaya** (UCLA), who lectures on Multiwavelength Anomalous Dispersion (MAD). Covering such an esoteric subject in a fifty minute lecture is challenging; using familiar concepts and real life examples is the key to successful teaching of this topic.

The focus then moved from biological crystallography to small molecules. **Dr. Bob Gould** (University of Edinburgh) gave an overview of the biennial British Crystallographic Association Chemical Crystallography School which has been running since 1987. Evolution of the course organisation over time has lead to an increase in the number of students and a decrease in the number of lecturers; this reduces the danger of experts contradicting each other! Bob stressed that in a course of this nature there should be a clear distinction between what students need to know, what they should be able to find out, and what they should have a feeling for. Fun events can be used in teaching; this particular alumnus of the School has fond memories of the crystallographic pub quiz!

Professor Bill Clegg (University of Newcastle) then covered the teaching of the dual headaches of disorder and twinning. As in other areas, it is important to use real life examples and tools that will be familiar to the student when covering these advanced topics. When teaching a topic that one may not be an expert in, it is important to make use of material available elsewhere, such as online. Clarity in the use of confusing terminology is very important; this is a particular problem in teaching about twinning.

Dr Larry Flavello (University of Zaragoza) addressed the problem of teaching chemists to be intelligent consumers of crystallographic results. Symmetry, particularly in the exploration of intermolecular contacts, proves to be a difficult concept for non-crystallographers to deal with. Larry showed several examples of increasing complexity that can be used to demonstrate the importance of symmetry in considering the intra- and intermolecular geometry.

The final talk of the session was given by **Professor George Sheldrick** (University of Göttingen) who gave an outline of the teaching of crystallography in Germany. Students are given real crystallographic data to analyse, providing a use for the "unwanted" structures (side products, starting materials) that otherwise would be forgotten. Apparently it takes some time for students at Göttingen to realize that Professor Sheldrick's native tongue is not German (in fact it is Fortran, as we all knew). For a more advanced course, an example was given of the use of PowerPoint to demonstrate the use of the Patterson superposition method in crystal structure solution.

Alice Dawson
University of Arizona

Advances in Computing Environments for Crystallography

www.hwi.buffalo.edu/ACA/ACA04/abstracts/S0603.html

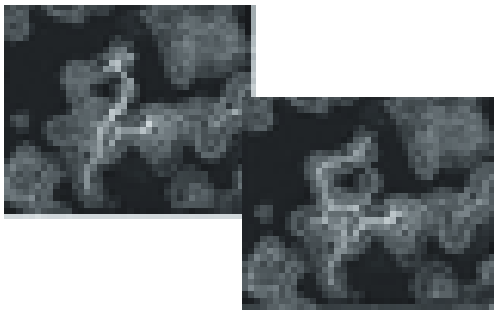
THE Computing Environments session, sponsored by the ACA General Interest SIG, contained a good range of talks covering the use of the GRID, distributed computing, protein model building tools, through to visualisation and integration of single crystal 3D raw data and comparative visualization of molecular and protein structures.

The first talk by **Russ Miller** (miller@buffalo.edu; co-authors: M.L. Green and C.M. Weeks) was about SnB (Shake-and-Bake)/BnP macromolecular structure solution and protein phasing software on the Grid (http://www.hwi.buffalo.edu/SnB/ http://www.ccr.buffalo.edu/grid/content/overview.htm). Russ clearly defined GRID computing and, in particular, what is not GRID computing, providing a breath of fresh air in laying down the law on the subject separating reality from hype and buzzwords. Pointing out that "The GRID" does not exist in the form that is commonly hyped and is currently under development, Russ elaborated on custom administrative tools written at the Center for Computational Research at SUNY-Buffalo in the context of the SUNY/Hauptman-Woodward Institute collaboration to make GRID computing practical for users and managers of GRID infrastructure. SnB/BnP is available via three existing GRID networks. Russ then gave a live Internet demonstration of submitting jobs to the SnB/BnP software via a standard web interface, followed by showing the tools that allowed users to check status of jobs, and quickly evaluate structure solution results. Software for collaborative examination and manipulation of molecular models via the Internet was also displayed. Queried during question time on whether authors of crystallographic software should make their programs GRID aware, Russ cautioned that unless you have a religious-type belief in the GRID, it might be too early to commit significant programming resources to GRID computing until the underlying systems management of GRID computing proves itself. Beta testers for the new SnB/BnP for GRID are most welcome and should contact Russ via the above address.

Anders Markvardsen (a.j.markvardsen@rl.ac.uk: co-authors: K. Shankland and W. David) of Rutherford-Appleton laboratory in the UK, then discussed the use of distributed computing in the role of finding optimal Hybrid Monte-Carlo parameters for structure solution from powder diffraction data. These optimal values can then be applied to structure solution software running on single workstations. Using distributed computing tools to link local workstations, results can be obtained in a couple of weeks that would have taken half a year or more using a single workstation.

Showing a healthy disregard for the forces of computing conformity and conference requirements for MS-Windows

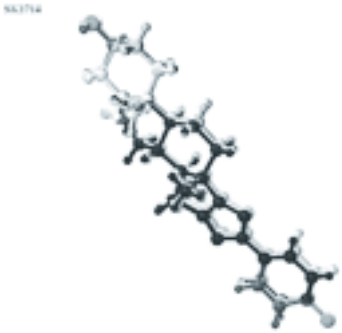
compliance, **Paul Emsley** (emsley@ysbl.york.ac.uk) from York, UK used his Apple MacOS X laptop to demonstrate the COOT ((Crystallographic Object)-Oriented Toolkit) Model Building Tools for protein crystallography. Coot is part of the CCP4 Molecular Graphics Project and has some features that resemble those of Frodo, O, Quanta and XtalView's XFIT. Paul's live demonstration showing COOT re-optimising the incorrect orientation of a residue in real-time drew "ooh's" and "ahh's" from the audience. The two screen images below show the before and after of this demonstration.



COOT (http://www.ysbl.york.ac.uk/~emsley/coot/) is freely available in source code form under the GNU GPL Licence, and compiled binaries for a variety of operating systems (SGI IRIX, Mac OS X, Redhat Linux) are available via (http://www.ysbl.york.ac.uk/~emsley/software/binaries/).

Dennis Mikkelson (mikkelsond@uwstout.edu: co authors: A. Schultz, P. Peterson, R. Mikkelson, T. Worlton, J. Hammonds, J. Cowan, Martha Miller, C. Bouzek, Michael Miller), a senior computer scientist at University of Wisconsin-Stout introduced a GPL'd user friendly software package for viewing raw neutron Time-of-Flight (TOF) single crystal data, with the option of indexing and integration (http://www.pns.anl.gov/computing/isaw/). Speeds of visualisation for reconstructed raw image files of reciprocal space collected with multiple detectors were stated as being performed within a second or so. Both manual and computer based indexing options were shown for handling multiple crystallites; and the software has the ability to perform integration of 3D diffraction spots. Various "wizards" to aid in analysis, and the *hkl* slice viewer are in the latest build (1.7.1 alpha 7) available on the above ISAW (Integrated Spectral Analysis Workbench software) website. The 3D reciprocal lattice view described in the talk is expected to be in the 1.7.1 "final" build by late August. Under the tyrannical direction of the session chair, Dennis quickly flicked through remaining slides to remain on time. Had the chair of the session (this humble scribe) been more on the ball and quick witted, he would have seen the error of keeping this talk to time and insisted that Dennis elaborate on a slide describing the future of this software, which included an invitation for collaborators to help develop the software. This software seems to represent not only an opportunity to the TOF single crystal community, but also X-ray CCD based crystallographers in providing the freedom to interact and integrate their raw single crystal data in a highly flexible manner. Free software aficionados will note the GPL definition of the word "freedom" is being used here.

The final talk of the session was that of **David Duchamp** (djduchamp@aol.com), showing the latest feature of CrystMol (Mac and MS Windows - http://www.crystmol.com/) for visually comparing potentially similar molecules from different structure files, or within the same structure where Z' is greater than 1; and protein examples. People comparing polymorphs or a chemically similar series of structures could find this very beneficial and time saving. Molecules can be compared automatically; using a point and click menu; or via the CrystMol scripting system. RMS differences are also listed. Following is an example of CrystMol comparing the Z'=4 structure from S.Thamotharan, V. Parthasarathi, R. Gupta, D.P. Jindal and A. Linden (2004), Acta Cryst C60, o405-o407.



Besides thanking the speakers for their presentations, thanks must also go to the staff of the Hyatt-Regency, Chicago for their effective assistance in the set up of presenter laptops.

Lachlan Cranswick

X-Rays, Crystals, Molecules and You

THIS session, for high school students and teachers, occupying a full day (0830-1930) on Sunday(!) was attended by about 30 teachers and 60 students covering the USA from Vermont to Idaho and Alabama to California, but the majority were from the Chicago area, half being from the state of Wisconsin.

Course lecturers and Demonstrators. *Left to right: Katherine Kantardjeff, Alex McPherson, Tim Herman, David Goodsell, Karen Lipscomb and Frank Allen.*

The objective was to show the possibilities for getting younger people actively involved in crystallography, especially from a biological standpoint. The first part of the day featured talks about basic crystallography by Katherine Kantardjieff and the information available from the various databases by Frank Allen and Karen Lipscomb of the CCDC and David Goodsell of the PDB. Listening to these, I was a little sceptical that the students would be able to cope with the implicitly assumed background, but I realized later, on talking to some of them, that they knew a lot more than I was giving them credit for! Much of the backing for this session comes from a group called "Students Modelling a Research Topic", known, unsurprisingly as SMART. This was introduced by Tim Herman, who emphasized the importance of solid models in early training, making concepts easier for younger people to grasp. His firm, 3D Molecular Designs & MSOE Center for BioMolecular Modelling manufactures or distributes a remarkable range of model types including the computer-generated layer type illustrated on the cover of the March Issue of Crystallography News. The scheme started in Madison, Wisconsin, and has been successful in persuading both teachers and students to give up after-school hours to devote to research problems involving structure modelling.

The afternoon sessions were practical; while the teachers were shown how to crystallize lysozyme, the students had sessions using the databases. In the evening, the students defended posters of their own in the poster session, and asked some very good questions of other poster presenters.

I was very impressed with what I saw. Essentially, the scheme turns normal teaching on its head by emphasizing structure, using virtual and real models of all sorts, before chemical reactions or biological function. These topics can then develop from molecular structure. How widely it could work – and it certainly is time-consuming – I couldn't say, but the enthusiasm and the achievement of the students at this meeting were as solid as the models with which they were working.

Bob Gould

Teachers crystallize. *Jeanene Crenshaw and Tracy Blackman from Jefferson Davis High School, Montgomery AL.*

Students pulsing: *David Brown and Seth Flaaten from the High School, Whitefish Bay WI.*

Students (roughly S1 level) presenting their research findings: *Michael Ruka and Anthony Benz, St Dominic's School, Brookfield WI.*

Model building: *Richard Garratt and Tommie Hata*

BCA 2004 Spring Meeting

Small Angle Scattering Session

THE SAS programme really started on Wednesday morning during the Instrument Calibration session with a talk by Dr. Manfred Kriechbaum from the Institute of Biophysics and X-Ray Structure Research, Austrian Academy of Sciences, on Practical Aspects of SAXS in Industrial Research.

In this talk the technical features, setup and application fields of a modern laboratory small-angle X-ray scattering camera in industrial research were presented. Emphasis was put on the nanostructural information content of SAXS in condensed heterophase (porous) systems, very common in industrial research and quality control, where SAXS can be an excellent complementary and even superior method (with respect to gas sorption methods) for the determination of inner surfaces and interfaces, as it 'sees' also enclosed pores and can be applied to wet samples. Industrial laboratories are also often faced with the task of high-throughput screening of multi-component formulations where the SAXS method can quickly yield nanostructural information when the SAXS camera is equipped with a flow-through sample cell attached to an autosampler. Furthermore, there is also the possibility to combine SAXS simultaneously with another thermal or spectroscopic method (*e.g.* simultaneous SAXS-DSC measurements).

Starting the first parallel SAS session was **Vladimir Kogan** of PANalytical with a presentation entitled Comparative SAXS Measurements Performed by Different Techniques. Nowadays modern laboratory x-ray diffractometers are being considered as possible platforms to perform SAXS experiments, challenging the performance of dedicated systems. Vladimir presented the preliminary results of comparative SAXS measurements on polymers and bio-polymers, obtained using different experimental set-ups.

This was then followed by Manfred's second talk of the day; Time-Resolved SAXS Measurements at Synchrotrons. The high-flux and brilliance of X-rays from modern 3rd generation synchrotrons enable us to follow the nanostructural development, the supramolecular assembling or molecular mechanism of phase-transitions *in situ* and in real-time with a time-resolution in the millisecond time regime by small-angle X-ray scattering. As examples, a variety of such time-resolved experiments, mostly on biological samples, performed at the SAXS beamline at ELETTRA, Trieste, Italy, were presented. Among them T-jump and p-jump relaxation studies on phospholipid phase-transitions followed by time-resolved SAXS as well as individual setups and current limitations were discussed.

This was followed by **Mary Vickers** with Solid Polymers to Particles in Solution which covered topics as diverse as: Oriented lamellae in blown polyethylene film; Lamellar repeat distances, tie molecules and mechanical properties; Lyocell (Tencel) and voids; Hair and breast cancer; $CaCO_3$ in fuels & lubricants; and $PbZrTiO_3$ particles in suspension.

The final SAS session of the afternoon was from **Andrew Harrison** of Edinburgh University with "*In-situ* diffraction studies of microwave driven processes in materials chemistry and biology". Andrew described how microwave heating is becoming increasingly important as a method of driving chemical synthesis and materials processes, both in solution, and in the solid state. He also highlighted the increasing concerns about the possible harmful effect that such radiation - as used in mobile 'phones - may have on biological tissue, over and above what might be expected from consideration of the likely heating effects at low exposure level. However, both aspects of this field are served by almost no direct experimental measurements of the nature of such effects.

The team at Edinburgh University have developed several different types of microwave reactor that enable them to perform X-ray or neutron scattering measurements on powders, single crystals, colloidal and liquid crystal systems during microwave irradiation, and to measure temperature accurately and precisely. He described the principles of designing and operating such equipment, and described some of their work on colloidal growth, and the potential to use such methods to probe the possible effect microwave radiation may have on the structure of proteins and biological membranes.

Thursday 8th April saw the Small Angle session kicking off with **Dmitri Svergun** of the European Molecular Biology laboratory - Hamburg Outstation With Small Angle Scattering Studies of Biological Macromolecules in solution. Small-angle scattering of X-rays and neutrons (SAS) is a fundamental tool in the study of biological macromolecules. SAS allows one to study the structure of native particles in nearly physiological solutions and to analyse structural changes in response to variations in external conditions. The scattering data bears information about the overall shape and internal structure at a resolution of 1-2 nm. The method is applicable to a broad range of sizes, from individual macromolecules to multi-domain proteins and large macromolecular assemblies. Recent progress in instrumentation and data analysis significantly enhances resolution and reliability of structural

models provided by the technique and makes SAS a useful complementary tool to high-resolution methods, in particular, in large-scale structural studies. Advanced methods to analyse X-ray and neutron scattering data from solutions of biological macromolecules were presented including: *ab initio* low resolution shape determination; modelling of quaternary structure by rigid body refinement; *ab initio* analysis of medium-angle data to obtain domain structure from X-ray data; the use of specific deuteration combined with contrast variation in neutron scattering to construct detailed inhomogeneous structural models; addition of missing loops and domains to high resolution protein models; quantitative analysis of equilibrium mixtures of oligomeric proteins. Practical applications of the methods were illustrated by recent examples.

This was then followed by a chap called **Richard Morris** from Huntsman Surface Sciences, Oldbury with; "He Scrubs Up Well - Doesn't He?" or, New Aspects of Expanded Lamellar Surfactants - Aqueous, Sugar Based Exfoliates. Currently there are two types of body scrub available; aqueous and non-aqueous. Aqueous scrubs contain insoluble abrasives e.g. shells, seeds or pumice and are sold as pastes, gels or thickened emulsions. Non-aqueous scrubs contain soluble abrasives i.e. sugar and salt. Oils, glycols and silicones are used in place of water. The disadvantages of these products are that the aqueous scrubs are viscous, difficult to manufacture and the insoluble abrasives may lead to bacterial contamination. The non- aqueous scrubs are pastes, which have an oily or greasy feel, difficult to spread and are expensive. However, it is now possible to produce water based sugar scrubs! It has been discovered that surfactants can be made to form liquid crystals in saturated sugar solution.

We can see from the SAXS data that the inter-lamellar spacing is in the region of 500 Å. These liquid crystals can support additional solid particles of sugar. The solid sugar crystals are suspended indefinitely and act as an exfoliate. The presentation demonstrated the application of SAXS in the development of new surfactant technology and Richard also gave a brief demonstration of how to make your own sugar scrub from everyday chemicals found in the kitchen.

Marcus Winter from Bruker then followed with SAXS from multi-functional XRD instruments; NanoSTAR - The Universe of Nanostructure Analysis that described the new Bruker XRD instrument.

Richard Heenan of ISIS at RAL delivered the final morning session; SANS - Practicalities and prospects. Small angle neutron scattering, SANS, remains a powerful tool in many areas of science, despite many advances in X-ray instrumentation. Accelerator based, pulsed neutron sources, such as ISIS, are the way forward for the future of neutron scattering. Major new pulsed sources are under construction in the USA and Japan and a second target station, optimized for cold neutrons, is to be built at ISIS which will enable a new world class SANS facility within the UK. The advantages of pulsed source SANS were outlined and examples given of SANS science from both LOQ at ISIS and the continuous source D22 instrument at the ILL reactor in Grenoble. SANS contrast variation, using deuterated components enables unique information to be obtained on increasingly complex systems. Complex sample environment such as pressure cells, flow and shear cells and stop-flow techniques are readily available to map system behaviour rather than simply measure single structures.

Thursday afternoon saw **Pete Laity** from Cambridge with Scattering from segmented Co-polymers - a reinterpretation of SAXS data. Small-angle X-ray scattering (SAXS) has been widely used to study the microphase-separated morphology exhibited by polyurethanes, which arises through the immiscibility of 'hard' and 'soft' chain segments. The results are often analysed on the basis of a lamellar model, which appears to be justified on the basis of the expected volume fractions of 'hard' and 'soft' microdomains. Peter's recent work has re-examined the SAXS data from a series of segmented co-poly(ether-urethane)s, using a number of alternative morphological hypotheses. The results suggest that a lamellar interpretation might not be the best model for polyurethane systems. On the contrary, the scattering data obtained from the co-poly(ether-urethane)s under various experimental conditions could be reproduced using 'globular' scattering models of the Zernike-Prins or Percus-Yevick types. This suggested relatively small volume fractions of hard segment microdomains and a significant persistence of segmental mixing. Analysing the SAXS data by curve-fitting these models has revealed considerable new insight into the morphological response to deformation in these materials and indicated possible links to mechanical and thermal behaviour.

Next up was **Mark Farnworth** from Pilkington Glass with X-ray reflectivity in the glass industry. Mark described how the techniques of XRPD, GAXRD, pole figures and X-ray Reflectivity measurements can be used to examine samples from all stages of glass manufacture, from the crystalline raw materials to the amorphous final product. GAXRD is used to examine thin coatings on the glass surface of hydrophobic coatings, which disperse water. Refractory materials are examined to determine how much non-crystalline material is present and the amounts of quartz, cristobalite and tridymite. Also, multi-layer stack coatings are examined *e.g.* Ti ZrO_2 Ag Si. Texture maps can be produced which show the degree of texture in the silver layer of the coatings and the thickness, density, top and bottom roughness of each individual layer can be measured.

Finally, **Richard Clapperton** of Huntsman Surface Sciences, Oldbury gave a fascinating insight into the world of detergent research with: SAXS Interpretation of Deflocculated Vesicles - The Route to Superconcentrated Detergents. Richard described how liquid detergents contain concentrated solutions of surfactants and their phase behaviour determines the key physical properties of the detergent, such as viscosity and storage stability. Whilst the latter can be measured through techniques such as rheometry, and phase can be identified by optical microscopy, there are few tools available

to the formulator to characterize the liquid on a molecular level. Small Angle X-ray Scattering (SAXS) is a fast, versatile technique that enables the finer details of surfactant phases to be determined. This includes confirmation of phase type and measurement of phase dimensions, such as water layer thickness between surfactant bilayers. The effect of additives on phase structure can be monitored by SAXS, thus assisting product development. The challenge of achieving superconcentrated detergents has been greatly simplified by SAXS characterization.

This concluded the SAS sessions and everyone agreed that it had been an enjoyable and successful event.

Richard C.E. Morris

Instrument Calibration Session "How to be a star"

INTRODUCTION - Dave Taylor and Jim Kaduk - The opening introductory session was shared by Dave Taylor and Jim Kaduk (the new ICDD Chairman).

Jim explained the criteria for a star quality pattern in the ICDD powder diffraction file. Dave went on to cover the standards available for instrument testing including non-ambient calibration and gave a reminder of the lists maintained on the IG web pages. The rapid expansion of the Powder Diffraction File (PDF) is a significant factor in driving us towards better instrument alignment to ensure that phase identification software pulls up the right matches with the push to tighter search windows. The need for testing was demonstrated with examples from the IG Instrument Sensitivity Round Robin and a new spreadsheet will be available soon to automate checks. The basics of instrument alignment were then covered. Dave also announced details of a new low angle Round Robin based on a Ag Behenate film being launched by the IG this summer. Jim rounded off by explaining the procedures for submitting "star" quality patterns to ICDD for all those new compounds currently missing from the PDF database.

Aspects of calibration in SAXS

Manfred Kriechbaum covered the difficulties of calibration for SAXS measurements with nothing in the way of absolute standards. Rat-tail (tendon collagen) with a spacing of approximately 67nm is used for checks but it is not very stable especially to moisture. He also gave an overview of the role of SAXS at the Austrian Academy of Sciences.

The European XRPD Standard

Steve Norval explained the background to this standard. For XRPD, there are different instruments, techniques and applications. It is not the easiest technique to standardize. The motivations for putting together a 'standards' document include good practice, a point of reference for producing acceptable data and demonstrating competence. The title of the document is 'X-ray Diffraction from Polycrystalline and Amorphous Materials'. It has been put together by a working group of a technical committee of the European Commission for Standardisation. 'General Principles' and 'Procedures' documents were released in 2003 under the following codings: BSEN 13925-1 and BSEN 13925-2 respectively. The aim is to release a third document 'Instruments' this year - BSEN 13925-3. Beyond that, documents on 'Reference Materials' and 'Terminology' will be released. Steve gave an overview of the contents of the 'Instruments' document. It covers issues such as types, components, calibration and testing. For the control of a diffractometer there is component selection, component configuration, alignment and testing. Procedures have been established for calibration and instrument alignment/verification.

Lined-Up or Spot-On? The Ups and Downs of Diffractometer Alignment

Martin Vickers gave a very useful and practical guide to the alignment of the equipment at Birkbeck College which includes both transmission and reflection geometry. Good alignment produces accurate 2-theta positions, maximises intensity and produces nice peak shapes. Useful tricks and a well thought out approach, designed especially to assist Bruker Users in the tricky art of alignment, were well received.

Stress Instruments

Judith Shackleton gave a good overview of the approach required for residual stress analysis and stressed the importance of accurate results when measurements rely on very small changes in high angle measurements. Additional complications arise with the complex shapes of the components for analysis. Stress is calculated from Hooke's Law [Young's Modulus – Stress/Strain]. In effect, the crystallographic planes act as an atomic scale strain gauge. A stress-free standard is not required and the method is easy to carry out, however, the method is only sensitive to the top few tens of microns of a surface. She explained how an algorithm developed in conjunction with Rolls Royce was being applied to peened samples.

Calibration for Silver Halides

David Beveridge explained the problems associated with the photographic industry and the difficulties of resolving phases which requires the very precise measurements of a few lines at moderately high angles. Calibrations are required for peak position, width and peak profile. Peak widths are often variable and depend upon chemical variability, strain and grain size. Often in-house standards are required as calibration aids.

The session ended with the chair **Jeremy Cockcroft** thanking the speakers for their contribution to an interesting session.

Mark Farnworth

Other Meetings

South West Structural Biology Consortium

THE third annual meeting of the South West Structural Biology Consortium (SWSBC) was held at the University of Southampton on March 23rd and 24th.

The meeting began with a buffet lunch during which members of the consortium could talk to each other informally, followed by a brief welcome and introduction by the conference's host, **Jon Cooper.**

A smartly dressed **Alan Purvis** (Reading) was the first speaker. He described the -glucan phosphorylases and their role in carbohydrate metabolism, before focussing on starch phosphorylase from *Corynebacterium callunae* and the structural basis of its phosphate-dependent stability as a dimer. **Hazel Evans** (Bath) then spoke about her PhD work on the C3stau2 ADP-ribosyltransferase from *Staphylococcus aureus.* Comparison of her structures of this protein with those of related toxins shows some divergence in the mode of binding the NAD cofactor.

The third talk was an overview of structural biology at Exeter, presented by **Jenny Littlechild,** one of the main architects of the consortium. She mentioned Exeter's interests in structural enzymology, chemical biology and bioinformatics, and described two examples of the first of these. The opening session was completed by **Liz Hooley's** (Bristol) talk on mammalian MAP kinase inhibitory proteins and their plant homologues.

After a short break for refreshments and poster viewing, the programme of speakers resumed with **Kirsty Line** (Exeter). She continued a theme mentioned by **Jenny Littlechild,** describing her PhD work on α-lactamase, which was carried out in collaboration with Chirotech. **Claire Limpkin** (Bristol) described the structure of a Type II polyketide reductase and went on to propose a mechanism for its activation in which the active site opens by 19° upon association with an acyl carrier protein. **Nick Hopcroft,** now at Reading, spoke about some of his recently completed PhD work at the University of York. His talk concerned the binding of GAG and UAG RNA repeats to the trp RNA-binding attenuation protein of *Bacillus subtilis.*

After a short break, **Harry Powell,** one of two invited guest speakers, gave a very interactive and well received demonstration of the data collection and processing software Mosflm. The first day of the meeting ended with the conference dinner at the university staff club, including an impromptu speech by **Jon Cooper.**

The following day began with **Jorn Werner** (Southampton) giving an overview of his NMR work on adhesion proteins, a reminder that this was a general structural biology meeting rather than a purely crystallographic one. **Matthew Baker** (Bath) then spoke about superantigens and the different ways in which they can crosslink MHC class II molecules and T-cell receptors. **Gus Cameron** (Bristol) described how inhibitors of *Plasmodium falciparum lactate dehydrogenase* are being developed, with the aim of finding new antimalarial agents. He then went on to talk about the plasmodial ATP-dependent calcium transporter, which is the target of some of the antimalarial drugs already available.

Stephen Connelly (Exeter) continued the schedule of talks after the break, talking about his mainly molecular modelling work on *human pyrrolidone carboxyl peptidase.* **Matt Crump** (Bristol) spoke about combined crystallographic and NMR studies of proteins involved in polyketide biosynthesis, whilst **Isabel Moraes** (Reading) focussed on the expression, purification and crystallisation steps when talking about her PhD work on a *dihydroorotate dehydrogenase.*

The morning session concluded with a description of the opportunities presented by the new Diamond synchrotron, presented by the meeting's second invited guest speaker, **Louise Johnson.** She explained that three tunable beamlines would be available for protein crystallography from the first year of operation, with others becoming available in later years.

After a buffet lunch that served as a final chance to view participants' posters, **Lawrie Skipper** (Reading) gave a talk on the SUR1 protein and its involvement in diabetes. **Michail Isupov** (Exeter) described the use of an intrinsic zinc atom in a MAD experiment to determine the structure of another α-lactamase and **Simon Kolstoe** (Southampton) completed the meeting's talks with a description of his PhD work on the pentameric pentraxin blood proteins.

The meeting was then brought to close with a few words from **Jon Cooper** and prizes for posters.

Dalton Discussion 7, 5-7 July 2004, St Andrews

WE recently attended the RSC Dalton Discussion 7 meeting on 'Ionic and Electronic Properties of Solids'; for both of us this was our first experience of a conference based in 'chemistry' rather than 'crystallography'.

After a not-so-long but typically annoying journey on the great British rail system, we arrived in St Andrews to find weather somewhat better than that in Durham, though we were soon to discover than no weather system lasts long in coastal Scotland.

The structure of the program was slightly unusual in that, as the name suggests, it was based around discussion, with the majority of talks only lasting five minutes. This was a refreshing format as the shorter length of the talks made people focus on the critical, and most interesting, points of their work. The chairs did an excellent job of highlighting the points that tied the talks in each session together, and bringing up many questions which were then vigorously debated.

Keynote lectures were given by eminent researchers such as **Professors C.N.R. Rao, Jean-Marie Tarascon, Bob Cava** and **Dr. Martin Jones** (on behalf of **Prof. Peter Edwards**) and covered such diverse subjects as ruthenium oxides, phase separation in manganates, transparent conductors and properties of electrode materials. These provided a more in depth insight into these areas of chemistry than the short talks.

At the poster sessions, held jointly with the British Zeolite Association conference, we each presented posters on our PhD projects and received several helpful comments and suggestions from others. It was good to be able to view and talk about work on a very wide range of topics in an informal setting.

The conference dinner, held in the historic location of one of the older college halls in town, was very enjoyable, and was followed by 'ethnic entertainment', of Scottish musical nature, back on the campus.

Overall it was a very helpful meeting as it gave us a chance to see things from a more synthetic/applications than structural perspective, and brought up interesting points about material design. Hopefully there will be more involvement from sold state chemists at the next BCA spring meeting, as more interaction between these two closely related research communities can only be a good thing.

We are very grateful to both the PCG and the RSC who awarded us bursaries which allowed us to attend this meeting.

Full details of the scientific content of the meeting can be found in the forthcoming Special Edition of Dalton Transactions, which will feature papers from each of the speakers.

Matt Hampson & Clare Crossland

Diversity Amidst Similarity: A Multidisciplinary Approach to Polymorphs, Solvates and Phase Relationships Erice – Sicily, 9th-20th June 2004

I WAS delighted to be asked to give a talk at the 34th International School of Crystallography in Erice as I had heard so much about the quality of these meetings. On arrival at Palermo airport in Sicily, a team of very cheerful people wearing bright orange scarves who belonged to the meeting organising committee welcomed me. After a one hour coach journey we arrived in Erice which is a rustic but charming small village remotely located on a hilltop with beautiful views to the sea and vales.

The course successfully delivered the multidisciplinary approach planned. The applications of crystallography in polymorphism were extensively explored as well as other spectroscopic, computational and thermodynamic methods. The talks were nicely balanced, covering historical facts, relevant general principles, technique fundamentals and practical applications. In addition to workshops, where I got hands-on experience on some of the techniques, there were also useful "ask the experts" lectures. In these sessions delegates were encouraged to put forward questions and problems they are experiencing with their own work so that the experts in the field could help them with a possible solution. The diversity and overall quality of the posters presented was good and the actual poster sessions held outdoors as thankfully the weather in Erice allowed so. I was very nervous about my oral presentation titled "In-situ monitoring of crystallisation by energy dispersive X-ray diffraction" as it was my first time speaking at a meeting of this size. However other delegates and the organisers gave me a lot of encouragement and my talk went really well on the day.

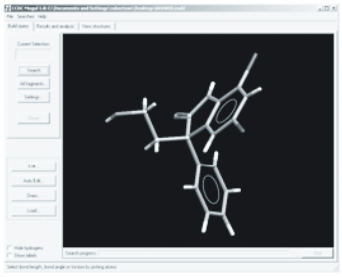
The social side of the meeting was also excellent. Erice locals were friendly and the atmosphere within the course was very informal and relaxed what made it easier to approach others. The organisers arranged different fraternisation events for most evenings and even an afternoon excursion to archaeological sites and to the beach. The long duration of the course made it possible for me to meet many other young and senior authorities in the field.

I am really thankful to the BCA and to NATO for their bursaries that allowed me to take part in this course that was a truly great experience. I learnt many new things that have helped with my work and I was sad to leave because I had thoroughly enjoyed it and met so many nice people.

Luciana De Matos

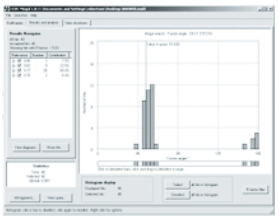
Press releases

Mogul - Easy Retrieval of Molecular Geometry from the Cambridge Structural Database (CSD).



THE Cambridge Structural Database (CSD) contains a wealth of experimental information on molecular geometries. However, accessing this information by means of conventional substructure searching can be time consuming. In consequence, these valuable data have been under-utilised. To remedy this situation the CCDC have developed a new program for the automated retrieval of molecular geometry data from the CSD, Mogul.

Mogul provides easy access to information on the preferred values of bond lengths, valence angles and acyclic torsion angles. The program uses a system of keys to encode the chemical environments of fragments (bonds, valence angles and acyclic torsion angles) in CSD structures. Use of a search tree indexed on these key values then enables the distribution matching any given query fragment to be retrieved, without the need for graph-based atom-by-atom matching. The search tree, together with a novel similarity calculation, also allows the retrieval of similar geometric features ranked according to a relevance score.



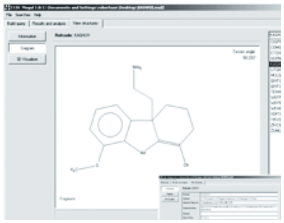
Histograms and summary statistics for retrieved CSD distributions are displayed interactively and the CSD structures that contribute to a histogram can be viewed. Searches can also be run automatically via an instructions file, thus providing a way of integrating Mogul with client applications.

Validation experiments indicate that, with rare exceptions, search results afford precise and unbiased estimates of molecular geometrical preferences (see: Retrieval of Crystallographically-Derived Molecular Geometry Information, Robin Taylor, submitted).

Mogul has many potential applications including:

- validating the geometries of libraries of modelled molecules or of newly determined crystal structures
- assisting structure solution from low-resolution (e.g. powder diffraction) x-ray data.

Mogul is now available as part of the CSD System, for further information please contact: admin@ccdc.cam.ac.uk or visit the CCDC website: www.ccdc.cam.ac.uk/products/knowledge_bases/mogul/



Gary Battle

International Centre for Diffraction Data

ROBERT L. SNYDER TO RECEIVE THE J.D. HANAWALT AWARD

THE International Centre for Diffraction Data takes pleasure in announcing that Dr. Robert L. Snyder, of Georgia Institute of Technology, Atlanta, Georgia, U.S.A. has been selected to receive the 2004 J.D. Hanawalt Award for excellence in the field of X-ray powder diffraction.

Dr. Snyder will present the Hanawalt Award Lecture entitled, "The Evolution of Total Pattern Analysis" at the 53rd Annual Denver X-ray Conference in Steamboat Springs, Colorado, U.S.A., 4 August 2004. The presentation of the award will precede the lecture.

The J.D. Hanawalt Award is presented every three years for important, recent contributions to the field of X-ray powder diffraction and phase identification published within the last several years. The award consists of a commemorative plaque, an honorarium, and travel funds to attend the meeting at which the award and lecture will be presented.

Previous recipients of this prestigious award include: Raymond P. Goehner and Joseph R. Michael, 2001; Herbert G`bel, 1998; Daniel LouNr, 1992; William Parrish, 1986; and Ludo K. Frevel, 1983.

Contact: Helen M. McDonnell
mcdonnell@icdd.com

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

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

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

2 September 2004
Workshop on Size/Strain and Quantitative Phase Analysis Software, Prague, Czech Republic, (part of above meeting)
www.lachlan.bluehaze.com.au/epdic-2004

4-8 September 2004
5th European Conference on Mineralogy and Spectroscopy (ECMS 2004) Vienna, Austria,
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
Symposium D of E-MRS Fall Meeting "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, Czech Republic
www.ssc2004.cz

14 September 2004
2nd Neutrons and Numerical Modelling Workshop: Student School, Institut Laue-Langevin, Grenoble, France
www.ill.fr/Events/N2M2

15-18 September 2004
2nd 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 Conference celebrating 30 Years of EMBL Hamburg. 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/congresso

21 September – 2 October 2004
VII School of Neutron Scattering "Francesco Paolo Ricci" Small and ultra-small angle neutron scattering: structural and dynamical studies.
Capra, Palau, Italy
www.fis.uniroma3.it/sns_fpr/>

1-8 October 2004
FEBS Advanced Course: Advanced Methods in Protein Crystallisation.
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

18-19 October 2004
SPINE (Structural Proteomics In Europe) Congress 2004, London
www.spineurope.org/page.php?page=home

18-20 October 2004
NOBUGS2004 Conference – New Opportunities for Better User Groups Software, PSI, Switzerland
www.ins00.psich/nobugs2004

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

29 October-5 November 2004
EMBO Practical Course on Solution Scattering from Biological Macromolecules, EMBL, Hamburg Outstation
www.embl-hamburg.de/workshops/2004/embo

10-13 November 2004
EMBO Conference on Structures in Biology, EMBL, 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

17-21 November 2004
SGO International Conference on Structural Genomics 2004 (ICSG 2004), Washington, DC.
(No website given)

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

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

29 November - 3 December 2004
Neutrons and X-Ray Scattering as Probes of Multiscale Phenomena, at the Materials Research Society Fall 2004 Meeting, Boston, MA, USA
www.mrs.org/meetings/fall2004

4-9 December 2004
Regional School of Crystallography and Diffraction, Havana, Cuba
www.cristalografia.net

6-7 December 2004
Micro- and Mesoporous Mineral Phases: Mineralogical, Crystallographic and Technological Aspects, Accademia Nazionale dei Lincei - Rome, Italy
www.icm3b.uhp-nancy.fr/cims/micromesoporous.htm

17-19 January 2005
Protein Crystallography in Drug Discovery: dedicated to structural genomics & proteomics, South San Francisco, CA, USA
www.protcrystconf.com

13-17 February 2005
Neutron Diffraction Characterization on Mechanical Behavior Symposium, Moscone Center, San Francisco, CA, USA
www.web.utk.edu/~hchoo/news/TMS05.html

14-18 February 2005
Australian X-ray Analytical Assn School AXAA 2005.
Fremantle, Perth, Australia.
www.pco.com.au/axaa2005

12-14 April 2005
BCA Spring Meeting, Loughborough
www.crystallography.co.uk

19-29 May 2005
Evolving Methods in Macromolecular Crystallography, 37th crystallographic meeting at Erice and a EuroSummerSchool, 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

3-7 July 2005
12th Convention of the Royal Australian Chemistry Institute (RACI), Sydney, Australia
www.RACIflyer.pdf

18-23 August 2005
IUCr Computing School (prior to the Florence 2005 congress), Siena, Italy,
www.iucr.ac.uk/iucr-top/comm/ccom/siena2005

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

27 November – 2 December 2005
International Conference on Neutron Scattering 2005.
Sydney, Australia,
www.sct.gu.edu.au/icns2005

9-18 June 2006
The Structure Biology of Large Molecular Assemblies: the 38th crystallographic course at the Ettore Majorana Centre, Erice, Italy
www.crystalerice.org/futuremeet.htm

7-17 June 2007
Engineering of Crystalline Materials Properties: the 39th crystallographic course at the Ettore Majorana Centre, Erice, Italy
www.crystalerice.org/futuremeet.htm