

Crystallography News

British Crystallographic Association



Issue No. 93 June 2005

ISSN 1467-2790



BCA Spring Meeting - Loughborough p6



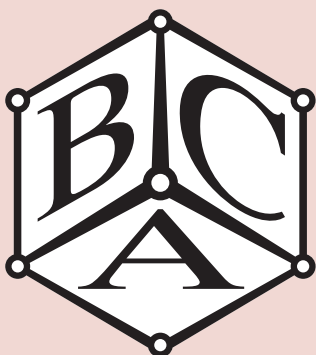
Exhibitors at the BCA Meeting p16-17

Robin Shirley 1941-2005 p18-19

Mary Rosaleen Truter 1925-2004 p20-21

Groups p26-27

Meetings of Interest p31-32



**BCA
Administrative
Office,**
Gill Moore,
Northern Networking
Events 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 **September 2005** issue are sent to
the Editor to arrive before **25th July 2005**.

Bob Gould

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

The British Crystallographic Association
is a Registered Charity (#284718) As
required by the DATA PROTECTION ACT,
the BCA is notifying members that we
store your contact information on a
computer database to simplify our
administration. These details are not
divulged to any others without your
permission. You may inspect your entry
during the Annual Meeting, or otherwise
by application to the BCA Administrative
Office. We will be happy to amend
entries at any time.

Designed & printed by Wm. Anderson & Sons Ltd.
34 Loanbank Quadrant, Glasgow.
Tel: 0141 440 2881
e-mail: enquiry@andersonprint.demon.co.uk

BCA News June 2005

Contents

From the President	2
Council Members	3
From the Editor	4
Prizes.....	4
Puzzle Corner/Corporate Members.....	5
Meetings	6-15
BCA Spring Meeting - Loughborough.....	6
Exhibitors at the BCA Meeting	16-17
Obituary - Robin Shirley.....	18-19
Obituary - Mary Rosaleen Truter	20-21
Other Meetings	22-25
Groups.....	26-27
BCA Accounts 2004	28-29
Profiles in Science	30
Meetings of Interest	31-32



***This month's
cover:***

*Photographs
from this year's
Spring Meeting.*

*Can you find yourself? Bet
you'll never forget that tree! The
inset shows a few non-ambient
pharmacists.*



From the President



WRITING this column immediately after a Spring Meeting, one tries to avoid too much repetition, since the President gets to say so much on so many occasions at that meeting. So let's keep this brief. The Spring Meeting in Loughborough was very successful, with an increased attendance

of over 320 delegates and a full Exhibition - this year we had to turn potential Exhibitors away. The participation of the XRF community in a parallel strand of the oral programme, and integrated into the Exhibition, was a success and one which we hope to repeat at future Spring meetings.

Following the success of the Young Crystallographers' satellite at the 2004 Spring meeting, we have asked our younger colleagues to be fully involved in planning their participation in 2006 and beyond. A proposal to establish a Young Crystallographers' special interest group was circulated informally in Loughborough and signed by over 50 young crystallographers; volunteers have also been found to begin organising the group. As a start to this, the Young Crystallographers will be represented on the 2006 Spring Meeting Programme Committee.

As I write, that Programme Committee is about to meet, under the chairmanship of **Paul Raithby**. The Programme Committee brings together representatives of the BCA subject groups and others, this year including colleagues from the British Association of Crystal Growth, to begin to

plan the detailed programme. I look forward once again to a full and interesting programme in Lancaster in 2006, and am pleased to be working with the BACG on exploring topics of common interest.

Two members of Council retired in Loughborough and are warmly thanked for their contributions to our organisation. Andrea Hadfield had been BSG group representative on Council for some years, and is succeeded by **Sheila Gover**. **Dave Taylor** is replaced by **Sheila Gould** as Treasurer; Sheila brings much past experience to the role, including as Treasurer of the IUCr XVIII Organising Committee in 1999 (Glasgow). I think it is acknowledged that the Treasurer's role is particularly important to an organisation and charity such as our own; Dave Taylor's extensive contributions in this role have made an enormous difference to the way in which the BCA is run and have been quite invaluable to the Association.

As I enter my last year as BCA President, minds may begin to turn to the election of my successor in Lancaster. As with all Council appointments, it is healthy (and more interesting!) if the elections for these are contested. I trust this will be so for the vacancy of President in 2006.

I look forward to a busy crystallographic summer ahead, with the IUCrXX meeting in Florence in August being an obvious focus; it will be my honour to lead the UK delegation to the General Assembly of the IUCr at that meeting. I look forward to meeting once again with many colleagues from the UK and elsewhere in our world-wide crystallographic community.

Chick Wilson



BCA Council: Front Row Christine Cardin, John Finney, Chick Wilson and Sheila Gould. Back row: Bob Gould, John Helliwell, Sandy Blake, Jeremy Cockcroft, Sheila Gover, Elspeth Garman, Georgina Rosair, John Evans and Peter Moody.

The BCA records the passing of colleagues **Jackie Truter** and **Robin Shirley**; they will both be missed. Obituaries can be found in this issue.

Robin's passing in particular has caused wide shock amongst his colleagues as he was still so active in the crystallographic world.

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 (2008)
Dr Sheila Gould
33 Charterhall Road,
EDINBURGH EH9 3HS
Tel: 0131 667 7230
treasurer@
crystallography.org.uk

ORDINARY MEMBERS

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

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

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

GROUP REPRESENTATIVES

Biological Structures

Dr Sheila Gover
131 Main Road
Middleton Cheney
BANBURY, OX17 2PW
Tel: 01295 711636
sheila.gover@tesco.net

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
Meriside
Alderley Park
MACCLESFIELD SK10 4TG,
Tel: 01625 516135
richard.pauptit@astrazeneca.com

Chemical Crystallography Group

Dr Simon Parsons
School of Chemistry
University of Edinburgh
EDINBURGH EH9 3JJ
Tel: 0131 650 5804
s.parsons@ed.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.org.uk

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

From the Editor



ISSUE number 93 is largely concerned with reporting our recent Spring Meeting, and I'm delighted to say that nearly all of this has been done by our bursars, who worked hard to get reports in quickly. We've been able to cover the major sessions from their reports, and I hope that my cutting and pasting hasn't resulted in any

mishaps. A few other items will be covered in the September Issue, and the main lectures will, of course, appear in due course in *Crystallography Reviews*.

For one thing I must apologise, and that is the absence of some pictures I took, they having been destroyed when I had a senior moment with my camera. I have **Sandy Blake** to thank for a memorable piece of *ex post facto* advice: "In future, Bob, remember that in the question 'Format OK?' the word *format* is a verb, not a noun." Which I shall do.

The two obituaries in this issue are of people I shall miss a lot. Jackie was well-established as a crystallographer

by the time I realised that I was one too, and was a great encouragement. She was also a very faithful supporter of the BCA long after her retirement. Robin's death was a bolt from the blue – like many others, I wondered why he wasn't at Loughborough. As someone said, "I assumed he must be saving up for Florence". As a keen scientist, a compassionate teacher and a hilarious eccentric, he will be greatly missed. I am very grateful to his Head of Department and to Mike Glazer for supplying their thoughts at short notice.

Particularly welcome are accounts of other meetings people have been to. One in this issue by **Robin Owen** is of a meeting in Japan. Its late appearance is my fault not his. Also included is a short report of the annual meeting of the DGK, our German counterpart, and there will be news from the ACA in the next issue. Please let me know of any such meetings you attend.

One small matter of housekeeping about submissions. *Please* send pictures with reports. They make the article and the journal much more readable. *Please*, however, *don't* embed them in a WORD document. Taking them out for the printer to use degrades them very badly. As a general rule, a .jpeg occupying 10-50kB will almost certainly be usable.

Bob Gould

Poster Prizes at the Spring Meeting



Richard Strange (BSG)



Gordon Barr (CCG)



Jacqui Cole (PSG)

Puzzle Corner

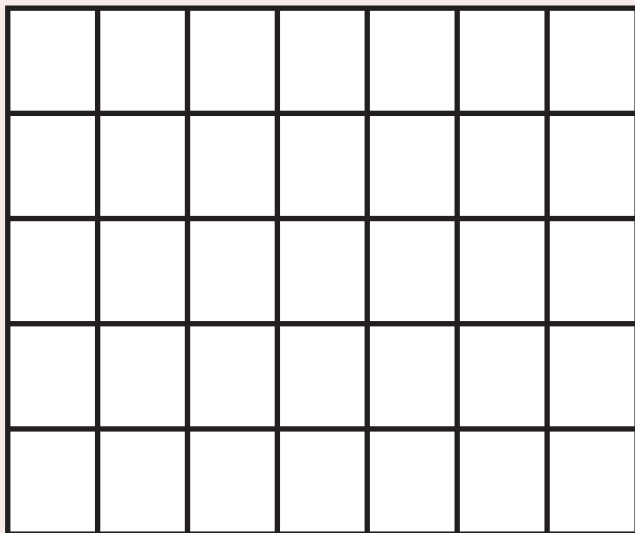
Last month's cryptogram got a good number of entries.
The actual text was:

"Symmetry and periodicity are among the most fascinating and characteristic properties of crystals by which they are distinguished from other forms of matter. On the macroscopic level, this symmetry is expressed by point groups, whereas the periodicity is described by translation groups and lattices, and the full structural symmetry of crystals is governed by spacegroups."

It is indeed from the Foreword to International Tables Volume A1, but is copied there from Volume A, which is its real origin.

More than one reader has criticised the policy of choosing "the first" as a winner, as this gives an unfair advantage to those who receive *Crystallography News* earliest. In fact, I sometimes get a reply before I have received my own copy! Consequently, I've drawn to choose the winner, who this time is once again **Jim Trotter**, to whom congratulations!

Now for a new one, keeping the symmetry theme going. Using the letters p,b,d,and q, fill up the following grid - one letter per square - so that it has the plane group $p2gg$. Arial (Helvetica) font is recommended! Blank spaces are allowed, but the more unit cells, the more points!



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 Events 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

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

BCA Spring Meeting

Spring Meeting - A student's view

THIS year's BCA Spring meeting was held at Loughborough University with its somewhat confusing maze-like campus consisting of many cricket, football and hockey pitches hidden amongst which were the university buildings, the Village Park accommodation complex and the James France Conference Centre, our new home for three days and located a handy half-hour stroll from the breakfast room (longer if/when you got lost).

BCA Spring Meetings in recent years have consisted of much science in a relatively short space of time. This year was no exception and again I found myself looking at the programme and seeing that some of the lectures which I wished to attend were happening concurrently. However the corridor at the rear of all bar one of the lecture theatres made hopping in-and-out of the sessions quite easy; sit at the back and you could slip in-and-out almost unnoticed.

The conference kicked off with an excellent plenary lecture by **Phil Coppens** which set the scene for the photocrystallography parallel sessions the next day. My personal favourite was by **Malcolm McMahon** who discussed the effect of high pressure on the crystal structures of metals and the peculiar host-guest like incommensurate structures which result.

Following **Anders Markvardsen's** CCDC prize lecture (incidentally a powder crystallographer has won this prize for the last three years - anyone see a trend?) we then had a Crystallography Exhibitor's Forum, something which I think is a first for a Spring Meeting and was a good chance for the large audience to learn of some of the new products coming onto the commercial market.

The evening poster session, always a highlight of any conference, was of particular satisfaction to me as my poster was considered by the judges to be good enough to receive an honourable mention at the award session. Close, but no cigar! However, I think most people who took the time to read **Gordon Barr's** winning poster would agree it was a worthy winner. Once again the Rigaku/MSO-sponsored wine was flowing freely and the ladies charged with ensuring that no-one's glass was ever less than half-full did a marvellous job.

Wednesday morning saw the start of several parallel sessions. In Photocrystallography, **Jacqui Cole** outlined the developments made in experimental technology over the last few years and also discussed the design and

construction, at SRS Daresbury, of a new chopper to allow picosecond time-resolved studies. Following-on, **Judith Howard** discussed the structural characterisation of some complexes which, under rather harsh conditions (30K and photoirradiation) undergo a transition from low to high spin and remain metastable at low temperature, and how this phenomenon can be harnessed in a variety of different applications.

Hopping into the *In-situ* diffraction session I heard **Roger Davey** present a talk on monitoring crystallisation *in-situ* by a variety of techniques, one of the neatest being the use of infra-red spectroscopy to predict which polymorph will crystallise (if there's a strong band in the IR spectrum corresponding to the OH wagging of a dimer in the solution, then it's a pretty good bet they'll be dimers in the solid state).

After coffee, **Richard Cooper** discussed using some of the features of CRYSTALS to apply general restraints during refinement. CRYSTALS is neatly interfaced with MOGUL to allow the application of appropriate geometric restraints based on information derived from the MOGUL library during problematic refinement, a very useful tool to have.

Most of the afternoon was spent sliding in and out of lecture theatres between the various parallel sessions and concluded with the BCA Prize Lecture given by **Andrew Leslie** who explained how the groundwork by **Alan Wonacott** and **Uli Arndt** allowed him to develop his career to his present position at MRC-LMB.

On Thursday morning **Mike Glazer** opened proceedings with a tutorial session on the physical basics of phase transitions. Presumably conscious that his was the first lecture of the day following the conference dinner, Mike kept his presentation nicely-pitched to be understood by relative novices, and I also came out of the lecture armed with ideas for practical demonstrations for my own seminars! Following the coffee break a parallel session built upon the basics of phase transitions already set out by Mike, covering ferroelectric and ferroelastic phase transitions, and also those induced by extremes of temperature and pressure. I ended the conference by attending the CCP14 WinGX workshop where, following a demonstration of the software by its author **Louis Farrugia**, attendees were able to try out some of the features in a hands-on session.

I am grateful to PANalytical Ltd for funding a bursary to cover the cost of the conference fee, accommodation and the meals. I am also thankful to my crystallographic colleagues across the country whose attendance at the BCA Spring Meeting make it all the more enjoyable.

Gary S. Nichol (University of Newcastle)

In situ Diffraction

The opening session, chaired by **John Evans**, began with a lecture given by **Matt Rosseinsky** on *In-situ diffraction in inorganic materials discovery and processing*, where he described work on materials used in mobile telecommunications, where oxides of transition metals lie at the centre of a \$4 billion industry. The most suitable materials have been found to be oxides of transition metals with a d^0 configuration, for example $\text{Ba}_3\text{ZnTa}_2\text{O}_9$ (BZT). This was a thoroughly enjoyable insight into the synthetic processes involved in the production of suitable materials, and indeed the analysis and monitoring of the sample in producing the desired product.

Joe Hriljac described *High-Pressure Studies of Zeolites*. With the example of Zeolite A, he showed that the application of pressure in an aqueous environment resulted in an initial increase in the unit cell volume of the structure before an overall decrease in volume as the pressure increases. In contrast, in an anhydrous environment, there is only the overall volume decrease. This has been shown to be due to the forcing of water molecules into the zeolitic cavities when the pressure is initially increased. In a further example of the use of pressure in the structural determination of zeolites, Joe showed that at low pressure, one zeolite has fluid-like, non-crystallised, guests held in the cavities which resulted in additional scattering in the diffraction pattern for the zeolite. The use of higher pressures in this example results in an increase in the crystallinity of the guest molecules, therefore improving the diffraction pattern of the material.

Roger Davey presented a talk *Using X-rays for the In-Situ Study of Crystallisation Processes*, describing studies of (amongst other compounds) tetrolic acid, a polymorphic compound known to crystallise in both the carboxylic acid dimeric and catemeric forms. He used a variety of techniques, including IR Spectroscopy. Analysis of the infrared spectrum of tetrolic acid showed that a peak at 900 cm^{-1} was due to out of plane "wagging" of the OH group within the centrosymmetric CO_2H dimer motif. Infrared spectra of tetrolic acid in various solvents allowed the comparison of the polymorphic structures, giving some insight into the nucleation and crystallisation processes. In dioxane, however, the IR spectra indicated a monomeric structure, but a solvate was crystallised, indicating



that some caution is necessary in solid state structure prediction based upon IR spectra.

The second section was based around perspectives from industry, giving the chance to see the relevance of crystallographic techniques to the wider world. A particularly enjoyable talk was given by **Gordon Tiddy** on *Surfactant formulation*, who was both humorous and engaging with his insight into the world of fabric conditioner. This was a product I had used (despite his explanation to PhD students that 'this is something your mum uses') without any thought as to its chemical complexity or properties.

The final talk was by **Simon Jacques** on *In situ crystallisation studies of pharmaceuticals*. Dr Jacques talked about TEDDI (Tomographic Energy-Dispersive Diffraction Imaging) and its use in monitoring batch crystallisation, using L-glutamic acid as a model structure. L-glutamic acid is known to exist in two polymorphic forms (α and β), both of which crystallise in $P2_12_12_1$ with similar structures, giving rise to similar diffraction patterns. 2D spatial mapping of stirred slurries of both pure and mixed phases were studied in time-resolved experiments. Despite various problems, it was clear that the different polymorphs behave differently. Crystallisation was studied by monitoring six points in the vessel by time- and space-resolved diffraction. Data quality was poor, and so more points need to be studied. At the moment TEDDI is suitable for imaging at steady-state, but not with time- and space-resolution.

Anna Collins (University of Oxford)
Sophie Dale (University of Newcastle)
Ross Harrington (University of Durham)
Gary Nichol (University of Newcastle)
Graham Stinton (University of Durham)



Non-Ambient Pharmaceutical Studies

Jonathan Burley opened this session, chaired by **Anne Kavanagh** with *Crystal structure and intermolecular forces from variable temperature PXRD*. The structure was that of Glipizide, a major drug for treating diabetes. Variable temperature data were used to confirm the index of the cell, and Jonathan recommended this as a facile method of ensuring crystals are correctly indexed when using powder diffraction. Since structure-property relationships are of interest, he investigated intermolecular forces quantitatively by working out the Debye temperatures along the cell axes. This temperature is a measure of the lattice stiffness, i.e. bond strength. The anisotropic lattice expansion was fitted to the sum of phonon modes. Jonathan showed that glipizide has single phonon modes along the *a* and *c* axes, which he attributed to π - π interactions and hydrogen bonding respectively, and the *b* axis is characterised by two phonon modes, which correspond to van der Waals interactions and steric interlock.



For a patent, every pharmaceutical requires characterisation; this is often achieved, at least in part, by powder diffraction. One of the questions **Jeremy Cockcroft** considered in his talk *Obtaining accurate non-ambient laboratory PXRD data for pharmaceutical studies* was whether the powder diffraction patterns always represent a polymorph of the material. In order to answer this, accurate data are required, ideally without preferred orientation. To get good data, the diffractometer configuration has to be considered and the calibration of the equipment checked. Low temperature diffraction is often a useful tool, providing turbulence, draughts and icing problems can be dealt with. LT work requires capillary geometry, which has the advantage of reducing or removing preferred orientation. Several case studies were presented.

Steve Cosgrove finished the first session with *Probing (De)Hydration Behaviour by High Resolution X-ray Powder Diffraction*. He described studies of a candidate drug, as its sodium salt, which was known to crystallise as four polymorphs, three hydrates and a number of other solvates. Steve discussed DSC and derivative TGA for probing dehydration and hydration of the compound. Mass spectrometry is also used, with monitoring of the $m/z = 18$ peak indicating the loss of water from the compound. Dynamic vapour sorption is also used to cycle the compound within various humidity environments to monitor moisture sorption and dehydration. This method can highlight stable higher hydrates, which would be more appropriate for manufacture as the risk of water sorption by a lower hydrate would cause problems during weighing stages.

After the coffee break, **Roy Copley** took the chair, and **Francesca Fabbiani** spoke on *Probing Polymorphism with High Pressure* based on a search for high pressure polymorphs of piracetam. Varying of pressure adds an additional dimension to the search for polymorphs of pharmaceuticals. Three approaches are available – direct compression (best for very small molecules), growth of crystals from the melt and recrystallisation from solution under pressure. Three new polymorphs of piracetam have been structurally characterised. Francesca used graph set analysis to demonstrate the differences in the hydrogen bonding patterns within the polymorphs, and also introduced the concept of Hirschfeld surfaces to differentiate between the polymorphs.

Emphasising the importance, and often difficulty, of understanding polymorphs and hydrates of pharmaceuticals, **Angus Foster** discussed *The Use of X-ray Diffraction in the Pharmaceutical Development of a Dihydrate API*, a compound with complex hydration behaviour, which readily loses water under typical manufacturing conditions. Many techniques, including single crystal and VT powder XRD, VT-FTIR and isothermal-TGA to investigate under which conditions the compound could be dried and still remain crystalline.

Peter Laggner finished the session by discussing *Monitoring non-ambient nanophase processes by TR-SWAXS*. He gave a description of the equipment used, and then went on to discuss lipid polymorphism. By using temperature jump and pressure studies on membranes he could show that cholesterol induces softening when present in low concentration, but at high concentrations caused hardening of the membrane.

Sophie Dale (University of Newcastle)
Katharine Bowes (University of Cambridge)

CCDC Prize Lecture at BCA Spring Meeting, Loughborough

THE CCDC/CCG Prize for Younger Scientists was awarded this year to **Dr Anders Markvardsen** of the ISIS Facility for his work on structure solution by powder diffraction methods. Dr Markvardsen presented a lecture entitled *Probability, Powders and Pathways*, in which he outlined some of his recent work; in doing so he gave the audience a valuable overview of recent algorithmic developments in the area of powder diffraction. Prior to his lecture Dr Markvardsen was presented with a commemorative trophy and a cheque by **Dr Frank Allen** of the CCDC.

The first part of the lecture was devoted to the problem of determination of the extinction symbol from powder diffraction data, an essential component of space group assignment. Because powder diffraction patterns are one-dimensional representations of three-dimensional diffraction patterns, systematic absences are usually obscured by overlap with other reflections. The quantity sought by the algorithm described is the probability that a given extinction symbol, E , is correct given a set of intensities, \mathbf{I}^p , obtained from a Pawley refinement. Application of Bayes' theorem reduces this probability to the integral:

$$p(E | \mathbf{I}^p) \propto \int p(\mathbf{I} | E) p(\mathbf{I}^p | \mathbf{I}) d\mathbf{I}.$$

The second term in the integral is obtained from the Pawley fitting procedure, and depends on the degree of overlap suffered by a particular reflection. The distribution functions required for evaluation of the first term in the integral are derived from Wilson statistics for reflections which are not systematically absent; for systematic absences the corresponding term is the delta function. In determination of the extinction symbol the probabilities of all possible symbols belonging to a given crystal system are evaluated, and the results output with a figure of merit for each symbol derived from $p(E|\mathbf{I}^p)$. The output obtained for dopamine was used to illustrate interpretation of the program output. The procedure takes ca 1-20 seconds in practice on a modern pc, and it has been shown to be extremely robust. It has been incorporated into the program DASH, and is available from <http://www.markvardsen.net>. A detailed report is available in *Acta Cryst.* (2001) **A57**, 47-54.

The second part of the lecture concerned the application of maximum likelihood in refinements of crystal structures against powder data. Least squares, which is the method usually used for crystallographic estimation, is really only appropriate when (i) measurement errors follow a Gaussian distribution and (ii) the model does not suffer from significant errors. Refinement in the presence of gross measurement errors was discussed later in the conference by **Prof. Bill David**. The problem of refinement of an incomplete model was addressed here.

Stated generally, the aim of maximum likelihood refinement is to determine a set of model parameters that maximizes the

probability of the data given the model. The method reduces to least squares if conditions (i) and (ii) above are met, but in other circumstances Bayesian methods can be applied to derive alternative procedures. The likelihood function L can be expressed as:

$$L \propto \int p(\mathbf{I} | \mathbf{I}^{frag}) p(\mathbf{I}^p | \mathbf{I}) d\mathbf{I}.$$

The term $p(\mathbf{I}^p | \mathbf{I})$ is obtained from a Pawley fit (see above); $p(\mathbf{I} | \mathbf{I}^{frag})$ is the probability distribution function of the intensities \mathbf{I} given the set of intensities that can be calculated on the basis of a partial model (\mathbf{I}^{frag}). The function minimized during refinement is then $-\ln(L)$.

The procedure was illustrated with refinement of a model of the pharmaceutical remacemide nitrate in which the nitrate ions had been omitted. Least squares was shown to fail because the algorithm attempts to mop-up nitrate density distorting the remacemide molecules. Application of the maximum likelihood method, by contrast, converges on the correct positions for the remacemide molecules. It was also noted that maximum likelihood is widely used in macromolecular crystallography to take into account model errors (in the modeling of the molecule and/or solvent water). It was concluded that maximum likelihood extends the range of models that can be successfully refined. A full description of the method described is available in *Acta Cryst.* (2002) **A58**, 316-326.

The third and final section of the lecture described the use of the Hybrid Monte-Carlo (HMC) method as an alternative to simulated annealing in solving crystal structures from powder data. The essential difference between the two algorithms is the incorporation of dynamics in the HMC procedure. The method was illustrated using a particle on a surface which contained several minima of different depths; the aim is to find the lowest minimum. The particle is placed at some arbitrary position on the surface, and then 'given a kick'. The particle moves across the surface sampling different minima as it does so. When inside a local minimum the particle has low potential energy, but by conservation of energy, it also has high kinetic energy, and it is this that enables the particle to escape local minima. In crystallographic applications the potential energy corresponds to χ^2 .

Taken alone this procedure tends to be fast but rather unstable, but when combined with the conventional Monte-Carlo algorithm, which is slow and stable, the outcome is a fast, stable method for global optimization. HMC was illustrated by reference to the solution of the crystal structure of capsaicin, which in addition to requiring the position and orientation of the molecule to be determined, also has 7 conformationally flexible torsion angles. HMC was shown to solve the structure more quickly than simulated annealing. Implementation of the algorithm was also found to be straightforward as it only requires the evaluation of derivatives to model the equation of motion of the 'particle'. This method has also been published in *Acta Cryst.* (2002) **A58**, 441-447.

We wish to congratulate Dr Markvardsen on the award of the CCDC Prize, and thank him for an illuminating presentation.

Simon Parsons

High Throughput Crystallography

THIS parallel-session lasted all the morning on the final day of the meeting.

Jim Naismith chaired the first part. The first speaker, **Dr. Michael Sundstrom**, spoke on *Directed structural genomics: a protein family approach*. He introduced the Structural Genomics Consortium (SGC), which is a not-for-profit organisation that determines three-dimensional structures of proteins of medical relevance and provides the information to the public domain. It attempts structure determination of up to 200 protein structures per year. There are about 900 targets including dehydrogenases, reductases and proteins involved in phosphorylation dependent signalling and membrane receptors. He took us through the process of how they go from targets to structures, through making a dozen constructs to testing solubility and scaling up and analysing sequences, to crystallisation trials and solving structures. Most of the steps are automated and are much faster than conventional methods. He concluded by encouraging collaboration on structures that they have already solved. The volume of results presented was breathtaking.

Our next speaker **Professor Keith Wilson**, talked about *Trying to speed up the 3D structure pipeline: SPINE - (Structural Proteomics in Europe)* which started in October 2003. It involves more than 20 partners in eleven European countries working together to build a

standard, streamlined decision-making process - known as a pipeline - for identifying protein structures important for new drug discovery. It aims to solve 300 protein structures in three years. So far, also very impressive, 105 crystal structures and 28 NMR structures have been solved. SPINE's main targets are human bacterial and viral pathogens, cancer and immune dysfunction diseases. Keith also mentioned some of the solved structures that have medical importance, e.g. Sars Coronavirus Nsp9, Carboxypeptidase M, and E. Coli tRNA Pseudouridine Synthase Trud. Automation was mentioned which can speed up the processes required such as cloning and clone confirmation (done in 3-4 days), protein expression (done in 5-6 days) and crystallisation (requiring only nanolitre drops).

Ending the first part of the session was **Dr. Jeff Blaney**, His talk was on *Structure-guided fragment based drug discovery*. He explained how SGX has developed FAST™, a proprietary technology for rapid identification of novel, potent and selective small molecule inhibitors (MW 150-200) for drug targets. SGX utilizes X-ray crystallography techniques to ensure fast structure solution, including the incorporation of selenium into proteins, and the use of a third-generation synchrotron (namely APS in Illinois), for MAD phasing. As SGX had developed the emphasis they had switched from MAD phasing of new proteins to high throughput ligand bound structures. These ligands usually incorporated a bromine atom and so by use of anomalous scattering (f⁺ data) the orientation of a ligand was quickly determined. The success of using FAST™ in fragment-based lead discovery was highlighted with results for



protein kinases (Syk and Gleevec resistant BCR-ABL) and proteases (Factor VIIa).

After the tea break, the talks, chaired by **Charlie Bond** continued with a presentation by **Samar Hasnain** entitled *Combined X-ray approach for studying metalloproteins function/misfunction: a powerful approach to metalloproteomics*. Metalloproteins make up some 30% of proteins in known genomes. Several X-ray techniques including protein crystallography, Solution X-ray scattering and X-ray absorption fine structure (XAFS) have been very useful in studying metalloproteins. The marriage of XAFS and crystallography has been beneficial for structure-function studies of metalloproteins. Furthermore, the NWSGC's beamline has for the first time brought together high throughput MAD and single crystal XAFS as well as on-line metal screening that is very useful for studying metalloproteins.

The second speaker was **Bill Duax**, President of the International Union, who was highly enthusiastic about his research on *Multiple open reading frames, codon bias and amino acid use and the evolution of the genetic code*. His work done on the genome of *S. Coelicolor* revealed that the antisense strands of 70% of the 7555 genes (5277) contained no stop codons and therefore could be open reading frames (ORFs). Bill also talked about the short chain Oxido Reductase (SCOR) enzyme family that revealed multiple ORFs (MORFs) and a bias in codon usage. The MORFs in the SCOR enzymes and *S. coelicolor* appeared to identify a subset of the codon system that evolved first, and a subset of amino acids that made up the composition of the earliest folded proteins. He concluded that the benefits of such results could enable one to express protein from the antisense strand to produce for example antibodies to treat autoimmune diseases.

The session ended with a talk by **Tom Oldfield**. He gave an overview of *the macromolecular structure relational database (MSD)*, at the European Bioinformatics Institute (EBI), where you can access, organise and store data on macromolecular structures. There are many useful sites and links available. The results can be viewed within the AstreXViewer™@MSD-EBI. Furthermore, the time of request is very short, not more than five seconds. There was enthusiastic discussion about these developments especially the way in which widely different audiences and users had been catered for; helpful tutorials were just one feature facilitating these very important developments for widening of the use of all the structural data now available.

Arefeh Seyedarabi (Queen Mary College)
Helal Ahmed (University of Manchester)

Modern Techniques of Crystal Structure Refinement

THE parallel session “Modern techniques for crystal structure refinement” took place on Wednesday, 13th of April. It was divided into two sections based on talks and a CRYSTALS workshop.

The first part of the session was chaired by **Charlie Bond** (Dundee), who elegantly introduced the first speaker, **Richard Cooper** (Oxford), who spoke on *Advanced techniques in structure refinement*. The talk was based on the use of the least squares statistical technique in modern crystallography. Starting with the basics of least squares including the use of the design and normal matrices along with weighting schemes he went on to explain the use of the normal probability plot in assessing the validity of weighting schemes and spotting potential systematic errors. He explained a number of advanced techniques in structure refinement including the use of restraints. Particular emphasis was placed on the treatment of hydrogen atoms, though it was pointed out that modern refinements packages allow much more freedom by providing facilities for ‘generalised’ restraints based on any choice of linear equation. Another advanced technique highlighted was the use of a sparse matrix, which simplifies the Normal matrix by ignoring off-diagonal terms between atoms not in close proximity. This greatly reduces the number of parameters needed and is thus particularly suited to large structures. Finally non-atomic electron densities were discussed, in which fragments of crystal structures can be better modelled using geometric electron density envelopes e.g. a torus, rather than standard spherical atom approximation. He detailed briefly the use of MOGUL to aid the application of chemical restraints to a model and described the difference between restraints and constraints. After this he demonstrated his points with a number of practical examples. The presentation closed with a hands on description of the handling of the normal matrix in structure refinement using the program CRYSTALS.

The next talk given by **Thomas Schneider** (Milan) dealt with the *Refinement of proteins as large small molecules using SHELXL*. The importance of parameter reduction was stressed and was humorously described as “Scottish” in nature by the speaker. He presented the case of modelling residues using appropriate restraints and limiting the number of parameters by using single site occupancy factor for structural fragments. For such systems, the estimation of the precision of refined parameters from full matrix inversion is not always a straightforward process since there are often strong correlations between the radial standard uncertainties for partially occupied sites. The solution to this situation is of course the use of appropriate restraints to stop these sites ‘fighting’ over parameters.

The final presentation in the session was by **Garib Murhudov** (York), on *REFMAC, recent developments towards automatic refinement*. The protein structure refinement program REFMAC draws upon prior knowledge of two types to aid structure refinement. These were described as *Chemical knowledge*, for example bond angles etc. and *Structural knowledge*, from the protein database. A description of REFMACS handling of protein building blocks and general structural knowledge was followed by a discussion of the protein database as a source of knowledge and its limitations and reliability. The emphasis then shifted to a discussion on the use of TLS in describing atom oscillation for atoms close in space compared to atoms far apart. The session closed with a snappy analysis of the use of B values in protein crystallography detailing their γ^{-1} distribution as well as the correlation between B values and atom spacing and a description of how knowledge from the protein database

this program based technique. Finally, as Charlie pointed out, if you are in any doubt, it's probably Zn^{2+} !

The next talk *Beyond least squares*, given by **Bill David** (ISIS), discussed why and when the use of least squares is appropriate. Least squares techniques underlie many of the day to day programs used in structure determination. Bill posed the question, how appropriate the application of least squares is to the problems where we routinely use it. When the data show that they fit a different model from the Gaussian distribution, how can we justify using standard least squares procedures? He then described a scale-invariant method known as Jeffrey's Prior which was able to fit data significantly better by greatly reducing the effect of outliers present in the data and thus removing the need to remove such outliers by some other arbitrary criteria. In summary he suggested: don't throw away your least squares models, just accept their limitations!



Finally, **Alan Coelho** (ISIS) talked about *TOPAS-Academic, programming ideas*, addressing computing issues when producing software. It was a far reaching and thought provoking discussion of the functionalities and future direction of scientific computer programming. Amongst numerous technical points regarding the future of academic programming there were a few themes running through the discussion. Firstly that the functionality of any program is limited by the user, secondly that it is important to consider the organization of a program as this will determine its longevity and ease of adaptation (the speaker had a strong preference for hierarchical tree organizations). Clearly the message is that we should concentrate not on building monolithic applications but on building software 'tools' that can be used in ways never anticipated by the programmer.

can be used to impose restraints on these B values. The second part of the session, chaired by **Simon Parsons** (Edinburgh), began with the talk *What's that blob? Identifying metal ions in protein crystal structures*, by **Charlie Bond** (Dundee). Seeing that half of all reported proteins contain metal atoms, this is of paramount importance in protein crystallography and, perhaps surprisingly, establishing their presence and identity is not as straightforward as might be expected. The speaker described numerous examples of ambiguous electron density that could be a metal ion and suggested two approaches to determining what is present. The first approach, X-ray fluorescence, was not discussed in detail due perhaps to its being covered elsewhere at the meeting. The second approach, using programs such as WASP to determine metal ions, presence was described in some detail and numerous real-world examples were detailed together with the outcome of the application of

The last part of the session was a the CRYSTALS workshop, given by **David Watkin** (Chemical Crystallography Laboratory, Oxford) on how to treat problems relating to refinement, such as disorder or high atomic displacement parameters, pseudo-symmetry and twinning.

Patricia Lozano-Casal (University of Edinburgh)
Robert Taylor (University of Bath)
Michael Turner (University of Durham)

Phase Transitions

The phase transitions talks were held on Thursday. The session began with a very valuable tutorial session entitled *Critical Aspects of Structural Phase Transitions* by **Mike Glazer**. Assuming little or no prior knowledge of this area of research, he began by explaining a phase transition as some form of change in a system while preserving its chemical composition, e.g. loss of symmetry within a solid. He illustrated displacive, order-disorder, and reconstructive transitions, and explained the Landau (Mean Field) Theory, an empirical description of the behaviour of crystals at phase transitions. He gave two practical demonstrations. The first illustrated critical opalescence as a clear mixture of aniline and cyclohexane was heated, and the liquids mixed to form a single phase cloudy suspension at the critical point. In the second, an Euler strut was used to demonstrate soft modes of vibration. The tutorial ended with consideration of strontium titanate, a much studied perovskite which undergoes a structural phase transition at 105K, driven by the rotation of the oxygen octahedra around one of the cubic axes.

After a much-appreciated tea-break, the session continued, chaired by **Pam Thomas** with **Jens Kreisel** (Grenoble), on *Pressure-induced phase transitions in relaxor-based ferroelectrics*. These concerned some ABO_3 type perovskites whose interesting dielectric behaviour is studied under electric field and as a function of temperature. This has been extended to pressure, a clean parameter acting only on interatomic distances. The structure $Pb_3ZnNb_2O_9$ (PZN) has a rhombohedral average structure at 300K, and undergoes a phase transition between pressures of 1bar and 7.3GPa. and two further phase transitions as the pressure is raised to 31GPa. These phase changes could be followed using Raman scattering and by following the progress of diffuse scattering features which show the development between ordered and disordered phases.

Julian Haines (*Stability of crystal structures of α -quartz homeotypes at high temperature*), discussed some homeotypes of α -quartz (GeO_2 , $FePO_4$, $GaPO_4$, and $GaAsO_4$). These are of interest as the piezoelectric properties of α -quartz are limited at high temperature, while $GaAsO_4$ is stable 1198K. These were studied by neutron powder diffraction and neutron total scattering to determine the thermal stability of the α -quartz equivalent phases.

Michael Carpenter described the *Role of protons in phase transitions in lawsonite*, a framework silicate in which paired tetrahedra of Si_2O_7 are linked by AlO_6 octahedra. The structure contains channels which can host water and calcium. It undergoes ferroelectric, coelastic, and ferroelastic phase transitions, the natures of which were explored using a combination of techniques. Phase transitions due to displacements and ordering of the H/D atoms were indicated by significant change of the transition temperature on H/D substitution. In the absence of this effect, the conclusion can be drawn that the phase transitions must be mostly due to framework distortions. At 9.5GPa, a high pressure form is observed which is a proper ferroelastic. From the Raman spectrum, this form is not accompanied by proton ordering, only displacements in the framework.

After lunch, **Laurent Chapon** discussed the *Magnetic phase transitions in $RMnO_5$* where the key to the magnetoelectric properties may be magnetic frustration. They are weak ferroelectrics in their ordered state and have a spontaneous polarisation along the b axis. They show some anomalies in the temperature dependence of the dielectric constant – in fact there are 4 transitions on cooling. The structure contains 5-membered rings of magnetic atoms which leads to magnetic frustration. The magnetic diffraction was followed as a function of temperature using powder neutron diffraction at ISIS on GEM. The structural changes could be mapped to the magnetic phase transitions.

Ivana Radosavljevic-Evans presented work on the material $La_2Mo_2O_9$ which shows high oxide ion conductivity at 1100K. These types of materials are technologically important with potential applications as oxygen sensors and pumps, membranes for oxygen separation, and solid oxide fuel cells. $La_2Mo_2O_9$ has a phase transition at 850K above which the conductivity increases significantly. The structure of this material at room temperature was solved from powder diffraction data. Despite having a simple formula, there are 312 crystallographically unique atoms in the structure making it one of the biggest structures to be solved by powder diffraction. Insight has been gained into the oxide migration pathways in the high temperature structure.

Anna Collins (University of Oxford)
Teresa Savarese (University of Bath)
Lynne Thomas (University of Cambridge)



Photocrystallography

Phil Coppens' plenary talk *X, Y, Z & time: introducing the time dimension into crystallographic research* was an ideal introduction to the photocrystallography parallel session. He spoke about the data collection strategies required for this technique, and presented his results on $d^8 - d^8$ and $d^{10} - d^{10}$ metal systems. Despite generating relatively low populations of the excited states within the crystal, changes in bond lengths observed relative to the ground state could be measured and are generally comparable to those predicted by theory.

After a good night resting from the poster session and a hearty breakfast, we started the Photocrystallography section on Wednesday with a lecture from **Jacqui Cole:** *Single-crystal X-ray diffraction studies of photo-induced molecular species*. She gave an overview of the various approaches to this technique, presenting results from the US and UK on metastable states, and specific work on ruthenium complexes so photosensitive that the work had to be done in a makeshift tent to prevent the safety lights from ruining the experiment. She described developments of a mechanical chopper which will create short X-ray pulses (40ms - 3 μ s) to allow time-resolved methodology to be applied. She concluded that with Diamond currently being built, the UK will have unique opportunities in the field of time-resolved crystallography.

From a woman with a sharp chopper to another with a big laser! **Judith Howard** talked about *Spin cross-over complexes: structures and photomagnetism of high spin, low spin and metastable states and the LIESST effect*. In the case of the iron(II) complexes discussed, irradiation of the crystal with red laser light resulted in an electronic transition from the low spin state (ground state) to a metastable high spin state (excited state) which were sufficiently stable at low temperature to enable the structures to be investigated using X-ray diffraction. Unlike the samples discussed by the other speakers in this session, the conversion to the new state is 100%. The crystallographic observations in these systems were a change in the mean Fe - N bond length and decrease in the ligand bite angle.

The session continued with three international speakers, all of whom gave outstanding talks. **Simone Techert** (Göttingen) presented some lovely work on *Perspectives of time-resolved X-ray diffraction with XFELS; studies of topochemical single crystal - single crystal transformations*, which showed that the crystals become amorphous during the reaction. Charge density analysis was carried out on these systems. The second part of the talk included a consideration of the potential use of XFELS (X-ray Free Electron Laser) for *in-situ* XRD investigations of dynamical processes occurring on the femto-second time-scale, such as ion-migration through solid-state structures, molecular relaxation processes, and photochemical reaction mechanisms.

After coming back from fighting the tea-ladies for a cup of tea, we heard **Eric Collet** (Rennes) tell us about *The key role of X-ray diffraction for the investigation of photo-induced phase transitions*. This involved the use of pico-second time resolved synchrotron X-ray diffraction for studying light-induced phase transitions, with particular reference to the transition between neutral and ionic phases observed in molecular charge-transfer materials. When they excited the material, it formed layers of alternating high and low spin domains. The relaxation was not a simple exponential which was due to molecules being interconnected, producing a cooperative effect.

Beatrice Vallone (Rome) gave a more biologically orientated talk, by discussing protein structural dynamics. In the example presented, this technique was used to study the mechanism by which sperm whale myoglobin functions as it is suitable for time resolved structure determination. In order to study the protein dynamics, the various intermediates can be trapped, or a single crystal of the protein can be used and time-resolved crystallography applied. In the example discussed, Beatrice used Laue diffraction.

The session concluded with a second biological lecture, this time given by **John Helliwell**, *The 15K neutron structure of saccharide-free concanavalin A*. The presentation was concerned with a low-temperature neutron diffraction study of this bean protein, using the Laue diffractometer at the ILL in France. John talked about the experimental procedures for collecting neutron diffraction data at low temperatures, and highlighted the benefits to be gained from this type of analysis.

Martin Adam (University of Glasgow)
Katherine Bowes (University of Cambridge)
Elinor Spencer (University of Durham)



Crystallography in Industry

Wednesday's afternoon session "Crystallography in industry" was chaired by **Judith Shackleton** and opened with **Michael Preuss** (University of Manchester) lecturing on '*Residual stresses in friction welded aeroengine components*'. He talked about the types of friction welding: friction welding has the advantage over fusion processes which cannot reliably weld many of the high temperature alloys now found in aero engine components: the inertia friction method is used to join discs/shafts and the linear friction method for joining blades onto discs. A consideration during friction welding however is the generation of residual stress, during joining, and stress relief during post weld heat treatment. Industry has turned to synchrotron high energy dispersive X-ray scattering to enable researchers to undertake systematic studies of the residual stress profiles in welds and improve the understanding of how welding parameters and post weld heat treatments affect the residual stress fields and the performance of the welded component. The talk was concluded with the fact that higher temperatures for annealing brings down stresses to acceptable levels.



Tony Fry (National Physical Laboratory) followed with his lecture on '*Residual stress measurements at NPL. Increasing confidence and development best practice*' in which he talked about the parameter study to find how robust the x-ray diffraction method is. He went through two projects undertaken at the NPL and ended with mention of the Good Practice Guide authored with the Projects Industrial Advisory Group. The talk ended with a good discussion from delegates in the room.

Martijn Fransen (PANalytical) ended this first session with an enthusiastic lecture on '*The problem of sample fluorescence when dealing with transition metals in industrial samples*'. The talk covered 1-D and 2-D detection systems and posed the question "Can you get good peak/background ratio?" He went through the best choices of the practical aspects from the monochromator to the detector as a function of the elemental composition of the sample.

The second part of the session, chaired by **Richard Morris**, opened with **Peter Laggner** (Graz, Austria) on *Bridging the nano-gap: simultaneous SAXS and XPD on*

nanomaterials. He covered a lot in his talk giving a range of examples such as synthesis of mesoporous materials and dissolution of drug-delivery C/R microspheres. He focused on the design of the HECUS-System3 SWAXS (small and wide angle x-ray scattering) and its use in different applications. The need for SAX for determining domain size and surface roughness and XPD for crystal structure and amorphous content was explained.

The session was brought to an end with an interesting lecture from **Ian Cope** (Imperial College). Ian explained his PhD research: *Using XRD to support the study of an iron oxide deposit*, called the Pic de Fon deposit. This deposit is a potential new source of iron ore located in the Eastern Republic of Guinea, West Africa. The aim is to combine XRD and geochemical analysis to constrain the process by which banded iron formation is converted to iron ore.

It was good because as a field geologist he knew little about XRD, but was interested in how it could help in his research. XRD results indicate that distinct crystallographic signature may exist for the different ore grade material types. Each ore-grade material type exhibits different physical properties, hard, biscuit and powder, which in turn will control the metallurgical performance of the final delivered product.

All the presentations gave a useful insight into where and how crystallography is used in industry and the different type of demands industry places on crystallographic hardware compared to academia.

Robert Davies (University of Oxford)
Nicola Turvey (Aston University)

At and in the Membrane

At and in the membrane was a single session, chaired by **Steve Prince** gave three complementary talks on membrane proteins from protein expression to structural features. **Steve Baldwin**, *Membrane protein expression in the genomic era*, related the problems associated with the expression of correctly folded membrane proteins and possible applications of high-throughput methods to increase the success rate and remove the current rule of thumb: the mass of protein obtained is directly proportional to the number of post-doc/student hours put in. **Piet Gros**, *Two outer-membrane proteins: translocation through a narrow beta barrel pore and a tilted beta barrel*, described the structure of two interesting proteins, NalP and PagL. The mechanism by which NalP translocates its N-terminal domain was eloquently described before the unusual tilt of PagL within the membrane was explained, partially by considering the position of aromatic residues within the protein. The session finished with **Pascal Egea**, substituting for Bob Stroud, on how selectivity filters function, allowing membrane proteins to, for example, conduct H₂O but not H⁺ ions.

Robin Owen (University of Oxford)

Exhibitors at BCA Spring M



Analysco



Alpha Helix Ltd



Beevers Miniature Models



Bruker Nonius



CyBio



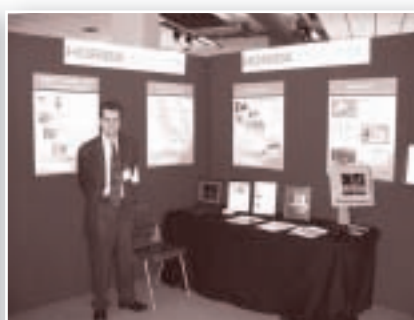
Fluidigm



Genomic Solutions



Hiltonbrooks



Horiba Jobin Yvon



ICDD



Malvern Instruments



Marresearch

Meeting, Loughborough



Molecular Dimensions



Oxford University Press



Oxford Cryosystems



Oxford Diffraction



Oxford Instruments



PANalytical



PerkinElmer LAS



Rigaku



Socachim-XRF Scientific



Spectro



Spex Certiprep



Taylor & Francis

Obituaries

Robin Shirley 1941-2005

(Two appreciations are given here - the first from Robin's Head of Department, the second from his long-time friend Mike Glazer. - Ed)

It is with great sadness that I have to announce that Robin died in hospital on Sunday, 27th March 2005. He had been suffering liver problems since contracting Hepatitis A last November and these finally proved fatal on Easter Sunday.

Robin was born in Harrow on 1st July 1941 and graduated from UCL in 1964 with a BSc in Chemistry. He joined the Department of Chemical Physics at Battersea College in 1967 as an Assistant Lecturer in Crystallography and moved to the Guildford campus shortly afterwards. Robin commenced a secondment to Psychology in 1988 as a Senior Research Fellow in Information Systems. This was combined with a collaborative arrangement with the Clarendon Laboratory at Oxford to allow for the continuation of his crystallography research activities in x-ray powder diffraction and crystallographic computational methods. The Psychology secondment continued until 1997 when Robin formally transferred over to Psychology in the new School of Human Sciences.

Robin assumed responsibility for teaching undergraduate statistics. Despite this being an unpopular subject, he was much loved by the students who valued his genuine concern to help them and his willingness to spend that extra bit of time explaining things. Robin was accessible to students and his student feedback often expressed gratitude for the pastoral role he willingly assumed. As well as his software development work for his crystallography research, Robin produced a complete integrated suite of instructional programs intended to promote understanding of statistical theory. It is unfortunate that more was not made of the software which was very innovative for its time. Robin was always keen to make improvements and he never regarded it as finished.

Although based in Psychology, Robin continued to develop and disseminate his work on powder indexing presenting his ideas around the world. He organised and contributed to the Crysfire 2001 suite of programs for determining powder structures which is widely used in the academic community and available in an industrial version. He continued to develop and demonstrate the programs up to the time of his death. Robin probably contracted the Hepatitis A during a visit to Egypt last November for a 5-day International Powder Diffraction Workshop at Assiut University. There his lectures went well but running his

software for the lab sessions proved to be difficult because the computers were running an Arabic version of Windows!

In various committees and boards of studies Robin was notable for arguing strongly for what was just and right. Unwilling to sit back and let events pass him by if he thought something was not being dealt with properly, he was sometimes in conflict with colleagues but his views often prevailed and he gained respect as a man of principle. These qualities were carried over into his Union activities. As Chair of the local AUT branch Robin was intimately involved in a wide range of activities and came into contact with many people across the University. Initially a reluctant Chair, he became an effective negotiator on behalf of AUT members. He was able to bring a rational, logical approach to union activity and negotiations without ever losing sight of his responsibilities to the members.

Robin will be remembered by many as someone who was very intellectually sharp. He had an endearing habit of arriving late for Psychology seminars yet would still be able to ask (usually the first) penetrating questions that often got to the heart of the debates at hand. This was all the more impressive as he was not, until relatively recently, trained as a psychologist and still saw himself as a crystallographer, computer scientist, and English poet. He had a genuine enthusiasm for ideas of all kinds.

Away from work he was External Activities Coordinator and then Chairman of the Wey Poets (Guildford & West Surrey Centre of the Poetry Society) and he organised and took part in poetry readings and participated at various festivals. He also lectured, published and broadcast on the subject of computer poetry and the programmed generation of language generally. He was a member of the Computer Conservation Society and used to maintain a gallery of microcomputer exhibits at the Computer Museum, Bletchley Park.

He will be remembered as someone who was always to be seen at social events whatever they were. He was a Father Christmas at the staff-student Christmas parties for a number of years and also the target of many a fond student 'sketch' in the annual party review. He was always portrayed sympathetically (not the norm for many staff) reflecting the warmth and esteem with which the students regarded him.

Robin was one of the great characters of the University and he will be missed.

Chris Fife-Schaw
HoD Psychology, University of Surrey

I was stunned today to receive the unexpected news that Robin Shirley had died on Easter Sunday, 27th March 2005. I had not known that he had been ill, and so this came as a complete surprise and a personal shock. It appears that he contracted Hepatitis A last November, probably during a visit to Egypt to attend a 5-day International Powder Diffraction Workshop at Assiut University, and this led to acute liver problems, from which he failed to recover.

Robin was born in Harrow on 1st July 1941 and graduated from UCL in 1964 with a BSc in Chemistry. In 1965, our paths first crossed, when I arrived in Kathleen Lonsdale's laboratory in the basement of the Chemistry Department of UCL to begin my postgraduate research. I well recall that on that first day there, I was surprised by a jovial bald-headed Lenin-lookalike with a loud voice bounding down the stairs from what we called the mezzanine floor. Robin had joined the lab a couple of years earlier to work on the crystallography of gall and bladder stones. Mrs Lonsdale had acquired a large collection of these stones, ranging in size from less than 1 cm up to one monster that was nearly as big as football, which Robin was most keen to show to me. If I recall correctly it was labelled "Mrs Olive Green". Needless to say, we quickly became friends, and "Mrs Olive Green" was often mentioned whenever we met in later years.

Robin, it has to be said, did not always hit it off with Mrs Lonsdale, and so he developed a kind of love-hate relationship with her (although many years later he did confide in me that looking back he realised how much he was indebted to her). Part of the problem was that he could sometimes appear to be abrasive, but this followed from a sharp and highly cerebral and critical mind. He was someone who did not suffer fools gladly. But at the same time he was warm and kind, especially to the other students in the group, and could always be approached for useful advice and help. It was Robin who first showed me how to use a polarising microscope, a technique that has remained with me to the present day.

In 1967, he was appointed to an Assistant Lectureship in Crystallography in the Department of Chemical Physics at Battersea College (later to become the University of Surrey). It was then that he turned his attention to the problem of automatic indexing of powder patterns and he wrote an influential review of all the techniques then available, which is still read today. However, it seems that he didn't quite see eye to eye with some members of the Department and in 1988 he moved to the Department of Psychology as a Senior Research Fellow in Information Systems. I was very happy during this time to be able to offer Robin and his PhD student laboratory space in Oxford while he sorted out his position at the University.

The Psychology secondment continued until 1997 when Robin formally transferred over to Psychology in the new School of Human Sciences. Here he taught undergraduate statistics, which, despite being an unpopular subject,

won the approval of his students. Indeed it is reported that they loved him for his genuine concern to help them and his willingness to spend extra time to explain things. I understand that he produced a complete integrated suite of instructional programs intended to promote understanding of statistical theory.

Several years ago, he was struck by serious personal tragedies that would have derailed most people, and indeed for a few years, he vanished from the Crystallography scene. I was delighted when he eventually resurfaced at a Crystallography conference to rekindle his involvement in the problem of powder indexing. As is well known, he began to put together the CRYSFIRE suite of programs, in which different powder indexing software was joined together in such a way that the user could easily migrate from one type of indexing program to another. CRYSFIRE rapidly established itself as an influential development, and very soon, Robin was invited everywhere that powder indexing was to be discussed and he was a popular figure at Crystallography conferences world-wide.

Readers may like to know that Robin was also a well-respected poet, having participated at several poetry festivals. He also lectured, published and broadcast on the subject of computer poetry and the programmed generation of language generally. He was a member of the Computer Conservation Society. A few years ago I was fortunate to be invited to the Science Museum to see the unveiling of a Ferranti Pegasus Mark II computer that he and the Society had managed to restore and get working. This was the very same machine that I, Howard Flack and Robin used during our graduate research, and I believe that it is now the only working valve computer in the world. Robin and I felt quite nostalgic when it was switched on to play Teddy Bear's Picnic and Rocking through the Rye (we used to play this during long hours at night working on this machine). You can see this for yourself today in the computer gallery of the Science Museum.

Robin was a larger than life figure, a real character, and I shall miss him.

Mike Glazer





Gordon Cox and Jackie Truter at the 1954 Paris IUCr

Mary Rosaleen Truter 1925-2004

Jackie Truter (Lady Cox) died from leukaemia on 26 November 2004. Her career in X-ray crystallography began in 1945 and at her death she was still active as Visiting Professor in the Chemistry Department at University College, London. She was the widow of Sir Gordon Cox FRS.

The following obituary draws heavily on the short autobiography she completed in March 2004 for her family and friends; direct excerpts are in quotation marks.

Mary Rosaleen Jackman was born on 19 December 1925, the only child of Douglas Jackman, research chemist and subsequently general practitioner, and Agnes Browne, lecturer in chemistry. 'Jackie' was the nickname she was given when a Girl Guide in London. She was a scholar 1936-1942 at St. Paul's Girls' School, which she loved. At the end of her first year at Imperial College, London she "got a first in the special Inter BSc exam for intending chemists, to the astonishment of people who assumed that with my looks I could not have a brain". She graduated in 1945 with a II₁ in chemistry.

A.J.E. Welch, who had given excellent lectures on crystal chemistry, started her on research with X-ray powder photography. After hearing **Sir Lawrence Bragg** at the Royal Institution she "was hooked on crystallography." In late 1946 she saw an advertisement for an assistant lecturer with 'an interest in, but no necessary knowledge of, crystallography'. She applied and got the job in the Department of Inorganic and Physical Chemistry at Leeds University, starting in January 1947. Her fiancé **Dr. Eric Truter**, whom she had met as a chemistry student at Imperial College, obtained a Fellowship in the Leeds Textile Department and they married in March 1947.

The University of Leeds 1947-1966

Her head of department **Professor E.G. Cox** "said that he would teach me and then I should teach the post-graduate students. I started a new research project and registered for the External PhD of the University of London. I did not want to be registered in Leeds because people would discover how young I was. I got the PhD in 1952".

"The PhD problem was to determine the crystal structure of nitronium perchlorate, $\text{NO}_2^+\text{ClO}_4^-$. The crystals had to be kept out of contact with air; for comparison I also studied Na^+NO_2^- . I took photographs, made visual estimation of the greyness of the spots and did the necessary computations with an electro-mechanical calculator and Beevers-Lipson strips." Soon she joined in the development of punched card methods and computer programming. She investigated S-O and S-C bond lengths in various valence states of sulfur. This led on to comparisons of bond lengths in small molecules in their crystals and as ligands in metal complexes. All the while she carried a heavy teaching load.

With her research students she achieved a considerable reputation with a series of papers on trimethyl platinum compounds, arising from syntheses by **R.C. Menzies** dating back to 1928. A paper in 1956 described a di(trimethylplatinum) complex involving three ethylene diamines, only one of which was bridging. Crystallographic methods had now reached a stage where C and N could be located and distinguished despite the presence of Pt and I. Of particular interest were the unusual structures of dimeric trimethylplatinum α -diketonates in which each α -diketone made two O-Pt bonds to one Pt and one C-Pt bond to the second Pt. New compounds were synthesised to study the character of the relatively long sixth Pt-C bond in the octahedral coordination around platinum.

As a close colleague of Jackie's at Leeds, I found her unfailingly cheerful and patient in tutoring me in chemical matters; reciprocally I appreciated the good use to which she put my contributions to mathematical and computational methods. My interest in tetrahedral oxyanions, and the heuristic $d\pi$ - $p\pi$ bonding hypothesis, arose directly from her structures. We were beneficiaries of Cox's leadership and his success in building up a strong and lively all-round group in chemical crystallography.

She was promoted Reader in Structural Chemistry in 1960. Shortly after, Cox left to become Secretary of the Agricultural Research Council. He was eventually replaced by an inorganic/analytical chemist. Her lab space was reduced, and teaching with larger classes became less pleasant. In January 1965 her marriage with Eric Truter broke up.

London 1966 - 2004

In 1966 she was invited by **Prof. Ron Nyholm**, Head of Chemistry at University College, London, to become Deputy Director of the ARC Unit of Structural Chemistry.

This was a new venture to allow him, as Honorary Director, to expand his research interests into alkali and alkaline earth metal compounds. Since there was insufficient space in College, the Unit started in October 1966 in a government office building in the Strand. By 1968 the place had been made into a proper laboratory with its own computer and automatic diffractometer. There were four post-doctoral members of staff as well as visitors and students.

"I had taken a big risk because the idea was to look for complexes of alkali and alkaline earth metal cations to see if we could understand and even emulate the discrimination shown by biological systems between e.g. sodium and potassium. We were not sure there would be any complexes but we soon made some and then had the good fortune to determine the crystal structures of several of Pedersen's crown ether complexes. [Pedersen, Nobel laureate 1987, had shown by 1967 that macrocyclic ethers extract metal salts into non-polar solvents and act selectively on these metals. He spent three months in the Unit in 1969.] Many papers were published. Ron was delighted with the progress of the Unit, and I was made a Professor of the University of London". Jackie's 1973 review in *Structure and Bonding* of 'Structures of organic complexes with alkali metal ions' was an ISI Citation Classic in 1989. She received a Chemical Society Award for Structural Chemistry in 1976.

In November 1962 **Gordon Cox's** wife Lucie had died of a heart attack. Jackie married Gordon in May 1968. He retired as Secretary of the ARC in September 1971.

In December 1971 disaster struck when Nyholm was killed in a road accident. The whole future of the Unit was uncertain, but eventually the ARC decided that it should be moved to Rothamsted Experimental Station in Hertfordshire. Initially scattered around the Rothamsted complex, the renamed Molecular Structures Department moved in 1977 into purpose built accommodation.

"Our work in Rothamsted remained the same as in London. We did a small number of crystal structure determinations for other people in the Agricultural Research Service (ARS), particularly the Unit of Nitrogen Fixation; we had already done some pyrethroid insecticides before moving to Rothamsted. The main thrust remained synthesising compounds with potential to complex selectively with alkali and alkaline earth metal cations" and examining the transport of these ions within biological systems, particularly membrane transport. At Rothamsted, "we changed from an animal (rat liver mitochondria in UCL) to a plant (opening of stomata in leaves) bioassay." The Molecular Structures Department was a happy group and highly productive in several areas.

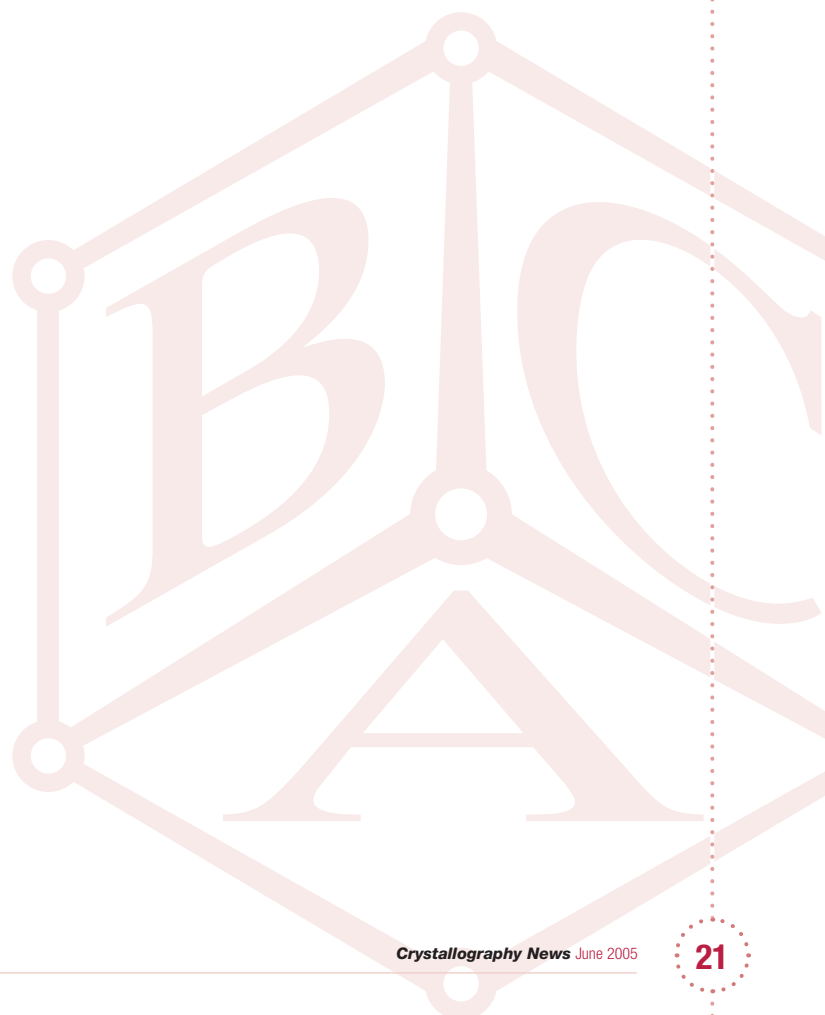
"When I joined Rothamsted officially, April 1973, morale was very high. It was the oldest, biggest and best agricultural research institute in the world. This continued during 1981 when the universities were hit by

Mrs. Thatcher's cuts. ... In the spring of 1983 the then Secretary of the ARC (**Ralph Riley**) visited Rothamsted and other institutes to warn of coming cuts. On Sept 7th 1983 the Director told me that I and all my staff were to be made redundant, essentially because our work was too basic with no immediate pay-off. His hope that we would all be gone by the end of March 1984 was not fulfilled as we fought back. The borrowed time allowed my staff to get other jobs and I was given 6 months notice in July 1984. In November 1984 I moved out of Rothamsted and into a room in University College."

There she did some teaching and, in the earlier years, continued with research more or less full-time. She had mutually valued relations with both her Jackman cousins and the Cox family. Gordon suffered increasing ill-health from 1992 and died in June 1996. Her own leukaemia was first diagnosed in 2002. In periods of remission, she continued to visit the College. She died in November 2004.

Especially as a younger woman, Jackie cut an attractive figure, elegantly dressed and independently stylish. At Leeds she entered fully into the general and social life of the University. She was a founder member of the BCA, a past chairman of the CCG and a trustee of the CCDC. At Rothamsted colleagues were always impressed with her dedication – to the work, to her staff and students and to the laboratory. Her many friends in the UK and around the world mourn her passing.

Durward Cruickshank



Other Meetings

Report on the South West Structural Biology Consortium meeting at Bristol, 20-21st March 2005

THE meeting was held in the impressive venue of **Burwalls**, a mansion house within view of the Clifton suspension bridge. The meeting was attended by around 80 participants from structural biology groups in Bath, Bristol, Exeter, Portsmouth, Southampton and Reading.

The meeting began with a few welcoming words by the meeting organiser, **Andrea Hadfield** (Bristol) who thanked the meeting sponsors CCP4, Oxford Diffraction, GE Healthcare (Formerly Amersham Biosciences), Molecular Dimensions Limited and UCB, some of whom were exhibiting. The first speaker was **Jim Spencer** (also from Bristol) who gave an overview of his research into β -lactamases of several classes (one of which was found to possess an interesting carbamoylated lysine residue at the active site) and a secreted proteinase (LasA) from *P. aeruginosa*. **Jenny Littlechild** (Exeter) then gave an overview of work in her group covering γ -lactamases along with an interesting example of a covalently bound trapped intermediate and gave the audience an insight into EU funding schemes under framework 7. The first session concluded with a presentation by **Marcus Winter** from Oxford Diffraction on applications of the Xcalibur PX Ultra instrument which operates from a sealed tube source with multi-layer optics.

Following a superb salmon lunch, **Ioanna Papapanagiotou** from Portsmouth gave an account of the structure and function of the C.AhdI protein – part of a bacterial restriction-modification system. Mutagenesis of the protein to introduce a single methionine residue allowed its structure to be analysed by selenomethionine MAD. Next, **Shalini Iyer** from Bath described the structure of a complex between human eosinophil derived neurotoxin (a ribonuclease) with human placental RNase inhibitor, along with the results of numerous mutagenesis experiments on the nature of the complex that these two molecules form. **Misha Isupov** (Exeter) gave an interesting account of how a very difficult molecular replacement problem was solved using the MOLREP program. Success hinged on use of an option which modifies the search model according to its sequence alignment with the target structure. **Nick Hopcroft** from Reading then gave an account of structural studies of metal-DNA interactions in structures occurring at Holliday junctions – an intermediate in the DNA recombination.

This was followed by a tea break and lively poster session in which around two dozen posters were presented in earnest and three commercial exhibitors (Amersham Biosciences, Molecular Dimensions and Oxford Diffraction) were present. The scientific sessions for the day concluded with a presentation on the DIAMOND source by **Liz Duke**. From an investment of 235 million, this source will provide 3 main protein crystallography beam lines and plans are afoot for another 3 catering for microfocus, high-throughput and sulphur-SAD applications. DIAMOND should be ready for users in early 2007. Following wine and posters, guests were treated to the splendid conference dinner and ensuing celebrations continued till the small hours.

Monday morning started sharply at 9.00 with a presentation by **Nathaji Thiyagarajan** (Bath) on novel inhibitor complexes of ribonuclease and this was followed by a talk from **Liz Hooley** (Bristol) on the binding of oxidized nucleosides to avidin. **Jed Long** (Southampton) presented the results of an NMR study to analyse the binding of a chemokine to its membrane receptor using peptides to mimic the extra-membranous loops of the receptor.



Structural Biologists gather between a left-handed helix and a cast iron pleated sheet



Just after much needed coffee, **Jon Cooper** (Southampton) gave an overview of projects including work on haem biosynthetic enzymes and extended studies of an aspartic proteinase by various techniques including neutron diffraction. This was followed by a talk by **Karen Atkins** from Bath on an immunoglobulin binding protein from *S. aureus*, known to play an important role in the virulence of this micro-organism, well-known to the NHS. **Chris Williams** from Bristol concluded the morning sessions by reporting the NMR structure of a domain from the insulin-like growth factor (IGF-II) receptor.

Following lunch, the final scientific session began with **Michelle Jenvey** and **Halina Mikolajek** from Southampton describing work on drug-binding to pentraxin proteins. This was followed by a talk from **Huan-Lin Wu** (Bath) who, whilst valiantly struggling with computer

gremlins, described the NMR structural studies of a guanine nucleotide exchange factor BopE, a protein important for the virulence of Burkholderia pathogens. **Kirsty Line** from Exeter gave an account of her work on human erythrocyte peroxiredoxin and sulfiredoxin as well as efforts to analyse the complex that both proteins form. Last but not least, **Anna Brogen** from Reading gave an elegant description of a number of interesting Holliday junction structures with various synthetic drug molecules and metal ions bound.

The final tea break was an opportunity for a conference photograph and for the award of poster prizes. The meeting closed with a few concluding words from **Leo Brady** (Bristol) and **Jenny Littlechild** (Exeter) who thanked **Andrea Hadfield** (Bristol) for her considerable efforts as meeting organiser and reminded everyone that the SWSBC meeting next year (2006) will be hosted by Bath.

BSR2004 report: Hear no evil, speak no evil, see no evil: a lab monkey's trip to Japan

THE 8th International Conference on Biology and Synchrotron Radiation (BSR2004) was held in Himeji, Japan at the start of September. Several obstacles presented themselves within the first few days of my visit, not least my lack of a grasp of Japanese. After sleeping through two earthquakes in the first two days, hopes were high that I could survive anything; the arrival of a typhoon the day before the conference was due to start challenged these hopes. Overnight refuge in Osaka, followed by an early morning bullet train to Himeji allowed everything to run smoothly and enabled me to reach the meeting on time.

The meeting itself was well attended by both Japanese and International participants. Over the space of four days, almost all aspects of biology and synchrotron radiation were discussed, providing interesting comparisons and parallels between different areas. The session entitled "new phasing and beamline techniques for protein crystallography" with talks from **M. Soltis**, **R. Ravelli**, **M. Weiss** and **R. Fourme** was of particular interest to me, complementing some of the ideas introduced in my own contribution to the meeting:



a poster entitled "Experimental tests of the theoretical radiation dose limit for cryo-cooled protein crystals". The session itself covered a broad range of subjects, the automation of beamlines was discussed by M. Soltis while R. Ravelli discussed the causes of, and the use for phasing of, radiation damage in protein crystals at synchrotron sources. The session ended with contrasting pleas for the use of longer and shorter wavelengths at synchrotron beamlines by M. Weiss and R. Fourme respectively.

Unfortunately the planned trip to Spring8 was cancelled due to typhoon damage, though the conference ended successfully with a hill top barbeque and the chance to sample a rather better blend of sake than that provided by the local bars.

My attendance at BSR2004 was generously supported by Keble College, Oxford and the organising committee of BSR2004.

Robin Owen

CCG School: Trevelyan College, University of Durham, 4-12 April 2005

THE 4th of April 2005 saw a horde of apprehensive students arriving at the unusually hexagon shaped Trevelyan College at the University of Durham. They were, of course, there to attend the Tenth BCA/CCG Intensive Course in X-ray Structural Analysis. Little did they know what they were letting themselves in for....

This course has now been running for almost 20 years and shows no sign of letting up. Even with a massive 80 places available, the school is always oversubscribed. The School is open to people from all over the world, with some students coming from as far as Finland, India and Malaysia. The only requirements are to have a good working knowledge of the English language and some experience with crystallography.

The lectures began on the afternoon of arrival (the meaning of 'intensive' became frighteningly clear) where the workings of matrices were revealed. The students are allocated to one of 10 tutors, with a total of eight students per group. These groups are the perfect size for discussion of problems at the end of lectures. The tutors, who had all given up their free time to assist, were absolutely fantastic. They needed incredible talent and skill to field the plethora of questions we threw at them and they all succeeded, despite being exhausted by the end of the week.

The Course covered all aspects of structure determination, including fundamental concepts of symmetry, diffraction, Fourier synthesis, direct methods, least-squares refinement and their application to solving and interpreting structures. Highlights included **Simon Parsons** (Edinburgh), a former tutor turned lecturer who gave an amazing breakdown of statistics and twinning, **Bill Clegg** (Newcastle), teaching symmetry with the help of art by Escher. **Sandy Blake** (Nottingham) gave a brilliant talk on data collection, while **Peter Main** unravelled the myth that direct methods are a black box technique and **David Watkin** (Oxford) explained what is really going on with refinement software.

The 10th School saw a revelation in that there were for the first time two female lecturers. **Jacqui Cole** (Cambridge) gave a storming lecture on data collection theory and the Ewald sphere and **Ivana Evans** (Durham) gave an introduction to powder diffraction.

The week revolved around lectures and tutorials in the day, followed by very useful surgeries before dinner. The evenings usually involved meeting in the bar, where we enjoyed activities such as a pub quiz or a Ceilidh. Drinking was optional but dancing compulsory! Just when the last few brain cells began to give out to the joy of direct methods, the students were given freedom!!! A whole afternoon to enjoy the sights of Durham, buy a new pair of shoes or even sleep off the effects of the previous evening. The students all returned refreshed and raring to go the next morning.



Amorphous tutors



Crystalline students

On Thursday evening it was the turn of the course students to give the presentations. These covered subjects tracking the history of crystallography and diffraction. The talks were generally quite light hearted yet informative (honest) and ranged from the history of diffraction, accompanied by **Roy** "Churchill the nodding dog" **Copley's** swingometer, to Monty Python's "What have the European crystallographers ever done for us?" Other presentations involved human synchrotrons throwing out sweets instead of X-rays, a crystal choosing a Blind Date with an X-ray or an electron and finally an appearance by Darth Vader describing crystallography in space and the myth of the R2d2 space group. The stars of the evening however were **Bill** "Cleggy" **Clegg**, **David** "Des Lynam" **Watkin** and others appearing in sock puppet form to answer questions on quasi crystals.

The Course finished with lectures and a session on the types of research available using databases given by **Elna Pidcock** of the Cambridge Crystallographic Data Centre. The Course Dinner followed, where those responsible for making the Course a success - sponsors, organisers, lecturers, tutors, students and local staff - were all thanked for their efforts and everyone had a chance to relax after a very busy week. Shortly after the dinner, the dance floor was given a good battering by all but especially by the tutors **Roy Copley** (Harlow, GSK) and **Jacqui Cole** (both on air guitar).

The venue was again a highly successful element of the Course. Trevelyan College offers lecture facilities in close proximity to accommodation, catering and social amenities, so that different aspects of the Course can be smoothly integrated.

On behalf of the Students we would all like to give a huge thank-you to: **Claire Wilson**, **Judith Howard** and **Amber Thompson** for the smooth running and flawless organisation; also to lecturers **David Watkin**, **Jeremy 'J-Dog' Cockcroft**, **Bill Clegg**, **Sandy Blake**, **Simon Parsons**, **John Evans** and **Peter Main** (what would we have done without the maths refresher!); and finally to all the tutors for all their courageous efforts.

Special thanks are due to organisations which generously provided financial support for the Course: EPSRC, IUCr, BCA Chemical Crystallography Group, Bruker AXS, Oxford Cryosystems, Chemical Computing Group Inc. and Rigaku MSC.

Alexandra Griffin (University of Bristol)
Richard Mole (University of Cambridge)
Teresa Savarese (University of Bath)

It's February, so it must be Germany - The DGK in Köln



THE German Society for Crystallography (DGK) held its yearly meeting in Köln from February 28 to March 4 this year. This was a joint meeting with Austrian Crystallographers, and like our meeting in 2004, with the German Society for Crystal Growth (DGKK).

The Society is a little larger than ours, (1066 members) and had over 400 at this annual meeting. Probably the main difference in structure is the much larger number of groups: Instead of our four, they currently have no less than 19 "Arbeitskreise" or work groups of widely differing sizes, although these are rather less formally organized. Ten of them had AGM's during the Annual Meeting. Two of them are particularly large, Structural Biology and Crystal Chemistry.

The venue for the meeting was a very large hall connecting the three Chemistry Institutes. Four lecture theatres opened off this, and it provided an excellent environment for the commercial exhibition and about half of the poster sessions. The rest were housed in the Physics Institute which was nearby, but far enough to make it something of a hike in the very cold weather. The timing of the meeting is to coincide with a break in the University year when there isn't a holiday but there are no lectures. This means that accommodation has to be entirely in hotels (or with friends if you have any in the vicinity!)

The first evening started with refreshments of beer – served in neat 200 ml glasses, but refilled regularly – and very large pretzels. During this a jazz duo of bass and saxophone arrived. The saxophonist had his instrument in one hand and a skateboard in the other. Their musical offering was very good, but sadly, the skateboard did not appear in it. The C Hermann medal was awarded to **Professor Peter Paufler** of the University of Dresden. The award of the Max-von-Laue prize had to be postponed, as the winner was unable to be present. Fortunately, the custom is to ask last year's prize winner to speak, and a lecture on the uses of EXAFS and related techniques to determine the structures of thin layers was given by **Dr D. Meyer**, also of the University of Dresden. The meeting was very much like the BCA in many ways. Every year, more and more of the meeting is conducted in English. All of the biological lectures and nearly half of the posters were in English, as well as about half of the abstracts. If you want to practise your German, the mineralogical sections are the best place to do it!

Next year's meeting is in Freiburg. More information is on the DGK website: <http://opal.kristall.uni-frankfurt.de/DGK/>

Bob Gould

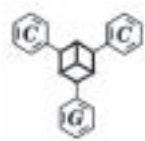


D. Meyer, winner of the 2004 Max-von-Laue prize



Der Dom zu Köln ist groß und schön!

Groups



CCG AGM Loughborough 12noon 13th April 2005

There were 45 members present at the AGM.

1) Apologies for absence:

Dr Michaele Hardie, Dr Andrew Bond, Dr Harry Powell

2) The minutes of the previous meeting

The minutes of the AGM held at UMIST in 2004 were accepted. There were no matters arising from those minutes.

3) Chairman's Report

The Chairman, **Dr. Sandy Blake**, spoke of the very successful Autumn Meeting entitled "In situ Crystallography" at Aston University.

He thanked Bruker AXS for sponsoring the meeting, Pfizer for sponsoring free student registration which they are minded to continue and **Dr Carl Schwalbe** for excellent local organisation and **Dr Simon Parsons** for organising the scientific sessions.

At this Spring meeting we had an excellent lecture by **Dr Anders Markvardsen** of ISIS, the winner of the CCDC Chemical Crystallography Prize for Younger Scientists.

Dr Sandy Blake thanked the retiring members of the CCG committee for their hard work and support, namely **Dr Simon Parsons, Dr Simon Teat, Dr Michaele Hardie, Dr Richard Cooper, Dr Katherine Bowes** and **Dr Carl Schwalbe** and all members of the committee for their work throughout the year.

4) Secretary/Treasurer's report

Dr Georgina Rosair (GMR) presented the Group's financial statement for 2004. The group's finances are in a healthy position. The autumn meeting made a modest profit, the final profit being £679. A one-off payment of £700 was made to the Durham Intensive Chemical Crystallography School to support the education remit of the BCA. There was a registration refund from the autumn meeting in 2003 which appeared in the 2004 accounts.

Dr Sandy Blake thanked the Secretary/Treasurer for her work.

There were no queries of the accounts.

GMR reminded the group for articles for Crystallography in the UK piece in the IUCr newsletter as there are many good things we can say about UK crystallography.

Dr Bob Gould said there was no deadline as such as he did not know in which issue the UK article would appear.

5) The 10th Intensive Course in Durham

Dr Sandy Blake gave an account of this course at Trevelyan College which had just finished and it was a resounding success. There were 80 students, 9 lecturers and 10 tutors.

A new format was tried with some optional lectures, and revitalised evening sessions. The student presentations which were both informative and entertaining.

The next Intensive Course is due to run in 2007 and will be held somewhere in the end of March to the beginning of April as the BCA Spring meeting is scheduled for mid April so that there will be no overlap of the Spring meeting and the Course.

6) Elections

Chairman:

Dr Simon Parsons (Edinburgh University) nominated by **Prof Bill Clegg** (Newcastle), seconded by **Dr Roy Copley** (GSK), period of office 2005 – 2007.

Member of Committee:

Dr Liling Ooi (Cardiff University) nominated by **Dr Georgina Rosair**, seconded by **Prof Paul Raithby**, period of office 2005 - 2008.

Member of Committee:

Dr John Warren (CLRC Daresbury), nominated by **Dr Simon Parsons**, seconded by **Prof Paul Raithby**, period of office 2005 - 2008.

Member of Committee:

Charlie Broder (CLRC Rutherford), proposed by **Dr Richard Cooper** (Oxford Diffraction), seconded by **Dr Katharine Bowes** (Oxford) period of office 2005 - 2008

7) Autumn Meeting

The CCG Autumn Meeting will be held on 16 November at Daresbury Laboratories and the local organiser will be Dr John Warren. The title is to be "Applications of computational methods to crystallography". Compilation of the programme is in progress.

8) AOCB

Dr Simon Parsons (SP) thanked **Sandy Blake** for doing an excellent job as chairman for the past two years. SP encouraged students to attend the autumn meeting. The CCG poster prize will be awarded at the BCA AGM this afternoon. He thanked **Prof. Bill Clegg** for his assistance in the judging of the poster prize.

Dr Andy Parkin (AP) asked the group whether they would in principle support the formation of a Young Crystallographers (YC) Special Interest Group. This was unanimously carried. **Dr Christine Cardin** asked whether there would be a YC meeting next year? Prof Bill Clegg said it would avoid a clash with the Durham school. AP suggested the format of another parallel session in the main Spring meeting in which graduate students would take part. **Bob Gould** mentioned that complaints had been made by YC participants that not enough older crystallographers were present at the YC satellite and that there were still problems in holding parallel sessions such that there was no easy way out of these problems. **Amber Thompson** spoke of the document circulated by AP which proposed a YC autumn meeting. **Prof Bill Clegg** added that this would be across the subject groups

9) Next AGM

The next CCG AGM will be held during the BCA Spring Meeting at Lancaster University (date and venue to be arranged)

The meeting closed at 12.40pm.

CCG Committee 2005

Chairman

Dr Simon Parsons (Edinburgh)

Deputy Chairman

Dr Richard Cooper (Oxford Diffraction)

Secretary/Treasurer

Dr Georgina Rosair (Heriot Watt)

Ordinary Members of the Committee

Dr Mary Mahon (Bath)

Dr Andy Parkin (Glasgow)

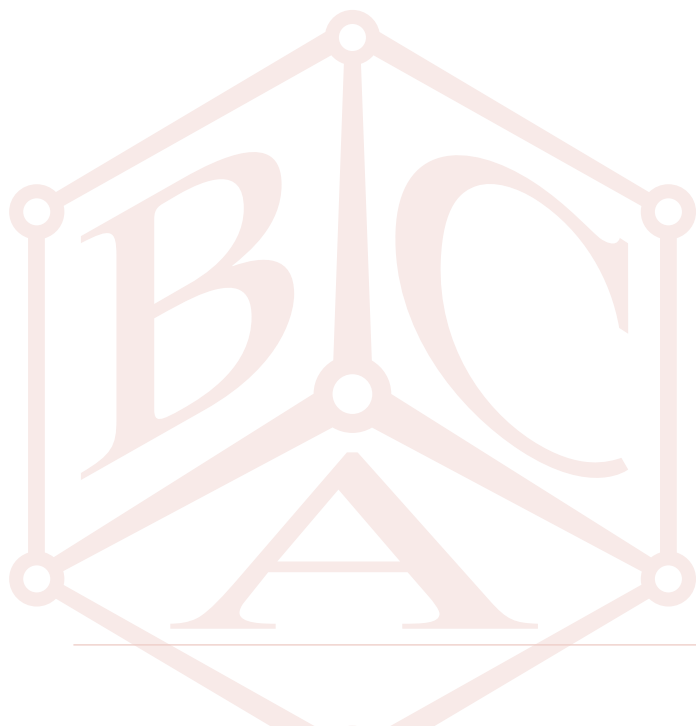
Dr Liling Ooi (Cardiff)

Dr John Warren (CLRC Daresbury)

Dr Charlie Broder (CLRC Rutherford)

Dr Andrew Bond (University of Southern Denmark)

Ms Alexandra Griffin (Bristol) co-opted student representative



BCA Accounts 2004

The British Crystallographic Association

Summary Financial Statements for year ended 31 December 2004.

Examining Accountant: R A Young, BSc, FCA.

The Young Company, Lakeview Court, Ermine Business Park,
Huntingdon PE29 6XR

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

INCOMING RESOURCES:

	2004	2003
Grants and sponsorship	2,300	6,240
Donations	1,633	553
Annual conference (5)	58,945	62,623
Meetings of groups	6,144	2,252
Newsletter	23,706	22,978
Membership subscriptions	17,322	19,704
Course fees	(600)	14,198
Net income from trading	(235)	-
Investment income	4,047	5,627
Interest received	2,746	2,358
IUCr Bursary	-	22,242
Sundry income	-	1,410
TOTAL INCOME	116,008	160,185

EXPENSES:

	2004	2003
Direct charitable expenditure (2)	116,125	116,508
Management and administration (3)	21,292	20,994
TOTAL EXPENDITURE	137,417	137,502

	2004	2003
NET INCOME	(21,409)	22,683
Unrealised gains (losses) of investment assets	3,305	2,422
NET MOVEMENT IN FUNDS	(18,104)	25,105
Balances brought forward at 1 January 2004	215,230	190,125
Balances carried forward at 31 December 2004	197,126	215,230

ASSETS:

	2004	2003
Fixed Assets		
Tangible assets	367	702
Investments	97,048	92,963
	97,415	93,665
Current Assets		
Stocks	425	743
Debtors	732	1,722
Cash at bank	113,280	124,868
	114,437	127,333
LIABILITIES: amounts falling due within one year	(12,818)	(3,543)
LIABILITIES: amounts falling due after more than one year	(1,908)	(2,225)
NET ASSETS	197,126	215,230
INCOME FUNDS:		
	2004	2003
Restricted funds (4)	71,158	89,305
Unrestricted funds (4)	125,968	125,925
	197,126	215,230

NOTES TO THE SUMMARY FINANCIAL STATEMENTS:

1. ACCOUNTING POLICIES.

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

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

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

2. DIRECT CHARITABLE EXPENDITURE

	2004	2003
Previous year conferences	45	-
Subscription to International bodies	3,701	3,903
Annual conference (5)	54,972	58,853
Meetings of groups	3,004	2,460
Newsletters	24,912	27,040
Course fees and accommodation	-	16,000
Grants and sponsorship	1,000	800
Prizes	1,050	364
Crystallography Reviews	4,000	4,428
Arnold Beevers Bursary Fund	1,200	2,660
Bursaries from restricted funds	22,241	-
	116,125	116,508

3. MANAGEMENT AND ADMINISTRATION

General expenses

	2004	2003
Depreciation	335	335
Administration fee	14,950	14,626
Accounting fee	3,143	3,298
Insurance	378	368
Bank and security charges	240	222
Spring Meeting Planning	-	796
Special Interest Group administration	553	481
Council members' expenses	612	128
Officers	759	378
Other Council expenditure	322	362
Total	21,292	20,994

The full BCA accounts for 2004 are available on request as an E-mail attached PDF file from the BCA administrative office.

The British Crystallographic Association

Summary Financial Statements for year ended 31 December 2004.

4. STATEMENT OF FUNDS	Brought Forward	Incoming Resources	Resources Expended	Gains/ (Losses)	Carried Forward
UNRESTRICTED FUNDS					
General fund	125,925	104,508	107,770	3,305	125,968
RESTRICTED FUNDS					
IUCr bursary fund	22,242	-	22,241	-	1
Arnold Beavers bursary fund	16,974	2,259	1,200	-	18,033
Dorothy Hodgkin prize fund	7,285	1,023	1,000	-	7,308
Chemical group teaching school	11,802	100	-	-	11,902
Chemical group fund	5,527	185	30	-	5,682
Industrial group fund	5,653	5,538	4,176	-	7,015
Biological structure group fund	19,822	2,395	1,000	-	21,217
Subtotal	89,305	11,500	29,647	-	71,158
Total of Funds	215,230	116,008	137,417	3,305	197,126

5. Spring Meeting 2004 Manchester	
INCOME	
Sponsorship	£4,955
Registration	£39,665
Exhibition	£12,675
Bursary	£1,650
Total	£58,945
EXPENDITURE	
Accommodation & Meals	£13,349
Facilities	£7,929
Catering	£6,224
Social Event	£2,716
BCA Speakers Expense	£2,199
Refunds	£1,200
Abstract Book	£2,765
NN Fee	£10,017
Administration	£2,798
Stationery & copying	£525
Bursaries	£5,250
Total	£54,972
TOTAL INCOME	£58,945
TOTAL EXPENDITURE	£54,972
MEETING SURPLUS	£3,973

All transactions for the 2004 Spring Meeting were made through the BCA account instead of the traditional University account. Consequently the detailed meeting accounts are reported as part of this financial report.

Treasurers Report 2004

The Association had a deficit of £18,104 during the year ended 31 December 2004 and has no material commitments or guarantees which could affect its future solvency. The major contribution to the reported deficit was the loan of £22,241 from the IUCr bursary fund to the 2005

The full BCA accounts for 2004 are available on request as an E-mail attached PDF file from the BCA administrative office.

Florence meeting. Positive contributions came from investments producing a healthy £6,793 of income. We also benefited from the transfer of the residual assets of the Residual Space Ventures Association and its associated trading company. This donation of £1,451 was authorised by the charity commission. £500 was allocated to bursaries, £500 to the Dorothy Hodgkin Prize fund and the remainder towards the 2005 BCA prize lecture. This boosted donations for the year to £1,633 up from £553 last year.

The unrestricted funds show a deficit of £3,262 over the year before revaluations. A revaluation of investment assets of £3,305 gives the unrestricted funds an overall surplus of £43. The Spring Meeting surplus and investment performance kept us in the black.

Council members have conducted a review of the reserves that the Association requires for sustaining its objectives. The major considerations are with regard to the long term funding of meetings, bursaries and underpinning projected deficits from reduced investment income. Existing investments of £97,048 are considered adequate to meet these needs.

A review of the major risks to which the Association is exposed has been conducted. The only consideration is with regard to its investments and to mitigate those risks the Association has all its investments placed with an independent professional management company.

Our agreement with Taylor & Francis to publish highlights of the Spring Meeting proceedings in "Crystallography Reviews"

resulted in all members receiving a copy in June 2004 at a cost of £4000.

Six bursaries totalling £1,200 were taken up this year. The Manchester Spring Meeting awarded bursary funding of £5,250 to benefit 35 students with 11 being commercially sponsored.

Crystallography News made a deficit of £607 this year on a turnover of £23,706. The additional postage costs incurred for the inclusion of Crystallography Reviews had a major impact on the deficit. The BCA owes a debt of gratitude to its advertisers and sponsors who generously support our activities.

Subscriptions to International bodies (IUCr & ECA) were £3,701, a little lower than last year due to currency variations. Administration costs are a little higher this year at £21,292, up by £298.

Membership income is down by £2,382 with eleven organisations paying Corporate Membership dues in 2004 (down from 13). The early membership renewals for 2004 reported last year did boost the income in 2003 but total membership numbers are down. Many of our members have signed Gift Aid declarations and a refund of £998 from the Inland Revenue was again allocated to the Arnold Beavers Bursary Fund. The Fund was also boosted by a transfer of £608 investment income from the BSG.

In my last report as Treasurer; I thank my colleagues on Council, the team at Northern Networking and our accountant Bob Young for their invaluable support over the last 5 years.

Profiles in Science

THE U.S National Library of Medicine has set up a website featuring twentieth century leader in biomedical research and public health. It holds archival collections of prominent scientists, physicians and others who have advanced scientific enterprise. It can be found at URL <http://profiles.nlm.nih.gov/SC/>

Collections for biomedical research include **Francis Crick**, **Barbara McClintock** and **Linus Pauling**. Here is a summary of their holdings on Francis Crick.

The Francis Crick Papers

The name of Nobel laureate **Francis Crick** (1916-2004) is inextricably tied to the discovery of the double helix of deoxyribonucleic acid (DNA) in 1953, considered the most significant advance in the understanding of biology since Darwin's theory of evolution. Yet, during a research career spanning more than fifty years, theoretical biologist Crick also made fundamental contributions to structural studies of other important biological molecules through X-ray analysis; to the understanding of protein synthesis; to the deciphering of the genetic code by which hereditary information is stored and transcribed in the cell; and to our conception of consciousness. Through force of personality and intellect, readily apparent in this online selection from his papers, he served as a one-man clearinghouse of criticism, ideas, and information for scientists the world over.

The Wellcome Library for the History and Understanding of Medicine in London is the repository for the scientific papers of Francis Crick (collection reference PP/CRI). The archive contains correspondence, lecture notes, photographs, laboratory notebooks, and published and unpublished articles, which range from 1938 to ca. 2002.

The section of the papers containing Crick's work in molecular biology (1938-1998) is catalogued and available for study in the Wellcome Library. The section of his papers on consciousness research is currently being catalogued and will be available in the future.

Individuals or institutions wishing to reproduce or request copies of the documents should contact the Wellcome Trust Medical Photographic Library at URL <http://medphoto.wellcome.ac.uk/>

As part of its Profiles in Science project, the National Library of Medicine has collaborated with the Wellcome Library to digitize and make available over the World Wide Web a selection of the Francis Crick Papers for use by educators and researchers. This site provides access to the portions of

the Francis Crick Papers of the Wellcome Library that have been selected for digitization.

Individuals interested in conducting research in the Francis Crick Papers are invited to contact the Wellcome Library, further details at URL <http://library.wellcome.ac.uk/>

This online Exhibit is designed to introduce you to the various phases of Dr. Crick's scientific career and professional life. It is divided into sections that focus on Crick's life and major scientific contributions.

- Biographical Information,
- The Discovery of the Double Helix, 1951-1953
- Defining the Genetic Coding Problem, 1954-1957
- Deciphering the Genetic Code, 1958-1966
- Embryology and the Organization of DNA in Higher Organisms, 1966-1976
- From Molecular Biology to Neurobiology, 1976-2004

Kate Crennell

Control and Prediction of the Organic Solid State

This is a Basic Technology project of the Research Councils UK, will be holding an Open Day on Tuesday 13th September 2005 at University College London. This day will be open to all those interested in polymorphism and computations in crystal structure prediction. Further details can be found at www.cposs.org.uk or by emailing **Louise Price** at l.s.price@ucl.ac.uk

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.

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

14-15 June 2005

CHESS 2005 Users' Meeting Cornell High Energy Synchrotron Source, Ithaca, NY, USA
www.chess.cornell.edu/Meetings/

15-17 June 2005

14th Croatian-Slovenian Crystallographic Meeting, Vrsar, Croatia
www.hazu.hr/kristalografii/vrsar05.htm

15-17 June 2005

Microstructure Analysis in the Materials Science, Technical University, Freiberg, Germany
www.wv.tu-freiberg.de/mk/bht

16-18 June 2005

X-rays and Neutrons: Essential Tools for Nanoscience Research, Washington DC, USA
www.sns.gov/workshops/nni_05/

17-22 June 2005

Molecular Crystal Engineering EuroConference on Evaluations and Predictions of Solid State Materials Properties, Helsinki, Finland
www.esf.org/conferences/pc05191

19-28 June 2005

7th EMU School: Mineral Behaviour at Extreme Conditions, Heidelberg, Germany
www.univie.ac.at/Mineralogie/EMU_School-7/

20-24 June 2005

International School on Mathematical and Theoretical Crystallography, Nancy, France,
lcm3b.uhp-nancy.fr/mathcryst/nancy2005.htm

20-24 June 2005

Summer School on Methods and Applications of Neutron Spectroscopy, Center for Neutron Research, Gaithersburg MD, USA
www.ncnr.nist.gov/summerschool/ss05

22-24 June 2005

CCP13 Annual Workshop - 14th Annual Fibre Diffraction and Non-Crystalline Diffraction Workshop, Cardiff
www.ccp13.ac.uk/

22 June - 3 July 2005

International School of Structural Biology and Magnetic Resonance - 7th Course: Structure and Biophysics - New Technologies for Current Challenges in Biology and Beyond, Erice, Italy
<http://smrl.stanford.edu/erice2005/>

27 June - 1 July 2005

Joint 20th AIRAPT and 43rd EHPRG: International Conference on High Pressure Science and Technology, Karlsruhe, Germany
www.air-ehprg-2005.de

3-7 July 2005

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

4-7 July 2005

IWORID-7: 7th International Workshops on Radiation Imaging Detectors, Grenoble, France
www.esrf.fr/News/FrontNews/IWORID7/

4-8 July 2005

X05: The 20th International Conference on X-ray and Inner-Shell Processes, Melbourne, Australia
www.chemistry.unimelb.edu.au/news/X05/X05.html

27-30 July 2005

2005 Trends in Microcalorimetry, Boston MA, USA
www.microcalorimetry.com/index.php?id=271

31 July - 19 August 20

Biological Membranes, current challenges Benasque Center for Physics, Benasque, Spain
www.physics.iastate.edu/staff/traveset/Benasque.htm

7-17 August 2005

ACA Small Molecule Summer Course, Pittsburgh PA, USA
www.hwi.buffalo.edu/ACA/ACASummerCourses.html

14-17 August 2005

Neutron Membrane Workshop, Indiana University, Bloomington IN, USA
www.iucf.indiana.edu/events/neutronmembrane/index.php

14-21 August, 2005

4th PSI Summer School on Condensed Matter Research - Spectroscopy/Microscopy, Lyceum Alpinum in Zuoz, Switzerland
sls.web.psi.ch/zuoz2005

14-28 August, 2005

The seventh United States National School on Neutron and X-ray Scattering, Argonne National Laboratory, IL USA
www.dep.anl.gov/nx/

18-23 August 2005

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

21-26 August 2005

27th International Free Electron Laser Conference, Stanford CA, USA
www-ssrl.slac.stanford.edu/lcls/fel2005/

23-31 August 2005

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

24-30 August 2005

Non-Commercial Crystallographic Software Fayre at the IUCr Florence 2005 Congress,
Florence, Italy
www.ccp14.ac.uk/projects/iucr2005-softwarefayre/

1-2 September 2005

Magnetism, Neutrons and High-Pressure, Edinburgh
www.csec.ed.ac.uk/NSG_main.html

2-8 September 2005

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

4-6 September 2005

Annual Conference, British Association for Crystal Growth,
Sheffield
www.bacg.org.uk

4-7 September 2005

Neutrons in Biology - A Satellite Meeting of the IUPAB/EBSA Biophysics Congress,
Grenoble, France
www.ill.fr/neutbio2005/

5-15 September, 2005

9th Oxford School on Neutron Scattering - An ideal introduction to the theory, techniques and applications of neutron scattering to the study of condensed matter,
University of Oxford
www.isis.rl.ac.uk/conferences/osns2005/

7-9 September 2005

12th CCP4 Protein Structure Workshop, Galashiels
www.ccp4.ac.uk

8-10 September 2005

Neutron Spin-Echo Workshop 2005, Institut Laue-Langevin,
Grenoble, France
www.ill.fr/YellowBook/IN11/NSE2005

13 September 2005

Control and Prediction of the Organic Solid State, University College London, Information from:
I.s.price@ucl.ac.uk

15-17 September, 2005

Murnau Conference - Structural Biology of Molecular Recognition,
Murnau, Germany
www.murnauconference.de

22-23 September 2005

The 13TH BENS Users' Meeting HMI, Germany
www.hmi.de/bensc

22-24 September 2005

7th International Meeting on Single Nucleotide Polymorphism and Complex Genome Analysis,
Hinckley, Leics
snp2005.nci.nih.gov/

25-30 September 2005

ICXOM 2005 - 18th International Conference on X-ray Optics and Microanalysis,
Frascati Rome, Italy
www.inf.infn.it/conference/2005/icxom/

6-7 October 2005

Watching the Action: Powder Diffraction at non-ambient conditions,
Max-Planck-Institute for Solid State Research,
Stuttgart, Germany
www.fkf.mpg.de/xray/

17-19 October 2005

3rd MECA SENS Conference on Stress Evaluation by Neutron and Synchrotron X-Ray Radiation,
Bishop's Lodge Resort,
Santa Fe NM, USA
ww.lansce.lanl.gov/mecasens2005/

19 November 2005

Canadian Light Source 8th Annual Users' Meeting, University of Saskatchewan, Canada
www.cls.usask.ca/enews/upcomingevents.php

27 November – 2 December 2005

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

4-6 April 2006

BCA Spring Meeting, Lancaster
crystallography.org.uk

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

9-13 July 2006

SAS2006 - The XIII-th International Conference on Small-Angle Scattering, Kyoto, Japan
www2.scphys.kyoto-u.ac.jp/sas2006/index.html

4-6 August 2006

ECM-23 Satellite Meeting on Mathematical and Theoretical Crystallography, Leuven, Belgium
www.lcm3b.uhp-nancy.fr/mathcryst/leuven2006.htm

6-11 August 2006

23rd European Crystallographic Meeting, Leuven, Belgium
ecm23.be

1-4 September 2006

EPDIC 10, European Powder Diffraction Conference, Geneva
www.sgk-sscr.ch/EPDIC10/EPDIC10.html

25-28 September 2006

PNCMI 2006 - The Sixth International Workshop on Polarised Neutrons in Condensed Matter Investigations,
Berlin, Germany
www.hmi.de/bensc/pncmi2006/

7-17 June 2007

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