



BCA Administrative Office,

Gill Moore,
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 **March 2005** issue are sent to the Editor to arrive before **25th January 2005**.

Bob Gould

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

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BCA News December 2004

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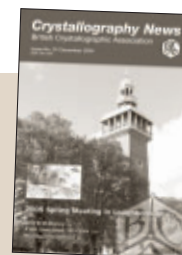
SR Summer School:



This month's cover:

Springtime in Loughborough where crystals have flourished since Pre-Cambrian times! Aside from fossils and bells, there will be a lot of science going on.

See pages 16 - 24



From the President



EDUCATION, EDUCATION, EDUCATION. An over-used and perhaps tired mantra, but one which reflects the driving imperative behind the status of the BCA as an Educational Charity. Of course, we are an organisation steeped in the delivery of Education;

arguably most of our activities can be regarded as educational in some sense. It is, however, vital in this modern world that one not only does, but that one records and publicises that one does.

For some time there has arguably been some confusion within the BCA and its membership of what "Education" means for our Association. Kate Crennell, for a number of years BCA Education Officer, worked hard in that position at delivering on an important part of that remit - what we have recently termed "early-stage" Education. It is clear, however, that delivery of our core remit at this point requires the evolution of a broader approach, underpinned by a coherent strategy. If one takes a moment to note down the Educational activities undertaken by the BCA in the last couple of years: Teaching Schools, Workshops, teaching-driven sessions at Spring Meetings, Young Crystallographers' initiatives, Crystal Growing events, etc, one arrives, over the full range of levels within the organisation, at an impressive list. To consolidate this, and promote the range of activity and to enhance it at all levels, needs a strategic approach for which the whole of Council, and the BCA subject groups, must take responsibility.

To help kick off discussions of such a strategy, with the agreement of Council, I convened a working group on Education comprising senior members of the community. The discussions were stimulating, the ideas and recommendations forward-looking, the conclusion that we do a lot but could do more; that we are currently not hitting all of our target audiences.

In the spirit of coordinating input from all parts of the BCA, and in developing a long-term strategy for continuing and enhancing delivery of our core remit, the President must ultimately be responsible. At its recent meeting, Council therefore agreed that in developing this strategy, for now I will be responsible for reporting to Council on educational

issues, with the specific responsibility to develop a future strategy in this area, and also to draw together, project and nurture our many current activities at all levels of our educational delivery.

To do this will require input from a range of people. From Kate Crennell, who we thank for her many years on Council as newsletter editor and latterly as Education Officer, and who we hope will continue from outside Council to provide her valuable contributions on early-stage education and archiving. From the subject groups. From individual members. And here we come to an appeal for input. How best to develop an Education strategy for the BCA? What is needed, what areas do we not currently deal with as fully as we might? To encourage you, our members, to engage in this debate, I will note here four possible ways forward emerging from the working group discussions: improved Teachers' resource pages on the web-site, focused on the curriculum; a sponsored "BCA expert gene pool" to deliver lectures to undergraduate science societies; expanded research level teaching content in Spring Meetings, continued harnessing of input from our "Young Crystallographers".

But there will be more, many more, suggestions. It is important that we develop this strategy in a timely manner - your thoughts, input and involvement are most welcome. As always, e-mails to president@crystallography.org.uk.

Enjoy this issue of Crystallography News, in which you will find many details of the evolving programme for the 2005 Spring Meeting in Loughborough. Vice-President John Finney has been working hard with his Programme Committee to develop this programme. I hope you agree with me that it looks exciting and tempting. As well as planning to come along yourself, why not draw this to the attention to colleagues who would not normally attend our Spring Meeting?

Finally, a sombre note. To lose giant Nobel laureates such as Francis Crick and Maurice Wilkins is sad and we mourn for their passing while also celebrating their achievements in long and distinguished careers. More shockingly, we record the sudden death of our colleague Sue Bayliss, at a tragically young age. An unimaginably sad loss, and one for which words are inadequate.

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
Department of Physics
& Astronomy
University College
London, 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. Andrea Hadfield
Department of Biochemistry,
University of Bristol
BRISTOL BS8 1TD,
Tel: 0117 928 7436
A.T.Hadfield@bris.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
Ms Judith Shackleton
Manchester Materials Science Centre
Grosvenor Street
MANCHESTER M1 7HS
Tel: 0161 200 3581
Fax: 0161 200 3586
judith.shackleton@man.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

Webmaster
Dr Jeremy K Cockcroft
School of Crystallography
Birkbeck College
Malet Street
LONDON WC1E 7HX
Tel: 020 7631 6853 (lab)
Fax: 020 7631 6803
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 7631 6853 (lab)
Fax: 020 7631 6803
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

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From the Editor



MUCH of this issue is concerned with the Spring Meeting in Loughborough, which is at an impressively good state of preparation. My particular thanks go to John Finney for his getting details to me so promptly and carefully - I hope that you will find the coverage here makes you want to be there!

As the President remarks, education is and must always be a hallmark of our Association. On behalf of Crystallography News, I am enormously grateful to Kate Crennell for her unflinching support in picking up educational matters and letting me know about them. I fervently hope that she will continue to do so, and, as always, I plead for more voluntary submissions from you, our readers. You'd be impressed at how high our publication rate is! Meantime, one of the features of CN is that we publish accounts of meetings from our bursars. In so doing, I hope we are helping them develop their communication skills and educating all of you as well!

There has been an absence of comment on Tony North's letter in the September issue on the subject of moving the pointer around on the screen in a Powerpoint presentation. Here is another call for suggestions. I, for one,

greatly appreciated the feature of the overhead projector (remember the overhead projector?) that allowed one to face the audience at all times while emphasising points on the foil with a simple pencil. Even then, however, there were some who preferred to wander around with a huge blackboard pointer to "make a point". Any ideas?

The main gathering since the last issue went to press was the excellent European Crystallographic Meeting in Budapest. The weather was a little on the damp side, but it was a good and well-balanced meeting, and there is certainly a lot to see and eat in Budapest! We have two accounts in this issue. Immediately after the ECM was EPDIC, the powder diffraction meeting, in Prague. I have been promised an account of it for the March issue.

As I mentioned last time, we are hoping to produce an issue in the IUCr Newsletter on Crystallography in Britain. (The current issue has an interesting offering on Russia.) I shall be coordinating this effort with assistance from John Evans (PCG), Andrea Hadfield (BSG), Georgina Rosair (CCG) and Judith Shackleton (IG). Any of us would be very grateful for any suggestions as to what should (or should not!) be in it.

Finally, I'm very grateful to John Bevington and Joan Halfpenny for their obituary for Sam Small. Sam was one of the founders of the BCA, and invariably a quiet, friendly presence at meetings. We miss him.

Bob Gould



Chick Wilson, Georgina Rosair, Jeremy Cockcroft, Judith Shackleton and Sandy Blake.



Bob Gould, John Finney, Elspeth Garman, Peter Moody, Andrea Hadfield, Christine Cardin and John Evans.

Puzzle Corner

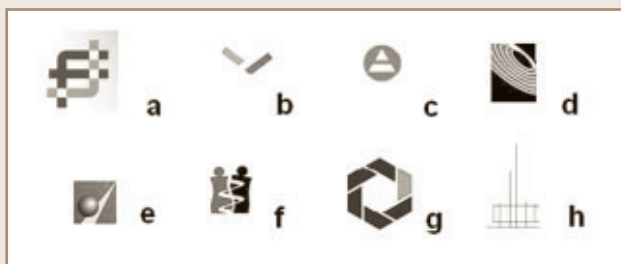
Congratulations, dear readers, last month's competition brought a bumper crop of entries! Most of them were nearly correct: our mystery crystallographers were:

1. Charles Taylor
2. Rosalind (Rosie) Franklin
3. Yvon Le Page
4. Sydney (Syd) Hall
5. Tiny (Herbert Marcus) Powell
6. Arnold Beevers
7. Lindo Patterson

Spelling CRYSTAL

The first fully correct solution was from **Richard Nelmes** - to whom congratulations. Various other people had helpful suggestions - one of the less helpful was improving the gender balance by making number 3 Yvonne Le Page. **Geoff King** gave a very good description of each, and several commented on having known several of them. Thanks to **Herbert Flack** for pointing out that there should be a space in Le Page. He also added: "PS Please Please Please Please Please get a new and better photo of yourself for page 4", which I hope that I have done.

Now for this month - this one was suggested by John Evans. Below are parts of the logos of eight of our corporate members. Can you identify them? Dare I suggest that this is a good time to have a look at our website? My apologies to other corporate members whose logos are unfortunately impossible to dissociate from their names!



From the Treasurer

I am not publishing the 2004 Spring Meeting accounts as usual in this issue. All the transactions this year went through the BCA bank account rather than the usual route of through a host University account. Consequently the Spring Meeting accounts will be an integral part of the full 2004 BCA accounts and be subjected to the scrutiny of our accountants. It is expected that a small 2004 Spring Meeting surplus will be announced at the 2005 AGM.

Dave Taylor - October 2004



BCA Corporate Membership

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

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

Gill Moore
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

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PANalytical
Rigaku MSC

Meetings

ACA Annual Meeting 2004 - Chicago

THE ACA MEETING was held at the Hyatt Regency centrally located in downtown Chicago within walking distance of many famous landmarks. However the number of potentially interesting presentations on offer ensured that much of my time was spent in the subterranean rooms of the Hyatt, considering crystallography.

The opening Sunday found me at the Interface between Powder and Single Crystal Diffraction, where **J. Kaduk** (BP) gave an insightful presentation into the determination of the crystal structure of guaifensin, a common expectorant, from powder diffraction data by simulated annealing. Problems with the Rietveld refinement highlighted errors in the conformation of the structure and quantum chemical geometry optimisation was required to ensure the correct conformation. Following on from this **S. Borrigger** (Purdue) discussed the phase transformations of Chloropamide. The crystal structure for form A was previously known and the structure of form C was determined from laboratory powder diffraction data by simulated annealing. Comparison of the two structures and consideration of the attachment energies for selected planes indicates a possible shearing mechanism for the interconversion. **R. Grothe** (UCLA) highlighted the information that can be obtained by consideration of texture from a sample and measurement with 2D detectors. The texture can be estimated from non-overlapping rings, which then can be used to reconstruct profiles in overlapping rings. After lunch, my time was split between the M.C. Etter Award

Session and remainder of the powder diffraction session.

L. MacGillivray (Univ. Iowa) was presented with the Etter award for his work on designing linear templates to direct solid-state reactivity and was followed by presentations from **W. Pennington** (Clemson Univ.) and **X. Wang** (Texas A&M) on the role of halogen bonding in crystal design, and the use of metal-metal bonded units to create geometrical shapes respectively. The powder diffraction sessions finished with **P. Lee** (APS) discussing the facilities available at the Advanced Photon source for powder diffraction and **W. Clegg** (Newcastle Univ.) covering microdiffraction at Daresbury station 9.8.

The transaction sessions, which ran over the Monday and Tuesday, were entitled: Crystals in Supramolecular Chemistry and further sub-divided into four sessions on Crystal Structure Prediction and Polymorphism, Crystal Growth Mechanisms, Crystal Structure Design and Applications of Crystal Design. The structure prediction session opened with presentations from **S. Price** (UCL) and **J. Bernstein** (Ben-Gurion Univ.) on the history and development of crystal structure prediction of molecular materials. **E. Pidcock** (CCDC) discussed a new model of crystal packing by considering the packing pattern of blocks of unequal size in a closed packed manner. Comparison with experimental structures in the CSD showed packings with a low surface area are preferred and the location of the molecular unit in the crystal system is constrained by the packing pattern. **Q. Gao** (Bristol-Myers Squibb) discussed a series of polymorphs and salt forms for an analog of MaxiPost. Finally in this session **R. Davies** (Univ. Texas) highlighted the role of thermomicroscopy in the phase analysis of co-crystal systems and the potential role of Hershfield surfaces in co-crystal analysis.

Call for Applications: The Jeffrey Award

A fund established in memory of George A. Jeffrey will be used to assist an outstanding student to attend the XX Congress of the IUCr to be held in August 2005 in Florence. Applications are invited worldwide. These must be from graduate students in good standing at the time of the Congress.

Applications must include:

1. A one-page letter explaining the student's background and any special circumstances in support of the application.
2. Letters of recommendation from the student's mentor and from one other person familiar with the student's crystallographic abilities and background. The mentor should state the expected date for the student's graduation.
3. A one-page biographical sketch of the student.
4. Copies of any reprints, preprints or abstracts in which the student is an author.
5. An abstract with the student as first author, which has been submitted for the program of the Florence Congress.
6. The student's e-mail address.

The original and two copies of the application (in English) should be mailed to -

B. Craven
Chemistry Dept.,
Indiana University of Pennsylvania,
Indiana, PA 15705, USA.

Applications must be received no later than April 27, 2005.

They will be judged by **B. Craven**, **H. Berman** (Rutgers U.) and **R. Stewart** (Carnegie-Mellon U.).

The important criteria will be the scientific excellence of the student's research, the student's financial need and the student's proficiency in English, the official language of the Congress.

The Jeffrey Award will cover at least the student's registration fee and the cost of student housing.

B. Kahr (Univ. Washington) initiated the Crystal Growth Mechanisms session, on testing Cairns-Smith's crystals-as-genes hypothesis by attempting to transfer screw dislocations from one crystal to another. **J. Swift** (Georgetown Univ.) then discussed the crystal growth of uric acid, the unregulated growth of which results in symptoms associated with gout. **T. Palmore** (Brown Univ.) and **C. Seaton** (Univ. Bradford) both discussed the directed epitaxy of molecular crystals. The first focused on inorganic complexes allowing crystals to grow with metal ions segmented into separate regions, while the second predicted organic interfaces by using the differential evolution algorithm. **R. Petrova** (Georgetown Univ.) and **J. Benedict** (Univ. Washington) ended the session with two short talks on the kinetic resolution of amino acids in agarose gels and optical molecular probes of crystal growth.

Tuesday was spent hurrying from room to room. The Crystal Structure Design and Applications of Crystal Design section of the Transactions sessions featured talks from **C. Åakeröy** (Kansas State Univ.) on development of supramolecular synthons for crystal engineering, **R. Rodgers** (Univ. Alabama) on using ionic liquids as a potential crystallisation solvent and **D. Braga** (Univ. Bologna) on the solid-solid and solid-gas synthesis of co-crystals. The final talks in this session covered the potential role of symmetry in crystal design by use of International Tables E by **J. Lauher** (State Univ. New York), while **L. MacGillivray** expanded on the applications of the systems discussed in his M.C. Etter award talk. Other sessions attended were Topics for the Young Scientist, where **F. Jurank** (Univ. California), **J. Kaduk** (BP) discussed careers in academia and industry while **N. McMillian** (Marshall, Gerstein and Borun LLP) covered Intellectual property and patents. In General Interest I, **D. Brown** (McMaster Univ.) highlighted the applications of graph theory in the analysis of inorganic solids to understand bonding.

Wednesday held the first sessions of the Trueblood Award symposium held in honour of **Richard Marsh**. They opened with the man himself giving a light-hearted review of the

developments in crystallography during his time, followed by **F. Herbstein** (Technion-Israel Inst. Tech.) on the various theories of first order enantiotropic solid-state phase transitions. **J. Bernstein** discussed the use of graph set analysis for the design of co-crystals. The Trueblood Award symposium continued the following morning with discussion of "Marshing" with **A.L. Spek** (Utrecht Univ.) giving an overview of problem and **F. Fronczek** (Louisiana State Univ.) covering the opposite problem of using too high a space group symmetry. This session concluded with **J. Glusker** (Philadelphia Univ.) highlighting the role that small molecule crystal structures and theoretical calculations can play in determining the role of metal ions in biological systems and **G. Battle** (CCDC) demonstrated Mogul, a new program from CCDC for rapid retrieval of molecular geometry from the CSD, covering both the computational work required to achieve fast searching and the potential applications.

The final session was General Interest III: Advances in Computing Environment for Crystallography, **A. Markvardsen** (ISIS) explained how the use of Grid computing allowed for the optimisation of control parameters for the application of the hybrid Monte Carlo algorithm to the problem of structure solution from powder diffraction data. The various parameter sets were farmed out to different nodes on the grid and the performance for each collected and analysed by the master node. **P. Emsley** (Univ. of York) wowed the audience with a real time demonstration of Coot's real time optimisation to electron density while adjusting the protein conformation. **D. Mikkelsen** (Univ. of Wisconsin-Stout) discussed the development of user-friendly software for the visualisation and reduction of single crystal TOF neutron scattering and **D. Duchamp** (Kalamazoo) demonstrated new features in CrystMol for molecular matching covering both small molecules and macromolecules in cases where there are multiple fragments in the asymmetric unit cell or polymorphic systems.

I would like to thank the ACA for inviting me to present my work at this meeting and the BCA for financial support.

Colin Seaton



22nd European Crystallographic Meeting, Budapest, Hungary, 26-31 August 2004

THE BURSARY awarded by the BCA contributed towards the cost of my attendance at the ECM-22 in Budapest.

I arrived a day before the official start of the conference to allow some time to visit many of the sights of the city. Unfortunately the terrible British weather of August appeared to have been packed in my suitcase, so much of the Thursday was spent dodging the rain, and “accidentally” locating the indoor market and its numerous cake stalls. The main shopping streets contained shops ranging from small, traditional shops to Marks and Spencers and C&A. During the week, I visited a number of the main tourist attractions, including St. Stephen’s Basilica and the Parliament building (the tour of the Parliament was particularly good). Probably the highlight of the tourist attractions would have to be a trip to the baths next to the Gellért hotel – amazingly relaxing and well worth the cost. I wasn’t so convinced with the rather attractive blue swimming cap/plastic shopping bag I was forced to wear though!

The opening ceremony of the ECM-22 was held at the conference centre and, after numerous welcome speeches, we were entertained by an excellent group performing traditional Hungarian music. What I expected to be a light buffet following the ceremony turned out to be an amazing spread of food and drink, a theme which continued in all tea breaks during the conference when a variety of drinks and cakes were available for delegates. The main (predominantly British no doubt) complaint was the severe shortage of “black” tea at the conference. As soon as tea break commenced, there would be a sudden rush of British people clambering for one of the few remaining cups of tea, to the amusement of the guy serving the drinks. A secret operation ensued involving the “borrowing” of teabags from hotels to ensure a good flow of tea during the day. I couldn’t possibly comment on which of the many distinguished scientists would have been involved in such blatant stealing!

The meeting was split into a series of parallel microsymbosia with two plenary sessions each day, which allowed for attendance of lectures on a wide range of subjects.

I presented a talk within the microsymbosium “Coordination chemistry: molecules and super-molecules” on the final afternoon of the conference. I was rather nervous; however, I have to be grateful to **Joe Reibenspies** whose talk preceded mine, as he had me laughing so much I forgot to be nervous! I am grateful to the ECM organisers for giving me the opportunity to present at such a big conference, and it was great to see other younger members of the BCA presenting at this conference, including **Iain Oswald**, **Anna Collins** and **Francesca Fabbiani**. Experience of presenting



at the Young Crystallographers’ satellite meeting at the Spring Meeting this year certainly appears to have given confidence to the younger crystallographers.

The conference dinner was particularly enjoyable and, uniquely, was held on a boat sailing on the Danube. Again, food and drink were aplenty and live music was provided for those that hadn’t eaten too much to dance! The view of Budapest at night from the top deck of the boat was beautiful. I really enjoyed the evenings, eating out at traditional and not-so-traditional restaurants. The evening concert performed in the Matthias Church was also amazing. It was lovely to catch up with people I had met in Durban last year as well as meet a whole new group of people. I’m looking forward to Florence already!

I am very grateful to the bursary committee for providing me with the financial support to allow my attendance at this very enjoyable meeting.

A review of some of the lectures I attended follows.

MS 31: Crystallographic Graphics Tools and User Interfaces

Clare Macrae (CCDC) gave an interesting talk on the development of the Mercury visualiser, a program I regularly use for the analysis of structures and the production of graphics. Clare highlighted the changes to the newest version of the program, to be released in the next few months. The ability to compare more than one structure in the same window was shown to be of use to researchers comparing polymorphs, while researchers analysing geometrical information such as torsion angles will find the ability to save this information in a spreadsheet format of great use.



Peter White (University of North Carolina at Chapel Hill) spoke on the problems of searching and locating archived data for structures dating back many years, long after the researcher responsible for producing the compound has moved on from the institution. Peter highlighted the need for institutions to implement a database-style archiving system with searchable fields and for the constant updating of the database.

MS 36: Chemical Use of Crystallographic Databases

Andrew Bond (University of Southern Denmark) presented on the occurrence of ring-stacking and ring-laddering of secondary ammonium halides in the organic solid state. Andrew highlighted the trend for the interactions within the stacks and ladders to be dependent on the steric demands of the R groups of the ammonium cation, and also on the directional properties of the $N^+ \cdots H \cdots halide^-$ hydrogen bonds.

Sam Motherwell (CCDC) presented on the use of the CSDContact database in the analysis of hydrogen bonding motifs, and showed the advantages of the database over similar searches performed using Conquest. For example, CSDContact allows the user to determine the average number of hydrogen bond contacts per atom, a search which would be tedious with Conquest.

Anna Collins (University of Oxford) spoke on the use of the program CRYSTALS in the comparison of structures having $Z'=2$. Anna described the use of the program to determine whether a structure contains pseudosymmetry operators.

Dirk de Ridder (University of Amsterdam) presented on the influence of ortho substituents on the twist angle of a carboxyl group with respect to the aromatic ring within a

molecule. This talk was particularly of interest, as I have carried out research during my PhD into the supramolecular assemblies of 1,2,3-trisubstituted carboxylic acid molecules, and have found similar effects in the twist angle of the central carboxylic acid group at the 2-position.

K6 Plenary Lecture

Jerry Atwood (University of Missouri-Columbia) discussed the concept of self-reassembly in the organic solid state, where self-reassembly involves a solid state to solid state rearrangement. Jerry used examples of calixarene structures to show such rearrangements do indeed occur, and highlighted the presence of two types of cavities in calixarene structures - continuous and non-continuous cavities - concluding that inclusion in one type of cavity can dictate inclusion in the other. Jerry also showed that the soaking of a crystal in a solvent in which the compound is not soluble can lead to crystal changes as the solvent moves through the crystal.

MS 24: Functional Supramolecular Assemblies

Gastone Gilli (University of Ferrara) began the microsposium with a very useful description of "smart hydrogen bonds", centring particularly on resonance and charge-assisted hydrogen bonds.

Michaele Hardie (University of Leeds) presented on the chemistry of cyclotrimeratriene (CTV), a rigid bowl-shaped molecule suitable for host-guest chemistry. Michaele showed examples of CTV acting as a ligand for group 1 metals cations, however derivitisation of CTV using pyridyl substituents increases the possibility for coordination to transition metals.

Iain Oswald (University of Edinburgh) presented on the attempts to produce high pressure polymorphs of compounds which match the predicted structures obtained from the CCDC blind tests. Iain discussed the methods of producing crystals using high pressure techniques and how the resulting structures compared to their predicted structures.

MS 29: Crystal Structure Validation: Challenges and Tools

Martin Lutz (Utrecht University) discussed the many sources of errors in X-ray crystal structure determination,



from crystal growth to crystal selection to data collection. Martin described the use of the software to validate the crystal structure, and also discussed the decision between obtaining data completeness or data redundancy.

Sandy Blake (University of Nottingham) gave a useful talk on the recent advances in structure validation using the CheckCif routines provided on the IUCr webpages. Sandy also highlighted a review of the submission procedures for Acta Cryst. C and E to allow interactive upload of figures after successful CIF submission rather than the email system used at present.

MS 23: Crystal Structure Prediction

James Chisholm (CCDC) and **Graeme Day** (University of Cambridge) both presented on the results of the latest round of crystal structure prediction blind tests. Both talks highlighted poor predictions with more complicated molecular structures, particularly those containing a greater number of hydrogen bond donor and acceptor groups, due to the increase in the options for the formation of hydrogen bonding motifs.

Sophie Dale (Loughborough University)

ECM22 - Materials Sessions

FROM the materials perspective there were a number of interesting microsymposia and keynotes at ECM22. These activities were organised in part by the recently formed Materials SIG12 led by Pam Thomas, of which more below.

The first main activity following Friday's opening lecture (on which I offer no comment) [*He gave it himself, very well - Ed.*] was a session on disordered materials chaired by Richard Welberry, which included contributions by many of the key contributors to this field. **Thomas Proffen**, author of the widely used DISCUS program, opened the session with a useful overview of the application of PDF analysis. The power of the technique is, as Thomas illustrated, the ability to investigate local correlations in a material. Thomas used the example of a powdered material containing 30% vacancies to illustrate this point. Bragg scattering, as analysed by the Rietveld method can't distinguish whether the vacancies are clustered or randomly distributed. This information is, however, contained in the diffuse scatter hidden in what's often merely considered as the "background" of the powder pattern. Thomas also described the application of long range PDF analysis (>100 Å) to studying 40 Å nanoparticles! **Thomas Weber** then described some imaginative and fascinating evolutionary algorithms for modelling diffuse scatter of molecular inclusion compounds and presented convincing arguments that a team of his evolutionary "ants" working competitively could model complex diffuse scattering patterns efficiently - provided they are kept "hungry"!

Dave Keen (Oxford/ISIS) then described Reverse Monte Carlo (RMC) and Molecular Dynamics (MD) approaches for studying cation motion and anion order/disorder phenomena in Ag_3SI superionic conductors over a wide temperature range. Dave expanded on these ideas and their application to the study of the dynamics of framework materials such as the piezoelectric GaPO_4 and SrTiO_3 in a second talk in Saturday's "Advances in Neutron Diffraction" session.

The disordered materials microsymposium was concluded with talks by **Susana Rios** of the Earth Sciences Department in Cambridge and **Mark Hostettler** of Bern. Susana described the amorphisation and phase segregation that can occur in materials such as ZrSiO_4 due to radiation damage, and Mark gave a clear explanation of the diffuse scatter caused by various models of stacking disorder in $\text{tris}(\text{bicyclo}[2.1.1]\text{hexeno})\text{benzene}$.

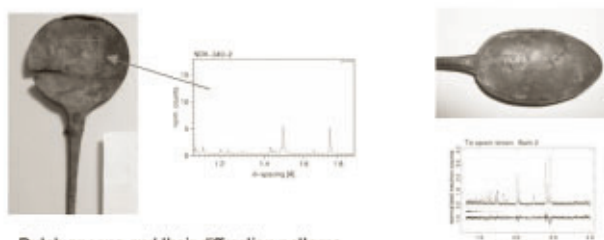
A second strong theme of both the oral and poster presentations was that of modulated materials. **Professor Petricek** (of Jana fame) had put together an excellent programme of speakers which celebrated the 40th anniversary of De Wolff's first publication on the structure of $\text{Y-Na}_2\text{CO}_3$. **Prof Aloysio Janner** gave an excellent overview of the importance of this contribution, as well as describing his recent work on geometric factors and their importance in biological and inorganic systems. A contribution from **Luis Elcoro** described an elegant application of superspace approaches to understanding the patterns of vacancy formation that can occur in both hypothetical and real materials. His "closest approach" geometric trick clearly could be applied to a number of packing/ordering phenomena in the solid state. Superspace arguments were also described by **Ivan Orlov**, a graduate student from Chapuis' group in Lausanne, who gave an equally elegant and clear description of how the structures of a series of complex hexaferrites could be described within a single structural framework.

The importance and prevalence of modulated structures was also brought out in Friday and Sunday evenings' keynote addresses by **Prof Van Smaalen** (Bayreuth) and **Malcolm McMahon** of the University of Edinburgh. Malcolm gave an excellent and stimulating overview of some of his recent work on the high pressure structures of metals. He described a number of fascinating modulated "host-guest" structures of the elements as well as touching on "simple" metal structures with up to 104 atoms in the asymmetric unit!

The materials SIG also helped organised a microsymposium on Saturday afternoon co-chaired by **M. Nespolo** and **Caroline Kirk** of the Natural History museum. Caroline presented work on identifying nitride inclusions in diamond and following hydration reactions using rapid laboratory microfocus diffraction methods. The session included a contribution on the use of neutron diffraction to probe the structure of tin spoons excavated in Amsterdam which was given by **Dirk Visser**. He showed how the non-destructive technique of neutron diffraction could be used to probe

the elements and alloys present in such spoons and in particular how the lead content varied with time, regulations and (presumably) the integrity of the manufacturer.

Jean Hodeau concluded the session with a fascinating description of "Rietveld Mapping" of fresco paintings. By collecting a series of diffraction patterns from 4000 pixels across the surface of the painting and performing Rietveld analysis of each, maps of the key pigments used across the painting could be created and a "crystallographic" image of the painting produced.



Dutch spoons and their diffraction patterns



Chemical uses of spoons, and some modern Belgian finger spoons

So, ECM22 contained some interesting science. Budapest is also a wonderful, cosmopolitan and beautiful city and was an excellent place to spend a sunny summer weekend at the end of August. Where else could one dine out on sauerkraut and "fowl skewer", with gipsy music in the background and the additional bonus of finding **Paul Raithby** on a nearby table? Were there any downsides to the meeting? Unfortunately, at least in my opinion, there was one. On several occasions the questions at the end of talks were overly "aggressive" in nature. Whilst scientific debate at a major meeting is vital, many of the instances I have in mind came from very senior members of the community following presentations by graduate students or young post docs and went beyond what I thought was reasonable scientific curiosity. This was something I hadn't previously encountered at a crystallography meeting and was (again in my opinion) both unnecessary and unwarranted. I hope not to see such things again!

Finally, on the subject of the materials SIG, **Pam Thomas** is currently coordinating a small group who will aim to promote the inclusion of various aspects of materials science at future ECM's. Further announcements and a web page will appear at some point in the future, but if people have suggestions or want to be involved in the activities of such a SIG I'm sure Pam would be delighted to hear from you!

John Evans

CCP4 Glasgow Protein Structure Workshop, "Heavy atoms - more than just a phase?", Galashiels, 1-3 September 2004

JOHN RAFFERTY opened the meeting on Wednesday afternoon with thanks to the sponsors and exhibitors, whose stands he encouraged us to visit, and a request to the audience not be shy with asking questions. He then handed over to **Neil Isaacs** as chair of the first session. Neil thanked John and his co-organisers (**Karen McClusky**, **Jim Naismith** and **Richard Pauptit**) for allowing him to enjoy this year's meeting without the pain of organisation, before introducing the first of the workshop's guest speakers.

Thomas Schneider, from the FIRC Institute of Molecular Oncology and European Institute of Oncology in Milan, explained how his program, ESCET, provides new tools for structure comparison by allowing us to quickly and easily superpose large numbers of structures in a meaningful way by automatically identifying 'invariant regions'. ESCET will be an essential aid to interpretation in these days of rapid structure solution, when one or two structures are no longer enough for a PhD thesis. **Nicola Ramsden** from Dundee followed with an introduction to structure-based lead discovery for the potential antimalarial target ispF, an enzyme from the parasite's isoprenoid biosynthesis pathway. Solution of co-crystal structures with a number of potential inhibitors showed that you can't always trust the results of docking simulations.

Axel Müller from York is working on the structural analysis of *Campylobacter jejuni* proteins involved in pathogenesis, and described the structure of the periplasmic binding domain of an ABC-type transporter of previously unknown specificity. Using the robotics available at the Oxford Protein Production Facility, he set up seven hundred crystallisation trials and, after some time, was delighted when an automatic e-mail alerted him to the growth of small, but well diffracting, crystals. Structure solution demonstrated serendipitous binding of cysteine at the active site, and consequently that the "approach from gene to structure to function is quite feasible". **Claire Middleton** (Dundee) closed the first session with the solution of the structure of the novel archaeal Holliday Junction resolving enzyme, Hje from *Sulfolobus solfataricus*. Claire is interested in that part of the resolving process "from the crossover down to the cleavage", and her structure goes some way to explaining the cleavage patterns observed for different resolving enzymes.

After a welcome break for tea, the afternoon session resumed under the chairmanship of **John Rafferty**, with **Andrew McEwan** from St. Andrews. Andrew continued the theme of archaeal DNA-modifying enzymes with his investigation into an archaeal DNA repair gene cluster: a work in progress. His work on the enigmatically named

protein 1399, which obligingly purifies “by the bucketload”, had so far led only to crystals that showed no diffraction, but were definitely protein; a situation no doubt familiar to many in the audience. Moving on to proteins 1439 through 1442, Andrew confessed to feeling once again close enough to “almost taste the structure”. A plea to the audience for help initiated an interesting and highly polarised debate as to the benefits or otherwise of seeding.

Remaining in the archaeal realm, **Jon Berrisford** from Sheffield described the structure of, and functional studies on, the novel *Pyrococcus furiosus* phosphoglucose isomerase (PGI). Jon’s structure confirms the metal dependence of the catalytic mechanism of the archaeal enzyme, a requirement which is not shared with the well characterised eukaryotic PGIs. **Daphne Kan** (Edinburgh) gave us a short account of her work on cyclophilin complexes, in which she has used crystal soaking and occupancy refinement to determine binding affinities for dipeptide substrates. **Marcos de Navarra**, from Brazil, currently a visiting student in Edinburgh, next presented an excellent overview of his work on iodine SAD phasing using a copper anode home source and quick cryosoaking derivatisation. He has used this method to solve two novel structures, including that of an enzyme purified from natural sources. A study of the effect of data multiplicity and resolution confirmed their importance for structure solution, and, particularly, successful autotracing.

Olivia Seator from UMIST then described her work on the expression of inwardly rectifying potassium channels, which she has chosen for structural study as they are the ‘simplest kind’ with only one transmembrane domain. Despite this, Olivia’s plans turned out to be “quite optimistic” and she apologised to the crystallographers in the audience for the molecular biology focus of her talk. She proceeded to introduce us to the delights of working with *Pichia pastoris*, a cheaper and easier alternative to using a mammalian expression system for the production of eukaryotic proteins. The session concluded with a valiant attempt from **Simon Hardwick** of Newcastle University to help us keep track of the complexity of proteins involved in the general stress signalling pathway in *Bacillus subtilis* and *Staphylococcus aureus*. His work is focussing on understanding the interactions between the various regulators of sigma B (Rsb) proteins in these two organisms.

The evening session, chaired by **Bill Hunter**, commenced with **Adrian Laphorn** from Glasgow, who convinced us that, nowadays, size doesn’t matter with his talk on small things (type II dehydroquinases) that come in big packages (multiple dodecamers in the crystal asymmetric unit...). Bill commented that “once upon a time every structure was like this, now only a few people are blessed with the opportunity” of tackling such challenges. **Changjiang Dong** from St. Andrews then presented the crystal structure and mechanism of a bacterial fluorinase, information that has been exploited for the synthesis of fluorine labelled compounds for use in brain imaging studies. **Paul Emsley** drew the official part of the first day to a close with an introduction to the trials and tribulations of developing his

molecular graphics program, COOT, entitled “COOT’s UI: wrong again!”. This was followed by a fun demonstration of the program’s capabilities in reading files, navigating around a structure, on-the-fly map calculation, ‘drag and drop’ fitting of residues to electron density (see BCA Autumn Newsletter, page 18), and locating and filling those “unexplained blobs” in your electron density map. Paul concluded with a request to the audience to think of COOT not as an “ugly water chicken”, but rather an eagle; “powerful, fast, elegant, free”, on which note further discussion was adjourned to the bar.

Thursday began with two excellent talks from the invited speakers, who were introduced by **Richard Pauptit**. **Thomas Schneider** gave a beautifully clear introduction to the theory of MAD phasing before moving on to discuss phasing using ShelX. “Things have moved a little bit in the past 5 years”, and phasing using ShelX is now as quick and easy as (ShelX)C, (ShelX)D, (ShelX)E. By use of numerous examples, both successfully solved and the still unsolved “protein from hell”, Thomas demonstrated that the key to solving your substructure is “to clean out the junk” from your data. **Gwyndaf Evans**, until recently of Global Phasing and now working at Diamond, again emphasized the importance of data quality to the success of structure solution. In his experience good quality data had not always equated with high multiplicity, and he illustrated this with numerous examples in his talk on phasing with triiodide solutions: Sharp and site-specific radiation damage.

After a brief break for coffee, we re-convened under the chairmanship of **Charlie Bond**, to hear an update from **Katie Evans** of Daresbury Laboratory on her characterisation studies of phytochromes from *Rhodospseudomonas palustris*. **Mads Gabrielson** from Dundee treated us to some Norwegian humour by way of introduction to the bifunctional enzyme ispDF, from the DOXP pathway of isoprenoid biosynthesis, another potential target for antiparasitic therapeutics. Analysis of the structures of the related monofunctional ispD and ispF enzymes allowed Mads to hypothesize, using an algorithm that he likes to call “arithmetic”, that ispDF should be a hexamer. The structure confirms this, showing a dimer of trimers where monomers are convivially linked by the “beta arm holding hands with its partner”.

Alex Theodossis from St. Andrews described his search for the determinants of the unusual lack of substrate specificity and stereoselectivity in *S. solfataricus* KDG (2-keto-3-deoxygluconate) aldolase. He has used the structure of this enzyme to pinpoint a number of targets for mutagenesis which he hopes will discriminate the ‘innocent bystanders’ from those residues actively involved in the catalytic mechanism. **Chris Anstey-Gilbert** from Sheffield posed the audience a “crystallisation conundrum” with his crystallographic studies on *E. coli* aconitase A, an iron-sulphur cluster containing protein, crystals of which, though perfectly reproducible, remain too small. His request for a “spectacular piece of advice” to help him grow larger crystals re-awakened the slumbering debate on whether or not seeding is the way to go. **Alastair McEwan** from Glasgow rounded off the session with an account of his

structural studies on plant glutathione S-transferases aimed at understanding herbicide and safener specificity.

A pleasant afternoon shinning up Black Hill with Lindsay, golfing with Gwyndaf, or kicking a football about with Karen, was followed by a splendid dinner of 'chicken-haggis'. We were then treated to a welcome reinstatement of the traditional after dinner speech, which was delivered by **Karen McClusky** assisted by the able script writing of **Magnus Althey**.

The final session on Friday morning commenced with **Lindsay Sawyer** announcing a last minute change to the program as **Julie Tucker** from AstraZeneca stepped in to deliver a talk on "top-secret" work solving the structure of the intriguingly named bacterial protein X..... This project had provided Julie with many interesting challenges, not least that of locating 96 seleniums. **Pierre Le Maguères** asked us not to shoot the messenger as he stood in for **Joe Ferrara** (unfortunately unable to attend) to describe new developments in Chromium phasing at Rigaku/MSC. **Jo Turner**, from York, has leapt "the phylogenetic chasm" in her bid to further understanding of the mechanism of viral assembly by studying the portal protein from the bacteriophage phi29. A little judicious protein engineering enabled her to improve the resolution of this large and rather beautiful tetradecameric assembly.

Emma Byres (Dundee) returned us to the search for effective antiparasitics with her quest for cocrystals of the mevalonate diphosphate decarboxylase (MDD) from *Trypanosoma brucei* with potential inhibitors. **Gareth Williams** from St. Andrews next recounted his success in carrying out structural studies of the two domains of ArnA, a bifunctional enzyme from bacteria involved in the synthesis of protective sugars. In contrast to the full-length enzyme (work which Gareth described at last year's meeting), the separated domains have proved most amenable to X-ray crystallographic investigation.

After a final break for coffee, **Jim Naismith** introduced **Tina Howard** from UMIST, who was overtaken by a "flurry of optimism" when she submitted her title, admitted that she hadn't quite got round to crystallisation, and so described the challenges presented by the expression, and purification of PSD95, a large, multidomain, membrane-associated guanylate kinase involved in the clustering of potassium channels in the postsynaptic membrane. **Buabarn Poonperm** (Edinburgh) continued the antiparasitic theme with a description of the crystal structure of phosphoglycerate mutase from *Leishmania mexicana* and the importance of bound metal ions for catalysis. **Antonio Ariza**, from Dundee, gave an account of his structural studies of RadA: an ATPase involved in the "wonderful" process of homologous recombination, which may provide a better model for eukaryotic recombinases than bacterial RecA. **Alex Merkel**, from St. Andrews, declined to tell us the story of EvaD, an enzyme involved in vancosamine biosynthesis in *Amycolatopsis orientalis*, referring us to her recent paper. Instead she gave us the tale of EvaA, a dehydratase from the same pathway, which remains a work

in progress as, despite overcoming the hurdles of expression and purification, her crystals don't yet diffract. **Mike Latcham**, from the University of Sheffield, drew the meeting to a close with his work towards molecular drug design using metallo-proteins. His first target, the miscellaneous Y gene product, YkuR, has been the 'bane of his life' for about a year, producing 'massive' crystals which reproducibly fail to diffract, whilst his second target, a methionine aminopeptidase with a "pitta bread fold", is proving reluctant to provide complex structures.

Next year's workshop will again be held at the Heriot-Watt University Scottish Borders Campus, School of Textiles and Design, Galashiels from 7-9 September.

Julie Tucker



Diamond Memorials?

IN OUR last issue (page 13) Kate Crennell wrote about the Firm LifeGem,

whose UK website is www.lifegem-uk.com, which offers to convert the carbon in cremated remains into a memorial diamond.

The process is certainly an interesting one, and is well described on the website. Kate, however, was particularly interested in where the carbon came from, as she (and I) had assumed that the carbon in the body was all converted to CO₂ in the process of cremation, leaving essentially calcium phosphate. A representative of Life Gem was interviewed on the Radio 4 programme Shop Talk on October 19, and did indicate that all the carbon in the coffin does indeed go in this way, but he, and the website, do maintain that it is carbon from the body which is converted to a diamond. To make a diamond weighing ¼ carat, that is 50mg, 200g of ashes are required from the approximately 3kg of ashes from an average person. From the website, the sentence which probably is most significant is the following:

The cremated remains are heated to extremely high temperatures under special conditions. During this phase, the carbon in the ashes coalesces with the natural carbon used in the diamond growth process, allowing the carbon from the deceased to be removed intact from the provided ash remains.

In other words, the quantity of carbon from the remains is unspecified, as is the proportion of "natural carbon" coming, presumably, from some other natural source.

Bob Gould

Bristol Protein Crystallography School

[Two students give their views! Ed.]

I WOULD like to thank all the people without whose help and support, the Bristol Protein Crystallography summer school 2004 would have not been possible.

It was the greatest opportunity for me, as a first year PhD student working towards solving structures of bacterial proteins using x-ray crystallography, to participate in this year's summer school and learn about a wide range of topics and areas that would definitely help me on my path towards solving structures.

I am very grateful to the lecturers who had travelled from far and near distances to provide us with their valuable information and experience. I would like to give a big thank you to **Professor Leo Brady** for organising the Summer school and making it an enjoyable week; a special thank you to **Elsbeth Garman** for her kindness to offer me the pair of gloves that she was recommending us all to buy in order to use when handling liquid nitrogen and a warm thank you to **Airlie McCoy** who helped us get through a flow chart we were trying to complete on the course.

The summer school provided me with both educational and social benefits and as well as learning great deal of valuable information, I was also able to meet and socialise with other people and make new contacts. I was personally able to get into a group of four people (including **Jitka Eryilmaz** from Birkbeck, **Yu Gan** from Reading, **Priya Rathinaswamy** from York and myself) and we spent several hours during the week (mainly in the evenings) getting to know each other and discussing the work we had covered during the lectures. This was very useful and it was interesting to see how different individuals with different backgrounds in the field came up with new ideas and suggested possible solutions to problems encountered by others.

We also had a chance to visit the Clifton suspension bridge, which was extremely beautiful with all the mountains and forests in the surrounding areas.

On the way back from Bristol, Jitka and I were fortunate to meet **Airlie McCoy** on the train towards London-Paddington where we got to further benefit from her suggestions and advice on some of the problems we were facing in our work.

Overall, this summer school was brilliant and I would sincerely thank everyone who made it happen. I would definitely recommend anyone who is in the field to make use of this wonderful opportunity and gain first hand advice and experience through meeting and listening to all the speakers and lecturers.

Arefeh Seyedarabi
(Queen Mary College University of London)



THE MEETING began on the Sunday afternoon with a session entitled "student stories", which consisted of five minute, two slide presentations by all of the delegates, briefly outlining their particular research areas. The student stories were broken up into four groups, interspersed with **Leo Brady's** short lectures on protein purification, expression and crystallisation.

The remainder of the week served as a comprehensive A-Z of crystallography, beginning on the Monday with excellent talks on X-ray sources, detectors, data collection, and a MOSFLM practical from **Elsbeth Garman**. The evening entertainment was a "cruise" around Bristol harbour, where our small vessel stopped at several pubs around the city allowing us ample time to fuel up.

Some of the delegates were a little worse for wear for Tuesday's talks on molecular replacement from **Jon Cooper** and **Airlie McCoy**, perhaps explaining why Airlie's simple explanation of maximum likelihood using dice seemed to confuse one or two people.

Wednesday started with a continuation of maximum likelihood, before a series of talks and computer practical sessions on phasing from **Martin Noble** and **Airlie McCoy**, covering maximum likelihood phasing, Pattersons, and MAD/SAD phasing.

Jon Cooper kicked off Thursday's sessions with a talk on phase improvement and averaging. Following this, **Paul Emsley** demonstrated the impressive Coot molecular graphics program in a practical workshop. The afternoon was rounded off by talks from **Nick Keep** and **Pete Artymiuk** on model refinement and validation, respectively, leaving us with sufficient time to scrub up for the conference dinner. The after dinner speaker, **Richard Pauptit** (AstraZeneca), gave a humorous summation of his scientific career to date, and then nearly all the delegates and tutors took a short trip into town to continue "scientific" discussions over a few more drinks.

Nick Keep's Friday morning session on other structural techniques gave a very brief introduction to techniques complimentary to crystallography, and the school finished with a short crystallography quiz. This was an excellent course for those new to crystallography.

Steven Hardwick
(University of Newcastle Upon Tyne)



Synchrotron Radiation Summer School 2004

CHESTER COLLEGE and Daresbury Laboratory played host for the second time to an international summer school in synchrotron radiation science in September this year. Six days of lectures and tutorials in Chester were followed by three days of practical sessions at Daresbury. Thirty research students and postdoctoral researchers came from a range of scientific disciplines, including physics, chemistry, materials science and engineering, biology, earth and environmental sciences, and from many countries in Europe and the Middle East, to take part. There was a particularly strong contingent from countries associated with the Sesame project to develop SR facilities in the Middle East.

Lectures and tutorials were given by synchrotron and other central facilities scientists from CCLRC (both Daresbury and Rutherford-Appleton) and the Diamond Light Source, and by major SR users. They covered topics in fundamental SR properties and operation, optics and detector systems, and relevant scientific theories and applications. We were very pleased to welcome **Professor Friso van der Veen** from the Swiss Light Source to give three keynote lectures. Apparently the students gave each of the lectures marks out of ten, but these were not published!

After a half-day break, which many of the participants spent in Liverpool, the SRS part of the school began with necessary user registration and safety training sessions, then each student took part in five half-day practical sessions in small groups, exploring various spectroscopic and scattering techniques, as well as having a tour of other SRS facilities. A final session included a look into the future, with topics such as free electron lasers.

The summer school was by no means all work and no play. The varied social programme included guided tours of Chester, a civic reception with the very friendly Lord Mayor, and a boat trip and barbecue. The highlight for most people was the medieval banquet at Ruthin Castle, with food served and entertainment provided by appropriately dressed staff, preceded by a journey through the hills of the Welsh borders on a sunny evening. We enjoyed fine



Not a lecture on synchrotron science!

weather throughout the time, even on the final evening in otherwise frequently damp Manchester for the closing dinner overlooking the airport runway.

The programme and facilities were scored generally very highly in a questionnaire completed by almost all the participants. Experienced SRS users will not be surprised that the lowest scores overall were for the catering at Daresbury, in contrast to that at Chester. Even the interruption of many of the practical sessions by beam problems following the SRS summer shutdown and restart did not prevent high marks for the experimental facilities. The social programme was narrowly beaten into second place for average score by the overall organisation of the school, and all said they would definitely recommend the school to others, almost everyone choosing the response "Enthusiastically".

The school's scientific programme was organised by **Bob Cernik** (Daresbury and Manchester) and **Bill Clegg** (Newcastle and Daresbury), and the social programme, together with most of the overall organisation, was once again handled magnificently by **Alison Hannah** (Daresbury), with support from **Stuart Eyres** and other colleagues. Stuart took large numbers of photographs, some of which were censored, but a collection can be found at <http://www.srs.ac.uk/summer-school/> and a few are shown here. We are very grateful to CCLRC, other UK research councils, and the EU for financial support.

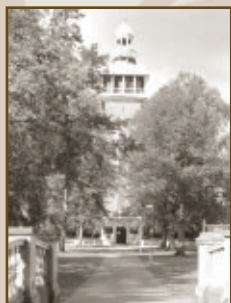
Bill Clegg



An attentive audience



Focusing on the sample



BCA 2005 Spring Meeting

Spring Meeting 12 - 14 April 2005 Loughborough University

THE UNIVERSITY of Loughborough, with its emphasis on sports science, is the location of our 2005 meeting. It's a modern campus university, within easy reach of the town. Loughborough is well served by road, rail and air. By rail it is only 90 minutes from London St Pancras, it is just 2 miles from junction 23 of the M1 motorway and 7 miles from East Midlands Airport, which has many scheduled domestic and international flights.

The BCA meeting itself starts at 10.45am on Tuesday 12 April 2005, and finishes with tea about 3pm on Thursday 14 April. There will be the usual Commercial Exhibition running from Tuesday to Thursday, and, of course, a poster session. As at UMIST last year, the posters and commercial exhibition will take place in the same area. This time, however, there will be a café in the corner of the exhibition hall to aid interactions with and between exhibitors, poster presenters, and participants generally.

The conference facilities offered by the University are excellent for both delegates and exhibitors. All scientific sessions, poster sessions and the commercial exhibition will take place in the James France Building. Building on the successful 2004 experiment with Satellite meetings on the previous day, there will be four such meetings on Monday 11 and the morning of Tuesday 12 April. Two of these will be workshops - one on White Beam Techniques, and another a hands-on CCP4 Workshop, while there will also be Daresbury XRD and ISIS CRY User Meetings. Tuesday morning's Joint Facilities User Meeting is another innovation. Issues will be discussed that are relevant to UK users of all the facilities. More details of these, and the main scientific programme, are given below.

For more information on the Exhibition and Sponsorship opportunities, or for any other enquiries about registration or accommodation, please contact Gill Moore at the BCA Administrative Office, 01355 244966 or e-mail bca@glasconf.demon.co.uk

Registration

Early Registration Costs (before 14 March 2005)

Full Registration:	£130.00
Student / Unemployed / Retired:	£ 65.00
Non-Member Surcharge:	£ 25.00
One-Day Registration (no concessions)	£ 65.00

Late Registration Costs (after 14 March 2005)

Full Registration:	£180.00
Student / Unemployed / Retired:	£ 65.00
Non-Member Surcharge:	£ 25.00
One-Day Registration (no concessions)	£ 90.00

Accommodation

Two types of accommodation are available at Loughborough University:

Standard B&B:	£ 28.00 per night
En-suite B&B:	£ 43.50 per night

All accommodation is located in the Faraday and Royce buildings in the Village area, a short walk from the main conference buildings. Breakfast and dinner will be served in the nearby Elvyn Richards Dining Room.

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

Catering

Morning coffee and afternoon tea will be served in the exhibition area, in the James France Building.

Breakfast and dinner (including the conference dinner) will be served in the Elvyn Richards Dining Room.

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

Packed lunch:	£ 5.50
Dinner on campus:	£11.50

Social Events

On Tuesday 12 April, The Poster / Exhibitors Reception will be held in the early evening. Wine and a Buffet meal will be served. Delegates will have the opportunity to meet with the exhibitors and poster presenters in a relaxed and informal setting. There will be no charge for the wine or buffet reception, but sponsorship is welcome.

The Conference Dinner will be held on Wednesday 13 April in the Elvyn Richards Dining Room at a cost of **£30.00 per person (£15.00 for students)**.

Car Parking

There is plenty of parking, free of charge, throughout the conference in Loughborough University grounds. Car parks can be found next to the James France Building and around the Faraday and Royce Buildings.

E-mail Facilities

Access to e-mail and internet facilities on designated terminals will be available during office hours in the Schofield building. Login passwords will be available from the Registration desk. Limited internet access is also available in the Halls of Residence for a small charge.

Abstract Submission

Submission of Abstracts will be electronic only. For instructions or any other queries, please contact Chick Wilson on bca2005@chem.gla.ac.uk. The Abstracts website will be: www.chem.gla.ac.uk/bca2005

Abstract Deadlines

Friday 14 January (Abstracts for consideration as contributed talks)

Friday 18 February (General abstracts and Bursary applications)

BCA Bursaries for BCA Spring Meeting

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

Council is again seeking commercial sponsors of Spring Meeting Bursaries at £155.00 per student and it is hoped that some Named Bursaries will be awarded at this meeting.

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

The closing date for all applications is Friday 18 February 2005. Only on-line applications via the BCA website: www.crystallography.org.uk will be accepted.

		Monday 11 April		Tuesday 12 April		Wednesday	
		SATELLITE MEETINGS					
08.30hrs				SATELLITE MEETING Joint Facilities User Meeting		In situ diffraction General (1)	Photocrystallography 1
10.00hrs				Coffee & Registration		Coffee & Exhibition 1	
10.30hrs				Opening Ceremony 10.45		In Situ diffraction Processing in industry	Photocrystallography 2
10.45 hrs	White beam workshop	CCP4 Workshop	Plenary session 1				
11.00 hrs							
12.00 hrs						AGM: Chemical Crystallography Group	
12.30 hrs	Workshop/User Mtg lunch			Lunch & Exhibition 12.30 - 13.30 hrs		Lunch & Exhibition 12.	
13.00 hrs						AGM: Physical Crystallography Group	Crystallography in Industry 1
13.30 hrs	White beam workshop	CCP4 Workshop	ISIS CRY Use Meeting	Plenary session 2		In situ diffraction General (2)	
14.00 hrs							
14.30 hrs						Tea/Exhibi	
14.45 hrs							
15.00 hrs	White beam workshop: tea & discussion	Tea		CCDC Prize Lecture		In Situ diffraction Central Facilities	Crystallography in Industry 2 15.00 - 16.00
15.30 hrs							
16.00 hrs	Daresbury XRD User Meeting	CCP4 Workshop	ISIS CRY User Meeting	Exhibitors' Forum		AGM:Industrial Group 16.00 hrs - 16.30 hrs	
16.30 hrs							
17.00 hrs						BCA AGM: 16.35 h	
17.30 hrs							
18.00 hrs						Prize Lec 17.30 hrs - 1	
18.30 hrs	Buffet for Workshops/ User Meetings/Council			Posters & Exhibition 18.30 - 22.00 hrs Buffet & Wine Reception 19.00 hrs		Conference 19.30 h	
20.00 hrs							

13 April		Thursday 14 April			
At and in the membrane	XRF: Liquid samples	Phase transitions 1 (Workshop)	High-throughput crystallography 1	Non-ambient pharmaceutical studies 1	XRF: Standards & calibration
0.00 - 10.30 hrs		Coffee/Exhibition 10.00 hrs - 10.30 hrs			
Modern techniques for crystal structure refinement 1	XRF Workshop: Awkward samples	Phase transitions 2	High-throughput crystallography 2	Non-ambient pharmaceutical studies 2	XRF: EDXRF applications
00 hrs - 13.00 hrs		Lunch & Exhibition: 12.00 hrs - 13.00 hrs			
Modern techniques for crystal structure refinement 2	XRF: WDXRF applications	Phase transitions 3	CCP14 workshop (hands-on session)		XRF: Combined XRF/XRD applications
AGM: Biol Structs Group					
AGM: Biol Structs Group 14.30 hrs - 15.00 hrs		Tea: 14.30 hrs - 15.30 hrs			
Modern techniques for crystal structure refinement: CRYSTALS WORKSHOP	XRF: Light element analysis				
00 hrs - 17.20 hrs					
Dinner: 18.30 hrs					
Dinner: 18.30 hrs					



BCA 2005 Spring Meeting
12 - 14 April 2005
Loughborough University
- Timetable of Events

Insight into Loughborough

THE MARKET town of Loughborough with a population of fifty thousand is the second largest town in the county of Leicestershire in the East Midlands.

It has a vibrant and thriving town centre. Attractions in the town include the Great Central Railway, Britain's only double track main line steam railway. Rides and dining on the steam trains are available. One attraction not to miss is Loughborough's unique war memorial in Queen's Park built in 1923 and incorporating the first grand carillon installed in Britain. The belfry of the 151ft tower was modelled on a medieval one at Moulins in France. It contains 47 bells, cast in Loughborough, ranging from 20lbs to 4 tons. A museum of bellringing is close to Loughborough in the heart of the English Countryside with the Charnwood Forest and the Peak District on the doorstep.

Crystallography and Diffraction at Loughborough University

Loughborough University has three Faculties; Engineering, Science, and Social Science and Humanities, the first two of which make extensive use of diffraction methods in their research activities. In Engineering, diffraction methods are used in many forms of materials analysis applicable to a variety of engineering projects. The Faculty of Science has three departments making major use of diffraction methods. In Physics, research is conducted in the fields of condensed matter physics, quantum structures and phase transitions, and materials physics and its applications. Many of the staff employ the techniques of surface EXAFS, grazing incidence X-ray reflectivity, normal incidence X-ray standing wave, and powder diffraction, with much of the work conducted

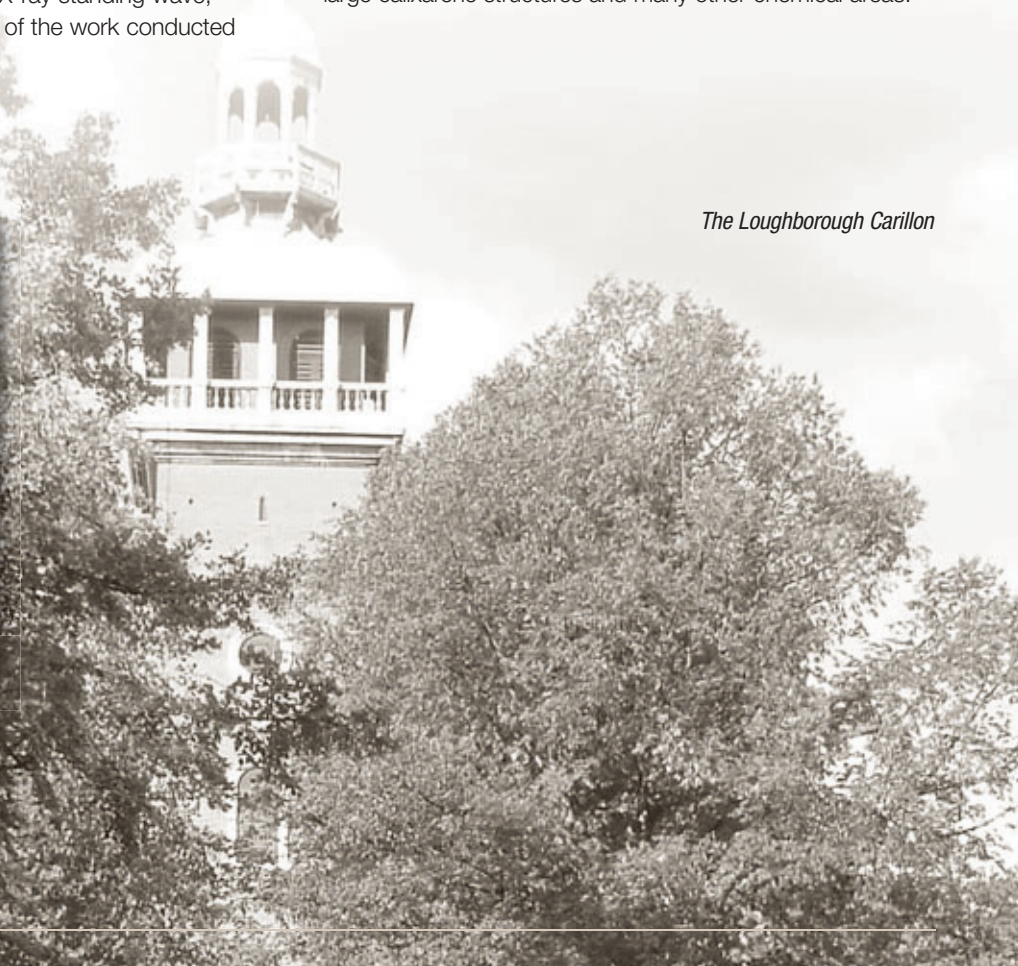


The local place to up your publications

at the SRS or neutron sources. The Institute of Polymer Technology and Materials Engineering (IPTME) is the home of the Loughborough Materials Characterisation Centre which has extensive facilities including powder diffraction, X-ray fluorescence, and small angle X-ray scattering which complement state-of-the-art equipment for surface analysis, advanced thermal analysis, and electron and optical microscopy. In Chemistry **Dr. Sandie Dann's** group run two powder diffractometers and make visits to neutron sources to support a range of solid-state materials projects including new pigments, zeolites, oxides and sulfides. **Prof. Vickie McKee** and **Dr. Mark Elsegood** jointly run two single crystal diffractometers and also use the SRS and ESRF to facilitate research projects in transition metal macrocyclic chemistry, large calixarene structures and many other chemical areas.



No deep-vein thrombosis in Loughborough!



The Loughborough Carillon

BCA 2005 Spring Meeting - Scientific Programme

“IN SITU and Non-ambient Crystallography” is the overall meeting theme that will be addressed in the four plenary lectures that open the meeting, and this theme is strongly evident in many of the other sessions. As trailed in the preliminary announcement in September's *Crystallography News*, an Exhibitors' Forum will provide an arena for exhibitors at the meeting to present their non-ambient and *in situ* kit in plenary session. By popular request following the successful teaching sessions and workshops last year (we never realised the space group diagrams in *International Tables* could be so popular!), there are a number of workshops planned, as well as teaching sessions integrated into the scheduled programme.

This year, we are particularly pleased to welcome participation from the RSC Solid State Chemistry group and the X-ray fluorescence community: the latter will be running a parallel session throughout the two days. We hope this will encourage interaction - and hopefully future scientific collaboration - between the two communities.

One further innovation this year follows on from the successful Young Crystallographers session at the 2004 UMIST meeting. The talk standard was impressively high - we want to have these talks integrated into the main programme this year so that everyone can hear them. So rather than set aside a particular session for talks by younger crystallographers, we are leaving slots unfilled in the programmes of the various sessions to be bid for. So when you submit your abstract (see details in an accompanying box), you will be asked to tick a box if you want your paper

Call for abstracts and bids for talks

AS FOR every BCA Spring Meeting, much of the discussion of new science takes place round posters. Please plan on showing a poster on your recent work, and encourage others in your group to do likewise - remember: posters mean prizes!

Please submit your abstracts on line at www.chem.glas.ac.uk/BCA2005

The deadline is Friday 18 February 2005.

This year, we have left open slots in the oral sessions for contributed papers from young crystallographers. We look forward to receiving bids for these slots - check out the sessions and see which one your talk will fit in to best! The bidding procedure couldn't be easier: when you submit your abstract on the web, just tick the tick box! Deadline for these bids is Friday 14 January 2005.



You could be speaking here next April!

to be considered for oral presentation. Your opportunity to wow us all!

Scientific Sessions

There is something for everyone in the eight sessions of the main scientific programme, plus the X-ray fluorescence strand and the workshops. This year there will be two Prize Lectures: the BCA Prize Lecture, given by an eminent crystallographer in honour of another eminent crystallographer, and the CCDC Prize Lecture. There will be a hands-on CCP14 Workshop, a CRYSTALS Workshop allied to the Modern Techniques of Structure Refinement session, and a WinGx 'interactive poster'.

There has been a significant expansion in the meetings that will run as Satellite meetings to the main BCA meeting. Monday 11th April will see two all day workshops, one on White Beam Techniques, and the other a hands on computer-based CCP4 Workshop. The afternoon of the Monday will also see ISIS and Daresbury crystallography user meetings, while a further innovation this year is a 'Joint Facilities' user meeting on the Tuesday morning where issues of common interest to users of the major central facilities to which UK scientists have access (SRS, ISIS, ILL, ESRF, and DIAMOND) will be discussed. If you want to attend any of these satellite events, just tick in the relevant box on the main meeting registration form.

Like all well-behaved liquids, the detailed scientific programme is now - thanks to the nucleating efforts of the various co-chairs - crystallising very well. The following summarises the planned sessions and the agreed speakers to date. It's particularly pleasing to see a good number of eminent scientists from outside the UK - this really will be an international meeting! Further details as they come available are accessible via the main BCA Webpage at www.crystallography.co.uk

Remember - we are leaving unfilled talk slots to be bid for by younger crystallographers! Submit your abstracts for posters and talk bids on www.chem.glas.ac.uk/BCA2005 Deadlines are 14 January 2005 if you want to bid for a talk slot, and 18 February 2005 for posters.

Plenary Talks

Phil Coppens (State University of New York at Buffalo):
X,Y,Z and Time: Introducing the time dimension in crystallographic research.

Malcolm McMahon (Edinburgh):
Pressure induced complexity in the elements.

Herbert Pöllmann (Halle, Germany):
XRD, XRF and in-situ investigations on anhydrous and hydrous cementitious materials - Some examples.

John Rafferty (Sheffield):
Structural studies of DNA Holliday junction resolvases.

Parallel sessions

In situ diffraction

(Co-chairs: **John Evans**, Durham; **Andrew Harrison**, Edinburgh; **Paul Raithby**, Bath; **Jeremy Cockcroft**, Birkbeck; **Steve Norval**, ICI).

Matt Rosseinsky (Liverpool):
In-situ diffraction in inorganic materials discovery and processing.

Poul Norby (Oslo):
In-situ synchrotron studies probing the synthesis/application of inorganic materials.

Mark Smith (Warwick):
The use of *in situ* diffraction to probe the processing of amorphous silicate-based materials from gelation to reaction with biofluids.

Pam Thomas (Warwick):
Synchrotron X-ray Studies of Ferroelectrics under applied Electric Fields.

Andy Dent (DIAMOND):
In-situ studies of heterogenous catalysts.

Simon Redfern (Cambridge):
How P modifies high-T disorder in oxides: observations with neutrons.

Gordon Tiddy (Manchester)
Title TBA

Geoff Moggridge (Cambridge)
Title TBA

Non-ambient Pharmaceutical Studies

Co-chairs: **Anne Kavanagh**, AstraZeneca; **Roy Copley**, GlaxoSmithKline)

Jeremy Cockcroft (Birkbeck):
Obtaining accurate non-ambient laboratory PXRD data for pharmaceutical studies.

Steve Cosgrove (AstraZeneca R & D):
Probing (de)hydration behaviour by high resolution X-ray powder diffraction.

Francesca Fabbiani (Edinburgh)
High pressure studies of pharmaceutical compounds.

Angus Forster (GlaxoSmithKline R & D)
The use of X-ray diffraction in the pharmaceutical development of a dihydrate API.

At and in the membrane

(Co-chairs: **Neil Isaacs**, Glasgow; **Steve Prince**, Manchester)

Bob Stroud (UCSF, USA)
Title TBA

Piet Gros (Utrecht, The Netherlands)
Translocation unit of autotransporter NalP from *N. meningitidis*.

Crystallography in industry

Co-chairs: **Judith Shackleton**, Manchester; **Mark Farnworth**, Pilkington; **Richard Morris**, Huntsman; **Martin Gill**, Natural History Museum)

Peter Laggner (Graz, Austria):
Title TBA

Spring Meeting Exhibitors Forum

FOLLOWING much demand from both our commercial Exhibitors and from the membership, 2005 in Loughborough will see a welcome return of the Exhibitor's Forum as a session at the Spring meeting.

Giving a short opportunity to address attendees in the lecture halls, the forum will provide each Exhibitor with the opportunity to present their latest developments and encourage participants along to their stands in the commercial Exhibition. It is serious, but entertaining and enlightening, and we encourage participants to provide a good audience for this valuable session, to be held following the Plenaries on the opening day of the main meeting.

Modern techniques for crystal structure refinement.

(Co-chairs: **Simon Parsons**, Edinburgh; **Charlie Bond**, Dundee)

Thomas Schneider (Milan):

Title TBA

Garib Murshoadov (York):

Title TBA

Charlie Bond (Dundee):

What's that blob? Identifying metal ions in protein crystal structures.

Bill David (ISIS)

Title TBA

Richard Cooper (Oxford)

Title TBA

A CRYSTALS workshop relating to modern refinement techniques will be held as part of this session.

Phase Transitions

(Co-chairs: **Pam Thomas**, Warwick; **Kevin Knight**, ISIS)

Jens Kreisel (Grenoble):

Pressure-induced phase transitions in piezoelectric lead-based perovskites.

Julien Haines (Montpellier)

Stability of the crystal structures of alpha quartz homeotypes at high temperature and at high pressure.

Photocrystallography

(Co-chairs: **Paul Raithby**, Bath; **John Helliwell**, Manchester)

Jacqui Cole (Cambridge)

Single-crystal X-ray diffraction studies of photo-induced molecular species.

Judith Howard (Durham)

Spin cross-over complexes: structures and photomagnetism of high spin, low spin and metastable states and the LIESST effect.

Eric Collet (Rennes, France)

The key role of X-ray diffraction for the investigation of photo-induced phase transitions.

High-throughput crystallography: more biology and new drugs

(Co-chairs: **Jim Naismith**, St Andrews; **Charlie Bond**, Dundee)

Stephen Burley (Structural GenomiX, USA)

Structure-guided fragment based drug discovery.

Samar Hasnain (SRS Daresbury)

Combined X-ray approach for studying metalloproteins function/misfunction : A powerful approach to Metallogenomics.

X-ray Fluorescence

(Co-chairs: **David Beveridge**, Ilford; **Dave Taylor**, BCA)

David Beveridge (ILFORD Imaging UK Ltd)

Determination of sulphur and chlorine in organic compounds by XRF.

Michel A. J. Davidts (Socachim-XRF Scientific)

Fusion for better analytical results in XRF analysis.

Graham Oliver (CTE, Ceram.)

Status of WDXRF in ceramic analysis.

Margaret West (West X-ray Solutions Ltd)

Setting the standards for calibrations.

Stanislaw Piorek (R&D Niton, LLC)

Field portable XRF for on-site screening and analysis of prohibited substances in plastics.

Martin Teasdale (GlaxoSmithKline)

EDXRF applications in the pharmaceutical industry.

Noel Thomas (WBB Minerals, Germany)

Combining XRF, powder XRD and structural modelling techniques: application to plastic clays and kaolins.

Latest programme information is posted on <http://bca.cryst.bbk.ac.uk/bca/ig/meet5xrf.htm>

Workshops

CRYSTALS

(Organisers: **David Watkin** and **Richard Cooper**, Oxford)

This will take place as part of the Modern techniques for crystal structure refinement session.

CCP14

(Organiser: **Richard Cooper**, Oxford)

This will be a hands-on workshop.

BCA
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Satellite Meetings

White Beam Techniques

(Contact: **Mina Golshan**, SRS Daresbury)

The workshop is expected to cover the following topics:

- Introduction to energy dispersive synchrotron diffraction
- Energy dispersive data analysis
- Engineering applications
- Tomography with white-beam
- RAPID TEDDI
- Small molecule crystallography with white-beam
- White-beam topography
- Behaviour and statistics for white-beam diffraction experiments

It will end with an open discussion.

CCP4 Workshop

(Contact: **Martyn Winn**, CCP4, Daresbury)

This will be a hands-on workshop.

Central Facility User Meetings

Two User Meetings will take place on Monday 11th April:

- **SRS XRD User Meeting** (Organiser: **Mina Golshan**, Daresbury)
- **ISIS CRY User Meeting** (Organiser: **Richard Ibberson**, ISIS).

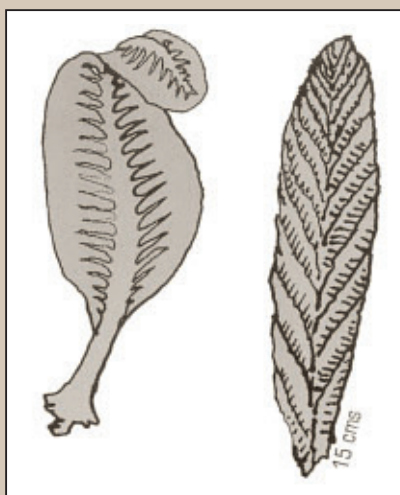
In addition, there will be a Joint Central Facility User Meeting on the morning of Tuesday 12 April to address scientific issues of interests to users of DIAMOND, ESRF, ILL, ISIS, and SRS.

BCA
2005
Spring Meeting

Try your hand at finding Pre-Cambrian fossils!

THOSE geologists amongst you will probably know that Loughborough sits on the edge of Charnwood Forest, which is famous for its Precambrian fossils. These are highly unusual – until recently, people were sceptical that soft body fossils of such age could actually exist. The Charnwood fossils, described as ancient sea pens, were discovered by a schoolboy in the 1950s - and named *Charnia masoni* after him.

Beacon Hill, which gives its name to the Charnia-bearing Beacon Hill formation, is within walking distance of the conference site. So after a pint or two, why not take a walk one evening to see if you can find a Precambrian fossil? Who knows? You might get it named after you also (*Charnia chickii*?? Mmmm.....)



Precambrian fossils, Charnia, from Charnwood Forest.



How Loughborough might have looked in Precambrian times...

Obituary

Ronald William Henry Small 1921-2004



“SAM” Small was born in Birmingham where his father was a builder who passed on many of his constructional skills. Sam’s scientific career began after he left school when he became an assistant in the Department of Chemistry at the University of Birmingham, working with Professor Gordon Cox. He studied part-time for a

London external BSc in Physics, followed by a PhD in Crystallography from Birmingham in 1947 and DSc in 1982. Although he had worked for Gordon Cox, Sam was never regarded as a “pippin” as he was not one of his research students, his PhD being supervised by F. J. Llewellyn after Cox had left Birmingham for Leeds.

Sam became a Lecturer and later Senior Lecturer in Chemistry at Birmingham and for nearly 20 years gave the course on general Physical Chemistry to new entrants and on crystallography to students in the final year. He was responsible for much of the practical Physical Chemistry throughout the programme for BSc. He had a lively interest in the students and their performance and he retained memories of most of the many hundreds with whom he had dealings.

When Gordon Cox left Birmingham, Sam set about re-establishing X-ray crystallography in the old Frankland building before moving into purpose-built accommodation in the new Haworth block. As for many crystallographers of that era, it was a case of do-it-yourself and adapting war-surplus equipment; the laborious hand calculations before the advent of computers were made somewhat easier by Sam’s construction of a machine, based on the rotation of gears and sliding of bars, for calculating \sin and $\cos 2(hx+ky+lz)$. This was later superseded by a well-worn set of Beavers-Lipson strips, and later still by use of very early computers including LEO and ENIAC. Sam and his research students were successful in their endeavours and their work became well known and respected, many of the students later obtaining lectureships in crystallography at other Universities or taking up research posts in the then new field of scientific computing. A very notable achievement of Sam while at Birmingham was his building of a complete 4-circle diffractometer and the associated HT generator and counting chain with the assistance of Steve Travers. The instrument was very accurate and led to the determination of one of the lowest R-values known at that time for a 3-D structure. Many modern instruments depend upon a closely similar design.

In 1964, Sam became one of the pioneers at the new University of Lancaster. He quickly established a working laboratory for crystallography in the temporary

accommodation in the former furniture factory of Waring and Gillow, before moving into the comparative luxury of the new buildings at Bailrigg, where an ICL mainframe allowed full advantage to be taken of developments in crystallographic computing. He was appointed to a Readership and with his research students worked very effectively up to and beyond his retirement in 1989. His last years were marred by Parkinson’s disease but he earned tremendous admiration by carrying on his work with courage and determination. It was a great disappointment when he lost his laboratory due to the University’s financially-driven decision to close Chemistry as an undergraduate course, despite Lancaster’s strong research performance and international reputation in polymer chemistry. Sam made sure that his remaining equipment was transferred to deserving institutions where facilities for crystallography had hitherto been limited. Thereafter he made use of instrument time provided by friends and former research students to obtain new data; like most crystallographers he also had a tremendous backlog of unpublished results to write up. Some of Sam’s most important studies involved explosives, in particular the polymorphs of HMX and complexes of RDX and BSX. Much of this work was regarded as highly secret and, to his regret, he was allowed to publish only a small part of his results. He was examining new complexes of HMX quite recently. His last publication was “An x-ray diffraction study of partially ordered electron density in clathrates of Dianin’s compound that include simple carboxylic acids” in 2003.

Sam was active in the IOP X-ray Analysis Group (later the Crystallography Group) and in the RSC Crystallography Group; he served as Secretary of both Groups at various times and was instrumental in organising many conferences. He played a major role in the formation of the BCA and in the organisation of the Inaugural Meeting at Durham in 1981; he was BCA Secretary from 1985 to 1987. Sam also had many interests outside crystallography: before his illness took hold, he was a keen player of squash and had earlier been an enthusiastic member of Kings Norton Rugby Union FC. He was interested in classical music and British birds and was accepted as an expert on Alpine plants, especially the genus *Primula*. He played a prominent part in the planning of sporting facilities and the introduction of a tutorial system at Lancaster. A few evening classes in Birmingham and a developing interest in the chemistry and crystalline properties of stoneware glazes led to Sam becoming an accomplished craftsman potter, manufacturing his own glazes for a multitude of useful and decorative hand-thrown items. The throwing wheel and kiln he constructed himself. As well as supplying his own household and those of friends and relatives with plates, bowls, coffee services and the like, he sold many items in aid of charity. After moving to the North West, the family first lived at Gressingham in the Lune Valley while their house at Denny Beck was being built. Sam turned his new garage into a pottery, and a field into a garden which was the envy of all who saw it.

Sam’s wife Mary died in 1991. He is survived by their three sons Nicholas, Richard and Jonathan and by his brother John who farmed in Pembrokeshire.

John Bevington and Joan Halfpenny

Books

Light is a Messenger; The Life and Science of William Lawrence Bragg

Graeme K Hunter

Oxford University Press, 2004

Price: £35.00 (hardback)

ISBN No. 019852921X, 322 pages.

THE THOUGHT has never crossed my mind that it would have been interesting to have had the chance to meet **Isaac Newton** or **Albert Einstein**. In the case of **Sir Lawrence Bragg**, who died in 1971, my entry into crystallography in 1974, just 3 years later, makes it somehow galling to have been so close, and yet so far, in time to have seen him in action. Obviously my point here, in mentioning **Newton** and **Einstein** in the same breath, is that he is such an iconic figure in the whole development of X-ray crystal structure analysis, and the many discoveries with which **Bragg** was closely involved in, that I feel one must rank him in the **Newton** or **Einstein** league in the history of science.

The author of this biography immediately explains his reason though for writing on **Sir Lawrence Bragg** ('**Bragg**'), which is that **Bragg** is still the youngest ever Nobel Prize-winner and that fact alone makes **Bragg** an icon. There is a 'however' though, which is that **Bragg** was Nobel Prize-winner in 1915 jointly with his father, **Sir William Henry Bragg**. His father specialised more on crystallographic instrumentation and apparatus, and was also preoccupied for several years in the early 20th century with the idea that X-rays were corpuscles rather than waves. But, skipping on a few years, and to press the point about the strength of this father and son team, they agreed to split the world of crystal structure analysis into organics for the father and inorganics for the son. **Sir William Henry Bragg** died in 1942 and **Bragg** broke away into the biological (organic!) world when he moved to Cambridge from Manchester to succeed **Rutherford** in 1938. Unexpectedly, **Bragg** teamed up there with **J D Bernal's** former student **Max Perutz**. Together they pioneered the development of protein crystallography until, with **Kendrew**, the protein structures of haemoglobin and myoglobin were eventually determined in the late 1950s. On the way, also under **Bragg's** patronage, **Watson** and **Crick** determined the DNA double helix structure in 1953, based on the fibre diffraction data from Kings College (**Franklin** and **Wilkins**).

This is a very quick sketch of the story, but leaving out the major precocious moment in 1913 of a very young **Bragg**,

i.e. as a Cambridge postgraduate, firstly deriving what became known as **Bragg's law** and then also deducing the first crystal structure, that of sodium chloride. **Bragg's** father meanwhile, converted to X-rays being waves by the crystal diffraction grating results of **Laue** in 1912, built the first X-ray diffractometer. **Bragg** is quoted by the author as referring to "the superior nature of data from your diffractometer, Dad,". This and many others are amongst the jewels of quotations that the author sets before the reader.

Indeed, the author has clearly worked extremely hard on this book. The title itself, a very good one, is a quote of **Bragg** from what seems to me a rather obscure lecture he gave in 1928; the full quotation being "Light is a messenger, carrying a story about the form of the object....". A proper measure of the author's labours though, rather than saying he had read even the obscure lectures, are in the 1008 historical references at the back of the book, and numerous further footnotes throughout the book. These not only list numerous archived letters of **Bragg** and others but also interviews with a variety of key players. One has a growing feel of privilege at reading this carefully prepared biography.

There were also tricky details for the author to get right, specifically the tensions between father and son, in spite of the obvious filial devotion that I have touched on already. Obviously, as someone who did not see this all unfolding I was left feeling that the author had given a credible, evidence-based treatment of this important aspect of **Bragg's** life story. But the author pushed this too far, I felt, in extrapolating to **Jim Watson** being seen by **Bragg** as equivalent to himself as the young overlooked genius behind the DNA double helix (with **Bragg** viewing **Crick** as playing the equivalent role of his father, in danger of getting all the credit).

I was surprised to learn that **Bragg** was subjected to bouts of depression and angry outbursts. This was brought out in several places in the book, with footnote evidence back up. I suppose I didn't want to believe this, spoiling as it did my rosy view of one of my science heroes. However I did already know that **Bragg** had had a nervous breakdown. Anyway, the genial smiling character on the front cover of this book doesn't reflect this aspect. Also, my prior readings of **Bragg** anecdotes, admittedly only two, from *A Random Walk in Science* (published by IOP) showed that **Bragg** had a keen sense of humour.

There were some aspects of the book that I didn't like. The exposition of the crystallography was overly long in the early chapters, I felt. Like **Bragg's** aunt, of a later chapter, who hadn't a clue when **Bragg** tried to explain his latest crystal structure, I could imagine that non-scientists reading

this book would be equally baffled by these details of the science. I am also still mulling over the tactic of not gathering the family life details of Bragg, as a father, into one chapter; it seemed on several occasions that the author had to mix this into many chapters to ease the science details along. The family details deserved a better focus. [The advantage for the author was of course to keep a strict chronology of the story.]

In retrospect, Bragg had three distinct career phases. These came after the precocious beginning and the First World War when he was a Major leading a team doing sound ranging to pinpoint the enemy guns. There were his Manchester period (1919 to 1937), his Cambridge period (1938 to 1954) and then the Royal Institution period (1954 to 1965). Manchester itself was thoroughly slated. The most memorable anecdote was that the fog was so thick it even prevented seeing the stage from the back of the theatre! Altogether, Manchester was apparently a dirty, grimy, indeed uncivilised place. Bragg's wife was glad to leave Manchester behind when moving south. [What a difference a few decades makes - Manchester today has no fog, has stone-cleaned buildings, and is a cultural scene of thriving orchestras, theatres and national sports facilities!]

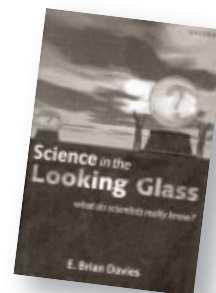
For anyone interested in the history of how our subject has come to where it is today, this book offers a feast of interesting details. In addition to the above history one must highlight the fascinating ins and outs of Bragg's rivalry with **Linus Pauling**. As one example, I mention their battle over their respective Nobel Prize nominations, leading up to the 1962 Nobel Prize awards for Perutz, Kendrew, Watson, Crick and Wilkins. This is revealed by the letters Bragg and Pauling wrote to each other, and into the Nobel Foundation, at the time. [Bragg won that tussle....]. There are also Bragg's major achievements in enthusing schoolchildren in science and discovery through his lectures, especially but not exclusively, in his period as Director of The Royal Institution.

As I arrived at the end of the book I admired the way in which the author left the last words on Bragg to **David Phillips**, who had worked with Bragg at the RI, by quoting from Phillips' Biographical Memoir of Bragg for The Royal Society. Indeed those last pages of this biography brought a crescendo of feeling about this great scientist and person, Sir Lawrence Bragg, whom I would never be able to meet; so close in time to the start of my career and yet so far. I was grateful for this book because I felt I had really got to see the person who had driven the science.

John Helliwell

Science through the Looking Glass - What do Scientists really know?

E. Brian Davies, King's College London
Oxford University Press, 2003
Price: £25.00 (hardback)
ISBN 0198525435, x+295 pages.



THE PHOTOGRAPH of the author on the dust jacket is a good introduction to this book. The author's enigmatic and attractive smile indicates that he is going to cover a huge number of topics and persuade his readers that they know a great deal less about them than they thought they did. In the meantime, he is going to have a great deal of fun, and to make sure that his readers do too!

In the preface, Brian Davies, himself a mathematician, makes this prediction:

In spite of the fact that highly mathematical theories often provide very accurate predictions, we should not, on that account, think that such theories are true, or that nature is governed by mathematics. In fact, the scientific theories most likely to be around in a thousand years' time are those which are the least mathematical - for example evolution, plate tectonics, and the existence of atoms.

And in all of his brushes with theories and theoreticians, philosophers and theologians, theories with which he disagrees are treated with respect and moderation. About the only time he uses the word anger is on page 72, where he presents a problem that is impossible to solve and comments:

I frequently hear mathematicians saying that such questions pose no problem 'in principle'. This phrase makes me quite angry. It might mean, 'I know it is not actually possible but would like to close my mind and pretend that I could do it if I really wanted to'. Another possible meaning is, 'I do not regard the difficulty of carrying out a task as an interesting issue.' Either interpretation leaves the speaker cut off from the mainstream of human activities.

Such attitudes make this reviewer angry too!

The book is a good mix of mathematics/science with linguistics/philosophy. There are chapters dealing with pure mathematics, probability theory, astronomy, geology and biological evolution, exploring the nature of knowledge about them. There must always be some mistake for a reviewer to find somewhere in a book, but I certainly have not spotted many. I can do no worse than point out that Davies is wrong in stating (p 211) that ^{13}C is a radioactive isotope. This isotope is indeed responsible for a lot of our knowledge about the world, but precisely because it is not radioactive! These "scientific" chapters are enclosed between the outer chapters on language and reductionism, and the whole is both convincing and enjoyable.

The final chapters are, naturally the most speculative. He attempts to explain the difference between “empiricist” and “realist” theories of science, and has to be content “with a description of science as it now is, and to attribute goals only to individual scientists.” (p. 270). One of the most delightful bits occurs in the discussion of anthropic principles, where Davies points out how easy it is to produce a bogus coincidence, and he supplies the one that he “found ... by playing around for a few minutes with powers of pi”: It concerns the ratio of the masses of the proton and the electron: $m_p/m_e = 6\pi^5$, with an in error of less than 0.002%. This is a matter which needs to be emphasised in all fields. Probably the most elegant spoof of all of this genre is R.A. Knox’s “proof” from remarkable cryptograms that Tennyson’s In Memoriam was actually written by Queen Victoria (*Essays in Satire*, Sheed and Ward, 1954).

His humane approach is gently put on p. 253: “Science is a system of thought, and should not claim to have a monopoly on the truth. But neither can its achievements be dismissed as of no import.” This has come a long way from Sigmund Freud’s noted summation: “No, our science is no illusion. But an illusion it would be to suppose that what science cannot give us we can get elsewhere.” (*The Future of an Illusion*, 1927).

Finally, a quote from p 213:

The most severe criticism of extreme religious fundamentalism is not that it is wrong (scientists are also sometimes wrong), but that it discourages people from trying to understand the marvellously complicated world around us.

For those who do wish to understand more about this world, here is a book that can be strongly recommended.

Bob Gould

Structure and Dynamics: An atomic View of Materials

Martin Dove, University

Oxford University Press, 2003

Price: £24.95 (paperback), **£47.95** (hardback)

ISBN 0198506783 (PB); 0198506775(HB) 352 pages.

THIS BOOK in the Oxford Master Series in Condensed Matter Physics is a very welcome addition to the armoury of textbooks in this area. It is particularly refreshing to see in the title the words “an atomic view” since so much of the emphasis in physics teaching is on the electronic view with the atoms simply providing a periodic (in the case of crystals) backdrop.

In this book, the author provides a clear, cogent and relatively self-contained late undergraduate (I would say third or fourth year)/first-year postgraduate grounding in the essentials of crystallography, crystal physics, lattice dynamics and phase transitions. Discussion of structure and bonding takes the first five chapters of the book, progressing from packing arguments to formal crystallography, including a nice summary of point group and space group symmetry. It is a pleasure to see

structures such as TiO_2 , ZrP_2O_7 and perovskites under discussion in a physics text-book – progression beyond the crystal structures of NaCl and diamond is a welcome advance! Furthermore, sections are included on disordered and amorphous materials too, and one of the examples of from the Diffraction chapter (Ch 6) is the structure of glasses from neutron scattering, an example that will disabuse physics students of the myth that diffraction techniques are only applicable to crystals.

From Chapter 7 onwards, the emphasis of the book changes to Physical Properties (Ch 7), Lattice Dynamics, their thermodynamic consequences and their Experimental investigation (Ch 8-10), Anharmonic interactions (Ch 11) and Displacive Phase Transitions (Ch 12). This necessarily covers a treatment of tensor properties, which runs the gauntlet of first-rank to fourth-rank properties in only 13 pages. Although this may be rather swift for the average student, it does accurately reflect the sort of period one has to try and teach this subject in a typical physics module, and there are sensible suggestions for additional reading.

The treatment of lattice dynamics is very clear with excellent diagrams for example, showing the atomic displacements in whole planes associated with longitudinal and transverse acoustic modes. After giving the monatomic and diatomic chains, which are standard undergraduate fodder, the author gives the generalisation for more complex cases, e.g. for a 2-D crystal of symmetry as low as $mm2$. These more difficult examples are most useful - whilst they can be omitted for the standard undergraduate teaching, they provide a useful primer for specialist final-year project teaching or even elementary post-graduate study. In this sense, the book can generally be used at more than one level. The final chapter on Displacive Phase Transitions is an excellent summary of what you need to know i.e., the knowledge you should not be without. It covers Landau and soft-mode theories and includes discussion of ferroelectric, ferroelastic and incommensurate phase transitions.

The numerous appendices A to N are a useful resource: A throws the spanner of reality into the works of the ideal crystal by admitting that not all crystals are perfect, introducing domains and domain walls amongst other defects. My own preference would have been to see this subject covered in the main text - however, it is present and clearly explained in the appendix. Most of the other appendices take the opportunity to explain theory, including theory of crystallography such as the Ewald sphere construction and the Wilson plot, in greater depth, which is entirely appropriate. The closing pages of the book are devoted to the answers to the well-posed problems found at the end of each Chapter. These constitute an additional resource for the busy lecturer and will certainly be widely used and adapted.

In summary, I found this to be a well thought-out, clear and modern book on the structural side of condensed matter physics. Whilst ideally suited to undergraduate physics students, I think much of the book could sensibly be used to teach equivalent modules in chemistry and, given the author’s background, I expect it to be useful for mineralogy/earth sciences also. On a personal note, I shall be recommending the book for my third and fourth year students in Ferroids next term.

Pam Thomas

News from the Groups



News from the Physical Crystallography Group Autumn Meeting

The 2004 Autumn Meeting of the BCA Physical Crystallography Group and the IoP Structural Condensed Matter Physics Group:

Neutron Scattering from Biological Systems will be held at Cosener's House, Abingdon, OXON on 13-14 December 2004, supported by the PCG and Rutherford Appleton Laboratory.

Organising Committee: **John R. Helliwell** (Dept. of Chemistry, University of Manchester), **Jeff Penford** (ISIS Facility, CCLRC), **John S.O. Evans** (Dept. of Chemistry, University of Durham) and **P.A. Thomas** (Dept. of Physics, University of Warwick)

IN THIS meeting we aim to give a broad overview of the contribution of neutrons to biology, with particular emphasis on neutron protein crystallography, 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. 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 expert alike. The meeting will start at 1:30 PM on December 13, 2004 and end at 12:30 PM on December 14, 2004.

We encourage graduate students to attend, and to bring posters for display at the meeting.

Confirmed speakers: **Mathew Blackley** (EMBL - Grenoble) **Giovanna Fragneto** (Institut Laue-Langevin), **Hermann**

Heumann (Max Planck Institute of Biochemistry), **Jayne Lawrence** (King's College London) **Bob Thomas** (University of Oxford), **Peter Timmins** (Institut Laue-Langevin), **Tim Wess** (University of Cardiff)

A registration form is available as an HTML document on: <http://bca.cryst.bbk.ac.uk/bca/pcg/reg2004.htm>

Paolo G. Radaelli
Local Organiser

AGM

The Annual General Meeting of the Physical Crystallography Group of the BCA/Structural Condensed Matter Physics group of the IOP will be held during the BCA spring meeting on Wednesday 13th April 2005 at 13:00. Elections will be held for the positions of Chairman, Vice Chairman, Honorary Secretary/Treasurer and one Ordinary Member of the committee. Nominations for these positions and any other items for the agenda should be sent to the Secretary (john.evans@durham.ac.uk) by 1/4/05 (after 12:00) or communicated to him during the spring meeting. Informal enquiries about the officers' roles should be directed to the President (P.A.Thomas@warwick.ac.uk). Current committee membership is:

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

John Evans

PANalytical Thesis Prize for Physical Crystallography - Call for Nominations



THE PHYSICAL Crystallography Group is pleased to invite entries for the first PANalytical Thesis Prize in Physical Crystallography. The prize will be awarded for the best use of techniques or methods of Physical Crystallography in a successfully-examined thesis submitted in the period from September 1st 2003 to December 31st 2004. The amount of the prize, which will be sponsored by PANalytical Ltd, will be £500. To be eligible for the prize, candidates must be a member of the Structural Condensed Matter Group of the IOP and/or the British Crystallographic Association (BCA). Non-members may enter the competition but will be required to join the BCA at the student rate (currently £7.00) to progress their nomination further.

To enter the competition, candidates must submit:

- (a) A copy of the Thesis on CD-ROM.
- (b) A personal statement of not more than 500 words explaining why the Thesis should be considered for the prize and including a clear description of the role of Physical Crystallography (as interpreted below or otherwise) in the research.
- (c) The names and contact details of two academic referees, one of whom may be the Thesis supervisor, who will be able to comment on the Thesis research of the candidate.

Nominations for the prize must be submitted to the Chair of the Physical Crystallography Group, Dr. Pam Thomas, by February 28th 2005 and the prize will be awarded at the 2005 BCA Spring Meeting in Loughborough, April 2005.

Remit of Physical Crystallography in connection with the PANalytical Thesis Prize

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

Pam Thomas

p.a.thomas@warwick.ac.uk



News from the Biological Structure Group

Biological Structures Group Winter Meeting 2004

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

David made fundamental contributions to the development of protein crystallography and also played a pivotal role in the formation of the British Crystallographic Association. The focus of the meeting will be on how protein crystallography continues to make major contributions to our understanding of biology at the molecular level. We are fortunate in welcoming among our speakers a number of David's early collaborators who worked with him on the development of phasing techniques and the determination of the first protease structure.

Speakers include: **Brian Matthews** (Oregon), **Tom Steitz** (Yale), **Michael Rossmann** (Purdue), **Jonathan Goldberg** (Sloan-Kettering), **So Iwata** (Imperial), **Dale Wigley** (CRUK) and **Richard Henderson** (MRC-LMB Cambridge).

The meeting is scheduled to last from 10.30 - 17.30. There is no charge to attend but the capacity is limited, and participants are strongly encouraged to become members of the British Crystallographic Association.

If you wish to attend you must register on-line before Friday 10th December at <http://www.bio.ph.ic.ac.uk/bc2004>

See the BSG website (<http://bca.cryst.bbk.ac.uk/bca/bsg/welcome.htm>) for further details of this excellent free meeting.

Biological Structure Group Vacancy

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 **Andrea Hadfield**, details opposite. Anyone interested in standing should get in touch - we can always help to organise a proposer and seconder if necessary!

Biological Structures Group Sessions at BCA Spring Meeting

Loughborough 11th -14th April 2005

BSG programme organiser, to whom scientific enquiries/comments should be addressed:

Prof. W. Hunter

E-mail: w.n.hunter@dundee.ac.uk

Co-organisers: **Prof. J. Naismith, Prof. N. Isaacs.**

This year we have an excellent programme with a number of overseas speakers from the USA and Europe. All potential registrants are reminded that the David Blow Poster prize (£100 plus a Blue John trophy) is awarded to the best BSG poster presented at the spring meeting. Bursaries will be available for students on a competitive basis. See meeting main entry for further details of this and the sessions outlined below.

Plenary Session

The meeting starts with an afternoon of plenary lectures, one from each special interest group within the BCA. These are designed to be of broad appeal across the crystallographic community. Dr. J. Rafferty (Sheffield) will contribute a plenary talk from the BSG with the title "Structural studies of DNA Holliday junction resolvases"

The parallel sessions of interest to the BSG include:

At and in the membrane

Speakers include **Prof. R. Stroud** (UCSF, USA), and **Prof. P. Gros** (Utrecht, The Netherlands) who will talk about the translocation unit of autotransporter NalP from *N. meningitidis*.

High-throughput crystallography: more biology and new drugs

Speakers from both academic and commercial backgrounds include **Prof. S. Burley** (Structural GenomiX, USA) "Structure-guided fragment based drug discovery" and **Prof. S. Hasnain** (SRS-DL) "Combined X-ray approach for studying metalloproteins function/misfunction : A powerful approach to Metallogenomics".

Modern refinement: big molecules with good data, small molecules with lousy data

Speakers including **Dr. T. Schneider** (Milan), **Dr. G. Murshudov** (York) and **Dr. C. Bond** (Dundee) "What's that blob? Identifying metal ions in protein crystal structures" will address some of the current challenges in protein structure refinement.

Twentythird Annual General Meeting

To be held at 1:30 on Friday 17th December during the BSG 2004 David Blow Memorial Winter Meeting at Imperial College.

Provisional Agenda

1. Minutes of 2003 annual meeting (Birkbeck 2003)
2. Matters arising on the minutes
3. Chairman's Report - Dr. Richard Pauptit
4. Secretary/Treasurer's report - Dr. Andrea Hadfield (including presentation of the preliminary accounts)
5. Committee Membership and Officers (2004-2005)
6. Any Other Business
Meeting to be adjourned until date to be arranged at BCA Spring Meeting after the end of the financial year.
7. Adjourned business: Acceptance of final accounts.

Draft minutes for the AGM 2003, along with reports for presentation at the AGM, should be available on the BSG Website in advance.

Arnold Beevers Bursary Fund

The Biological Structure Group has again contributed interest accrued over the year to this BCA bursary fund. Remember that as members of the BCA, BSG members are entitled to apply for bursaries to attend meetings from this fund. See the BCA website for details. Remember to use gift aid to enable the BCA to reclaim tax on your subscription - the money reclaimed in this way is also paid into the Bursary Fund.

Andrea Hadfield (a.t.hadfield@bris.ac.uk)
Secretary/Treasurer

BCA/CCG Durham Course

The tenth Intensive Course in X-ray Structural Analysis will be held in Durham from 4-12 April 2005. Information and application forms from **Claire Wilson**. (claire.wilson@nottingham.ac.uk)

From the Secretary

Announcement of Election to Council - Treasurer

This year we have a vacancy on BCA Council for the Office of Treasurer. After 5 years of service, the current Treasurer, **Dave Taylor**, is standing down to assume another role outside the BCA. Please send your properly seconded nominations for this position to me as soon as possible. I will accept nominations until two weeks before the date of the AGM on 13th April 2005. If you nominate someone, it is your responsibility to make sure that the person you nominate is willing to stand for election.

Christine Cardin, Secretary to Council

Biological Structures Group Annual General Meeting

DRAFT Minutes of the Twenty-second Annual General Meeting of the Biological Structures Group which was held at 12:00 am on Friday 19th December 2003 during the BCA Winter meeting at Birkbeck University.

Present:

Some 100 members of the group were present. Apologies were received from **Dr. Andrea Hadfield** (Secretary/Treasurer).

1. Confirmation of the minutes

The Minutes of the previous Annual General Meeting of the Biological Structures Group held at the BCA Spring meeting in York were approved. (A188)

2. There were no matters arising from the minutes. (A189)

3. Chairman's Report

The Chairman reported that the Group was involved in three principal activities, viz the Spring meeting, the Summer School (alternating between Bristol and St Andrews) and the Winter meeting.

- (i) The Spring meeting has a new format which has been pushed by the BSG; it will be shorter and cheaper than in previous years.

Arnold Beevers bursaries are available for students; all BSG students who applied were awarded bursaries this year (2003). The meeting had had a good programme which had been organized by **Gideon Davies** (York) who was thanked. There had been interesting sessions, and it was a great success. The Chairman noted that the Spring meeting is more oriented towards crystallography, while the Winter meeting is more biological.

- (ii) The Summer School had been held at St Andrews; funded largely by the CCP4. There had been 10 teachers and 35 students (and was oversubscribed).
- (iii) Free membership of the BCA was offered to students who attended the Winter meeting (forms were supplied). There was a new mailing list available to those who do not wish to become members. (A190)

The Chairman thanked **Richard Pickersgill** for organizing the Winter meeting.

He also presented the plans of the Group for next year. The Spring Meeting would be held in Manchester, and the BSG themes were:

- (i) molecules in medicine
- (ii) methods in macromolecular crystallography
- (iii) non-covalent interactions
- (iv) a Plenary on catalysis presented by **Jim Naismith**

Next year's winter meeting might take place in Birmingham. (This has subsequently been arranged to take place at Imperial College, London, as a memorial to **Professor David Blow**).

The 2004 Summer School would take place in Bristol; further details would be available on the web pages. The 2005 BCA Spring meeting will be held in Loughborough. The BSG will change from having a "local" organizer to a "programme" organizer. Loughborough is billed as being in a "convenient place" with "good facilities". (A191)

4. Secretary/Treasurer's report - Dr. Andrea Hadfield (Finalised at Spring Meeting, Manchester 2004).

During 2003 our accounts accrued £610.09 in interest, an increase of 34% over the previous financial year after consolidating our accounts with the Charities Aid Foundation bank. Following disappointing attendance at the excellent winter Meeting in 2002 held in Warwick, which proved to be an expensive venue, we made a £1011.20 loss which contributed to an overall reduction in capital of £856.07 over the year. A notable item of expenditure was the payment of the interest accrued in 2002, £454.95, into the Arnold Beevers Memorial bursary fund. This BCA-administered fund supplies travel grants to young BCA (and therefore BSG) members. The qualification and application details can be found on the BCA website.

In view of the assets of the BSG, and the desire of the members to support meeting expenses for young crystallographers, it was proposed that we should once again transfer our interest to the Arnold Beevers Memorial Bursary fund. This suggestion was approved by the members present. (A192)

5. Committee Membership and Officers (2004-2005)

There were no candidates for the position of Vice-Chairman which therefore remains vacant.

The current committee is therefore as follows:

Chairman	Dr. Richard Pauptit (2003-2006)
Vice-Chairman	Vacant
Secretary/Treasurer	Dr. Andrea Hadfield (2003-2006)
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) (A193)

6. Any Other Business

There was no other business. (A194)

Andrea Hadfield



Report on BCA Industrial Group - Pharmaceutical SIG Meeting on 5th October 2004

THIS MEETING of the Pharmaceutical Special Interest Group was superbly organised by Anne Kavanagh (AstraZeneca) and Roy Copley (GSK), and hosted by AstraZeneca at the company's picturesque Alderley Park site.

After a warm welcome to the meeting by Anne, **Rebecca Booth** (AstraZeneca) explained the importance of hydrate formation in the development of new drugs and the strategies available for screening compounds for hydrate formation. Whilst vapour sorption studies are very valuable for studying hydration processes that are governed by fast kinetics, they are not so useful for investigation of hydration processes that are under thermodynamic control and for which the kinetics may be slow. Such systems are best studied using a slurry method that relies on the activity of water being directly related to relative humidity. Rebecca illustrated the advantages of the slurry method using two case studies, theophylline and an AZ compound. For both cases, the slurry method proved much faster at assessing the relative stabilities of hydrates and anhydrous forms.

Chris Hunter (University of Sheffield) then explained how ^1H NMR methods can be used to study crystal nucleation in solution. The technique was originally developed to obtain structural information from the changes in chemical shift caused by complexation between two components to form a weakly bound complex. Chris explained how the technique can be extended to obtain structural information about molecular aggregates during the initial stages of precipitation. Chemical shifts are calculated *ab initio* for small molecules and then these are applied to larger molecules. A genetic algorithm approach is used to refine the chemical shifts allowing the structural model to be optimised by comparison of calculated and observed chemical shifts. The technique was illustrated with sulfamerazine, for which the solution-phase aggregate matches very closely the X-ray crystal structure, and carbamazepine for which the solution-phase structure is solvent dependent. In general, the method works well for relatively rigid molecules and for those for which there is an abundance of chemical shift information.

After coffee, **Gareth Lewis** (AstraZeneca) introduced the importance of salt selection studies in order to optimise the physicochemical properties of a drug. Interestingly even taste can be an important factor, especially for paediatric medicines. Gareth illustrated how remacemide, a potential antagonist for epilepsy, Parkinsonism and Huntington's disease, was crystallised as a variety of salts that were subsequently investigated by X-ray diffraction. The crystal structures clearly showed hydrophobic and/or hydrophilic regions depending on the nature of the counter-anion. The hydrogen-bond motifs were also analysed. Interestingly, the size and shape of the anions appeared to have very little effect on the types of structure observed.

Ed Collier (formerly UMIST, but now The University of Manchester) continued with the theme of salt selection and described the work performed during his PhD. This involved the preparation of a further 23 salts of the pharmaceutical compound (1R, 2S)-(-)-ephedrine using combinatorial techniques. Ed highlighted that during these crystallisation studies, several of the acids showed variations in their apparent acidity that depended on the solvent. From these salts, 19 crystal structures were obtained and the hydrogen-bonding networks and structure-property relationships were analysed. In addition to hydrogen-bonded motifs it is clear that π - π stacking interactions play an important role in many of the structures. The work has provided a starting point for a salt screening strategy and has improved understanding of the reasons for success and failure of commonly used anions to provide stable, crystalline salts.

After an excellent lunch and photo opportunity, **Chris Gilmore** (University of Glasgow) kicked off the afternoon with a presentation about how to identify polymorphs from the results of high-throughput screens that involve computer-controlled crystallisation and data-collection methods. Such data are frequently complicated by the presence of mixed phases, broad diffraction peaks, and preferred orientation. Chris explained how his program PolySNAP can be used to circumvent these problems. The technique relies on point-by-point matching of powder patterns rather than simply by matching peaks. A combination of non-parametric (Spearman) and parametric (Pearson) statistical methods are used to obtain a correlation matrix. This is then used to generate a distance matrix, which acts as a source of classification to generate dendrograms, multidimensional metric scaling, silhouettes, fuzzy clusters and minimum spanning trees. These tools allow the data to be partitioned into clusters of related patterns. The program is very powerful and can readily detect mixtures of phases or components. Chris and his team have extended the technique to include additional data from Raman, infrared, and DSC measurements.

Doug Minick (GSK, North Carolina) then described the chiro-optical technique, of vibrational circular dichroism (VCD) to aid in the assignment of absolute configurations of chiral drug molecules. In VCD, polarised infrared spectra are first recorded for a compound in solution. Because of the time-scale of the infrared technique, contributions from all of the conformers present contribute to the observed spectra. Molecular mechanics calculations are therefore used to identify possible conformers and then *ab initio* calculations are then used to obtain the relative proportions of conformers present and most importantly the contribution each one makes to the VCD infrared spectra. After correction of gas-phase frequencies to solution-phase frequencies, the experimental and theoretical VCD spectra are compared and conclusions can be drawn about the absolute configuration of the chiral compound. Although the technique has some limitations, Doug currently reported a 96% success rate and he has had 15 assignments subsequently confirmed by X-ray diffraction.

Colin Pulham (University of Edinburgh) finished off the day with a presentation about the use of high pressure as a means of searching for new polymorphs and solvates. Although high pressure is widely recognised in the Physics and Geosciences communities as a powerful means of inducing phase changes, it is not a technique that has been widely

explored by the chemical or pharmaceutical communities. Colin illustrated how recrystallisation in diamond anvil cells can be used to prepare and characterise new polymorphs and solvates of phenanthrene, paracetamol, and piracetam. These experiments can be scaled up and in some cases bulk quantities of these polymorphs and solvates can be recovered to ambient pressure. He also demonstrated how the technique can be used to screen for polymorphs by showing that the 3 known forms of piracetam plus a new form can be selectively recrystallised simply by changing the pressure.

Roy Copley concluded the day's proceedings by thanking the speakers and participants, and urged everyone to support the Spring BCA Meeting that will include two sessions on the subject of non-ambient pharmaceutical studies.

Colin Pulham

XRF Sessions at the BCA 2005 Spring Meeting

HELP! Please help us promote this new venture by passing on the details to your XRF colleagues. The XRF sessions are being organised through the Industrial Group.

This is a snapshot of the programme in late October, for the latest programme information - check out the dedicated XRF web page at: <http://bca.cryst.bbk.ac.uk/bca/ig/meet5xrf.htm>

XRF Session Details

Tuesday 12th April 2005

IG PLENARY: XRD, XRF and in-situ investigations on anhydrous and hydrous cementitious materials - Some examples. **Herbert Pöllmann**, Halle Univ. Germany.

XRF Exhibitors Session. 15:30-18:00

Presentations by exhibitors to give delegates a chance of updating their product knowledge from a spectrum of suppliers.

Wednesday 13th April 2005

Liquid samples. 08:30-10:00

Please offer a talk on your liquid application in this session.

WORKSHOP - Awkward Samples. 10:30 - 12:00

What are your awkward samples like? Do they decompose under irradiation? Are they sticky messes that sediment given half a chance? Come and tell us how you cope with them.

WDXRF Applications. 13:00 - 14:30

Determination of sulphur and chlorine in organic compounds by XRF.

Dr David Beveridge, ILFORD Imaging UK Ltd

Fusion for better analytical results in XRF analysis.

Mr Michel A. J. Davidts, Socachim-XRF Scientific

Status of WDXRF in Ceramic Analysis.

Dr Graham Oliver, CTE, Ceram.

Light Element Analysis. (Li-F or $e > 1.3\text{nm}$). 15:00 - 16:30

Light element analysis is routine for many people - share your experience by offering a talk in this session.

Thursday 14th April 2005

Standards & Calibration. 08:30 - 10:00

Setting the Standards for Calibrations.

Margaret West, West X-ray Solutions Ltd.

EDXRF - Applications. 10:30 - 12:00

Field Portable XRF for On-site Screening and Analysis of Prohibited Substances in Plastics.

Dr Stanislaw Piorek, R&D Niton, LLC.

EDXRF applications in the pharmaceutical industry.

Mr Martin J Teasdale, GlaxoSmithKline.

Combined XRF/XRD applications. 13:00 - 15:00

This session is for applications where the combined power of XRF and XRD is needed to resolve materials science applications and will be of interest to all Industrial Group members.

Combining XRF, powder XRD and structural modelling techniques: application to plastic clays and kaolins.

Noel Thomas, WBB Minerals, Germany.

Discussion Forum

We will wind up the programme with an informal discussion session which will allow you to ask all the questions that haven't been answered so far in the sessions. Finally, we will seek your views on the future of XRF within the BCA.

To offer a paper in the XRF sessions please contact:

David Beveridge: Tel: 01565 650000 Fax: 01565 872734

Email: david.beveridge@ilford.com or **Dave Taylor**: Tel: 01744893108 Email: djtaylor@lineone.net or simply fill out the web form (<http://bca.cryst.bbk.ac.uk/bca/ig/admin/xrfmail.htm>)

From the Industrial Group A Low Angle Instrument Calibration Round Robin

THE BCA Industrial Group has launched a NEW low angle XRPD calibration round robin.

The round robin is being coordinated for the Industrial Group by **Dave Taylor** and 16 participants have already registered.

The sample being used is a thin Silver Behenate film on a Polyethylene terephthalate (PET) substrate. It will be distributed as a 30mm square specimen and can be easily cut to size with scissors to fit your specimen holder. Participants in the round robin will need to measure the specimen from 1 degree to 40 degrees 2 theta for Copper Radiation or the equivalents for other wavelengths.

The instrument conditions are left to participants with a recommendation of a minimum of 0.01 degree steps with a 1 second per step time interval and taking just over an hour. A template will be supplied for reporting results which will include instrument parameters and the measured data as an angles, intensity - x,y list.

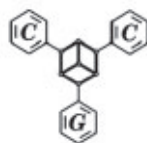
Each participant will be given a unique number to protect their identity in the final report but allow them to see how their data compared with the rest. It is expected that information on angular displacement, peak intensities and line profiles will form the basis of the data evaluation. All participants can keep their test specimen as a valuable instrument calibration resource. Subject to the results of this UK Round Robin the exercise may be rolled out worldwide and the test specimen may become a certified reference material.

Why use a Silver Behenate film?

The material orients on the substrate to give multiple orders of the basal Bragg reflection. The fact that it is a reproducibly deposited film will allow direct comparison of the intensity and line profile of each instrument with no contribution from the sample or its preparation.

Register on line or get more details from the Industrial Group web page at: <http://bca.cryst.bbk.ac.uk/bca/ig/admin/newslarr.htm>

The BCA gratefully acknowledge the support of **Tom Blanton** at Eastman Kodak Company, USA, for supplying the material used in this round robin exercise.



The CCDC Prize and Lecture

THIS PRIZE and lecture for Younger Scientists in Chemical Crystallography is sponsored annually as part of the BCA Spring Meeting. CCDC Prizes are awarded for original research in the following subject areas:

Chemical crystallography, including advances in instrumental, experimental or computational techniques. Applications of small-molecule crystallographic information in, e.g., structural chemistry, molecular modeling, materials design, structural biology or chemical informatics.

Candidates for crystallography awards should not be more than 35 years of age on 1 January of the year in which the award is made. Nominations must be made to **Dr Georgina Rosair**, the secretary of the BCA Chemical Crystallography Group.

Please see the CCG website for details - <http://crystallography.org.uk/CCG/ccg.html>
You can download nomination forms from the website.

The 2004 prize was won by **Dr Maryjane Tremayne**, University of Birmingham. Please remember that completed nomination forms and supporting material must reach me by Friday 7th January 2005.

Georgina Rosair (g.rosair@hw.ac.uk)

News Flash

World News

Rigaku

THE RIGAKU SUN

VOL. 122, NO. 190 SEVENOAKS, MONDAY, DECEMBER 6, 2004 SEVENTY-FIVE PENCE

MINI ON THE MOON

The Rigaku MiniFlex allows you to analyze samples on site. No matter where!

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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 December 2004

Regional School of Crystallography and Diffraction, Havana, Cuba
cristalografia.net

5 - 8 December 2004

International Workshop on the Physical Characterization of Pharmaceutical Solids, Chiba, Japan
www.assainternational.com/workshops/iwpcps_6/iwpcps_6.cfm

6 - 7 December 2004

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

17 - 18 January 2005

Protein Crystallography in Drug Discovery: dedicated to structural genomics & proteomics, South San Francisco, CA, USA
protcrystconf.com/

27 January 2005

The 7th Sinq Users' Meeting, Paul Scherrer Institute, Villigen CH
sinq.web.psi.ch/sinq/usmeet_7/meet7.html

13 - 17 February 2005

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

14 - 18 February 2005

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

21 - 24 February 2005

The 4th Pharmaceutical Powder X-ray Diffraction Symposium, Barcelona
www.icdd.com/ppxrd

28 February - 4 March

Annual Meeting of German and Austrian Societies for Crystallography and Crystal Growth, Cologne
www.kristall2005.uni-koeln.de/

7 - 11 March, 2005

International School on Crystal Growth: Fundamentals, methods and applications to biological and nano crystals, Puebla, Mexico
www.ifuap.buap.mx/ISCG05/school.html

4 - 12 April 2005

10th BCA/CCG Intensive Course in X-ray Structural Analysis, University of Durham. Please contact:
claire.wilson@nottingham.ac.uk

10 - 14 April 2005

Physics, a century after Einstein, University of Warwick
www.physics2005.iop.org

12 - 14 April 2005

BCA Spring meeting and X-Ray Fluorescence Meeting, Loughborough
crystallography.org.uk

2 - 6 May 2005

Practical X-ray Fluorescence, International Centre for Diffraction Data, Newton Square PA, USA
www.icdd.com/education

12 - 22 May 2005

Evolving Methods in Macromolecular Crystallography, 37th crystallographic meeting at Erice and a EuroSummerSchool, Erice, Italy
crystalalice.org/futuremeet.htm

28 May 2005

Powder diffraction software workshop (Sattellite of ACA), Walt Disney World, Florida, USA
www.chem.tamu.edu/xray/acawork/acaworkshop.html

28 May - 2 June 2005

ACA Annual Meeting, Walt Disney World, Florida, USA
hwi.buffalo.edu/ACA/

5 - 10 June 2005

7th International Workshop on the Physical Characterization of Pharmaceutical Solids, Kona, Hawaii
www.assainternational.com/workshops/iwpcps_7/iwpcps_7.cfm

6 - 10 June 2005

Fundamentals of X-ray Powder Diffraction, International Centre for Diffraction Data, Newton Square PA, USA
www.icdd.com/education

13 - 17 June 2005

Advanced Methods in X-ray Powder Diffraction, International Centre for Diffraction Data, Newton Square PA, USA
www.icdd.com/education

20 - 24 June 2005

International School on Mathematical and Theoretical Crystallography, Nancy, France
icm3b.uhp-nancy.fr/mathcryst/nancy2005.htm

3 - 7 July 2005

12th Convention of the Royal Australian Chemistry Institute (RACI), Sydney, Australia
RACIflyer.pdf

18 - 23 August 2005

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

23 - 31 August 2005

XX Congress of the International Union of Crystallography, Florence, Italy
iucr2005.it

2 - 8 September 2005

Electron Crystallography School 2005 - ELCRYST 2005, Brussels, Belgium
www.elcryst2005.de

27 November - 2 December 2005

International Conference on Neutron Scattering 2005, Sydney, Australia
sct.gu.edu.au/icns2005

2006

9 - 18 June 2006

The Structure Biology of Large Molecular Assemblies: the 38th crystallographic course at the Ettore Majorana Centre, Erice, Italy
crystalalice.org/futuremeet.htm

4 - 6 August 2006

ECM-23 Satellite Meeting on Mathematical and Theoretical Crystallography, Leuven, Belgium
www.icm3b.uhp-nancy.fr/mathcryst/leuven2006.htm

7 - 17 June 2007

Engineering of Crystalline Materials Properties: the 39th crystallographic course at the Ettore Majorana Centre, Erice, Italy
crystalalice.org/futuremeet.htm