Crystallography News

British Crystallographic Association

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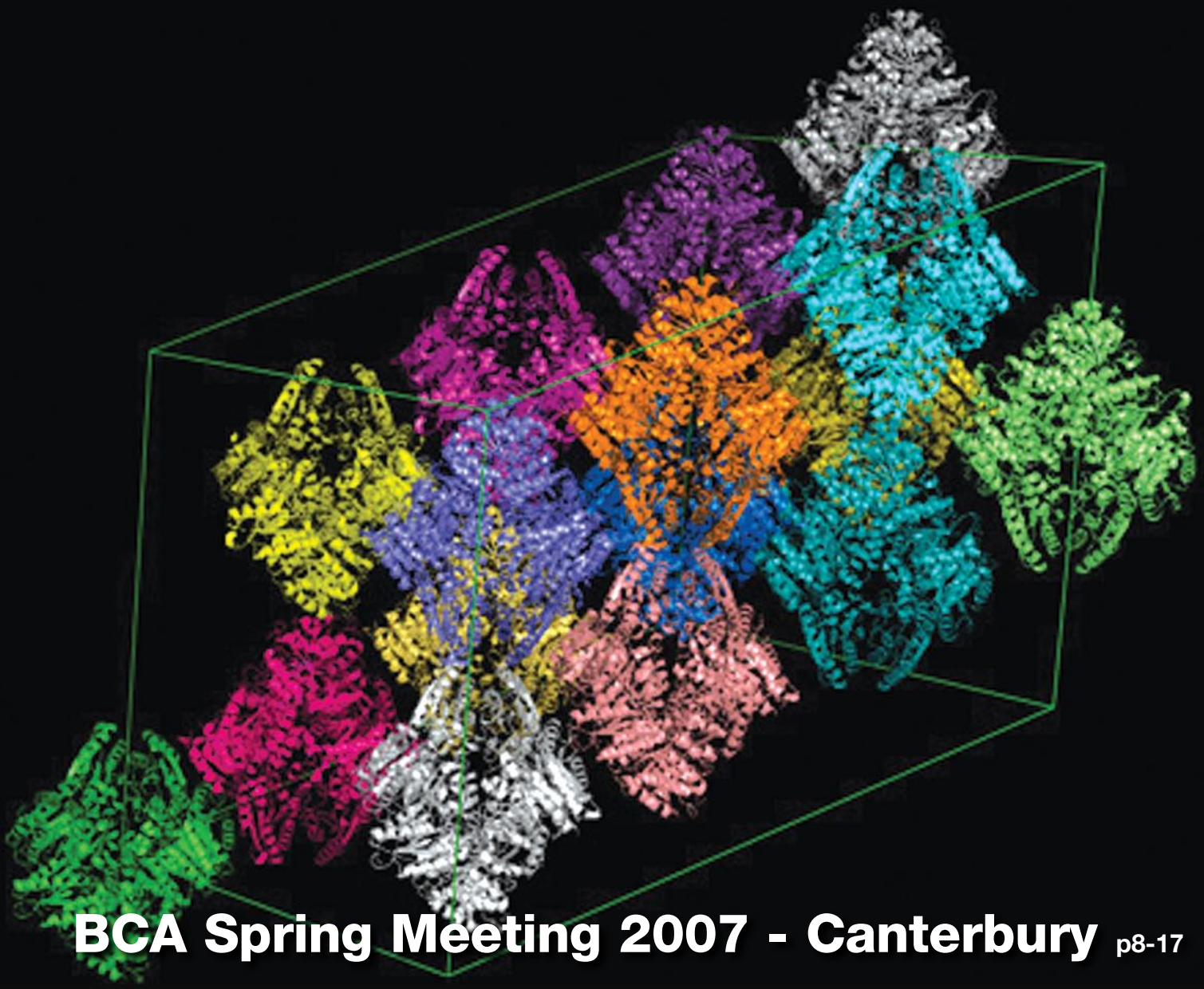
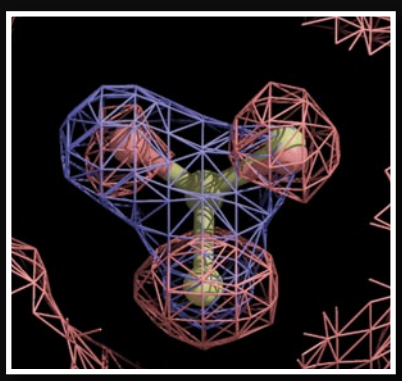


BCA Spring Meeting 2007 - Canterbury p8-17



Crystallography News March 2007

Contents

This month's cover:

Sixteen dodecamers occupy this P1 cell described by Adrian Lapthorn (p 31). The small picture represents the identification of a threonine molecule by Kevin Cowtan (p.30). Both were presented at the December meeting of CCP4.

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by William Anderson and Sons Ltd, Glasgow. 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 June 2007 issue are sent to the Editor to arrive before 25th April 2007.

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From the President

IT is a particular pleasure and a privilege for me to be able to write the opening article in what is a very special issue of Crystallography News. It is issue 100 and is published at the beginning of the BCA's Silver Jubilee year. As such it will hold a very special place in the history of the Association. The issue will be distributed during March, shortly before the focus of our celebrations at the 25th Anniversary Spring Meeting to be held at the University of Kent at Canterbury from 17th-19th April, 2007.

At this special moment it is important to remember how the BCA has developed over the past 25 years and to look forward to the future. The BCA has its origins in the "X-ray Analysis Group" of the Institute of Physics, which was founded in 1943. In 1969 the name was changed to the "Crystallography Group". Then in 1981, the BCA was conceived by the amalgamation of the Crystallography Groups of the IoP and the Royal Society of Chemistry, and had its formal inauguration on 6th April, 1982, at the Durham Meeting. At the first Council Meeting on 7th April, 23 Founder members signed up, and by the next Meeting, at Royal Holloway College, the number had risen to 52. The four groups of the Association, the BSG, the CCG, the PCG and the IG formed within the first year, and the BCA as we know it was off to a flying start. Since then additional membership categories of Student Member, Ordinary Member, Overseas Member, Corporate Member and the special category of Honorary Member have been added, and the BCA now proudly boasts over 1000 members.

The quality of science delivered by BCA Members has always been of the highest standard so that British crystallography is truly world-leading. Reflecting this success, a vibrant programme of Named Lectures has developed at the BCA Spring meetings commemorating some of the giants of British Crystallography. The BCA has always been inclusive and other groups with structural interests have joined the Spring Meeting, as exemplified by the British Association of Crystal Growth last year and the XRF Group this year. Special Interest Groups covering topics such as Education and the Use of Synchrotrons have also flourished. Crystallography News has, under the guidance of a series of dedicated editors grown into a highly professional and informative magazine. The future seems equally bright with the formation of the Young Crystallographers group. I beg to suggest that there is no other Association or Society that has such a large and enthusiastic group of young scientists, and I look forward to watching the BCA continue to grow from strength to strength over the next 25 years.

The healthy state of the BCA is entirely due to the dedication of its Members and Officers over the last 25 years. The current Officers and I would like to express our thanks to all the members, past and present, for their untiring efforts. We are also most grateful to all the sponsors, both academic and industrial, who have made personal or corporate donations to the BCA. And this was, perhaps, most evident at our hugely successful hosting of the IUCr Congress in 1999. Without their support the BCA would not be on such firm financial ground.

To return to the present, the schedule for the Spring Meeting at Canterbury is now complete, and the details are published in the following pages. I would like to thank **Lindsay Sawyer** and his team for putting such an excellent programme together. In the context of the meeting, the AGM will be held on the afternoon of Wednesday 18th April. At the AGM we have to elect a new Vice President, and Secretary, as **John Finney** and **Christine Cardin** are coming to the end of their terms of service. So the Council officers and I look forward to receiving nominations for these key vacancies of Vice-President, Secretary and the new formal post of Education Coordinator.

I look forward to seeing you in Canterbury. We certainly have a lot to celebrate!

Paul Raithby

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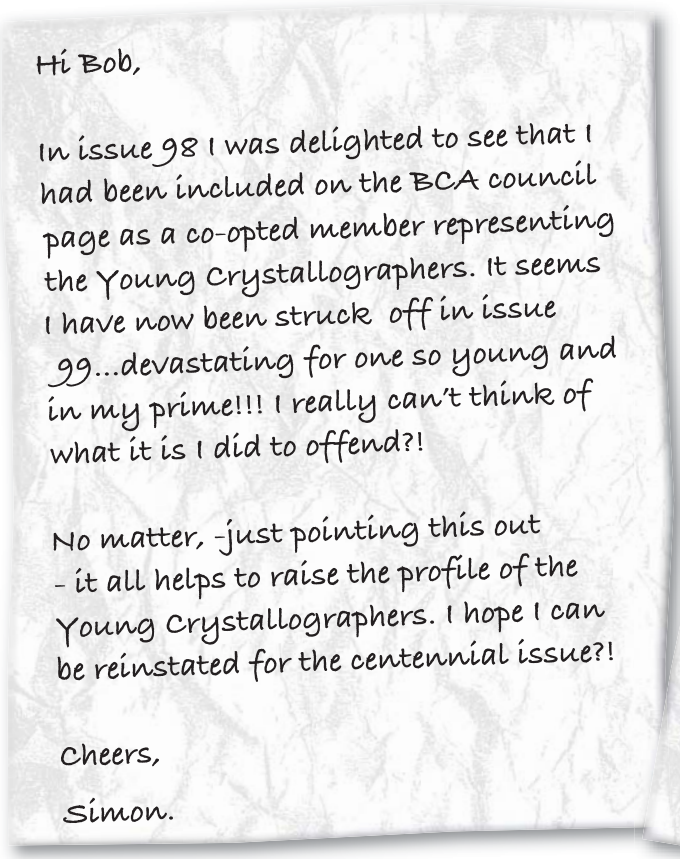
Letters to the Editor

LETTER FROM DR SIMON COLES



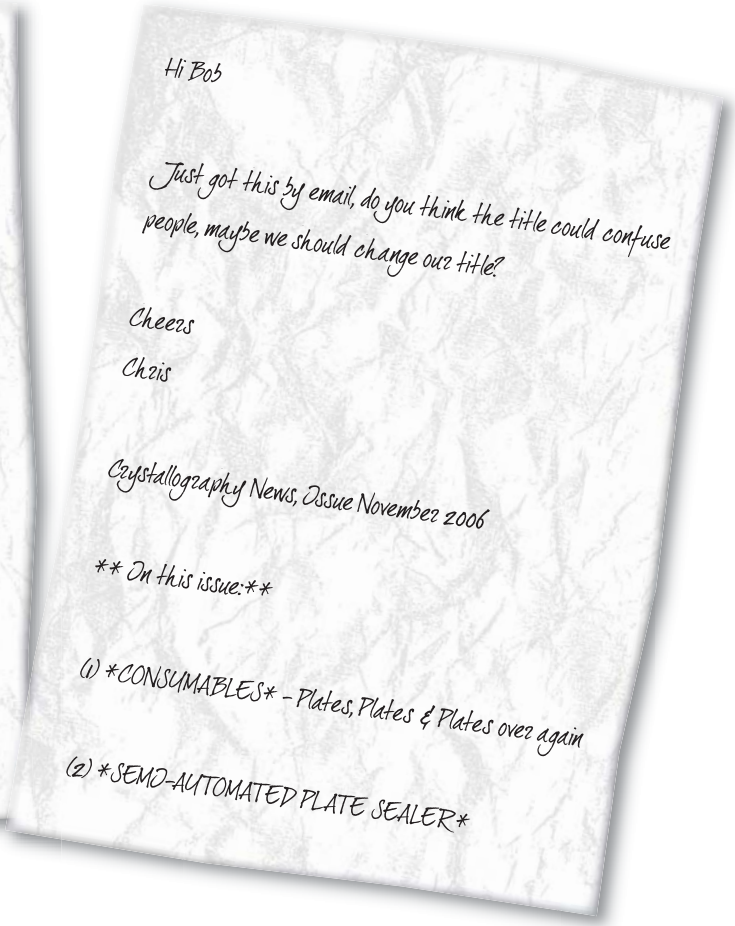
Dear Simon,

My fault, I fear. Very sorry, driving you into oblivion was not my intention. Unfortunately, I didn't notice that the reformatting of the Council page had made you disappear under a blurb. I must be extra careful next time! And, I'll make sure that in this issue, you go on as a Group Representative, not a co-optee!

Happy New Year

BOB

LETTER FROM PROFESSOR CHRISTINE CARDIN



Hi Chris!

Isn't it lucky that we don't have a November Issue?

All the best

BOB

St Patrick Was A Crystallographer

OCCASIONALLY, I accidentally open a spam message, where the random verbiage does catch my attention. Here was a bit of one I saw:

The methods and applications topics are grouped within the following categories; diffraction; spectroscopy, imaging. The beamline is intended for single-crystal diffraction and resonant magnetic scattering experiments for the study of ordering phenomena, phase transitions and materials science. Born somewhere in western or northern Britain, he was brought to Ireland as a slave when still a teenager. What's a photographer in his digital darkroom to do?

What indeed?

Bob Gould

From the Editor

WELCOME to the hundredth issue of Crystallography News! And those of us old enough to be able to do mental arithmetic will note that as we have four issues per year, this must, indeed be the 25th anniversary of the BCA! For this edition, we sent the lovely **Samantha** - on secondment from the Radio 4's I'm sorry, I haven't a Clue – to search the archives for some interesting bits from that 25 years, and she has come up with four offerings which she hopes that you will enjoy, starting on page 21. They begin with a very upbeat letter from **David Phillips**, our first President, in issue number 1, and it is good to see that **Paul Raithby**, our current president, is equally upbeat about the future of us and our science.

One thing I discovered was that we have always been *Crystallography News*, not, as some refer to us, the *BCA Newsletter*. I'm glad to say that that publication never existed. In fact *Crystallography News* is older than the BCA, as five issues with that name came out under the joint responsibility of the crystallography groups of the IoP and the RSC, although the numbering restarted at the inception of the BCA. It has survived so far with five editors: **Moreton Moore**, **John Squire**, **Kate Crennell**, **Jo Jutson**, and **Bob Gould**, all of whom have left their mark on the journal. Like the BCA itself, we rely much more on professional services that we did in the beginning. I particularly want to thank **Barry Brown**, **Michael Barron** and **Ross Mushet** of William Anderson & Sons Printers for their brilliant formatting and typesetting.

Much of this issue, as in every March issue, is devoted to the programme for the Spring Meeting. The main programme is flanked by a very impressive Young Crystallographers session and an equally impressive session of tributes to **Sam Motherwell**. The programme and timetable are as up-to-date as we can make them, and I am very grateful to **Lindsay Sawyer** for this help in getting them to this stage.

An unusual but very welcome feature of this edition is that we have a real original scientific paper which should be of general interest. **Kirsty Anderson** asked us to publish a flyer for the project Z'>1, structures with more than one molecule in the asymmetric unit, and agreed to expand this into a short article. The widespread significance of this work is illustrated by **Adrian Lapthorn's** picture on the front cover, of a protein which seems blissfully unaware of the advantages of crystallographic symmetry.

I look forward, camera at the ready, to meeting you in Canterbury, and particularly the hardy bursars who do so well at writing up what will happen there!

Bob Gould

BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
- A 10% discount on exhibition stands 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 **£750.00** per annum

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

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Puzzle Corner

FOR our hundredth issue, we return to what is clearly our readers' favourite for puzzle corner – the substitution cryptogram. Each letter in the text always represents the same letter. Capitalisation has been suppressed, but punctuation left intact. Please identify the source of this uplifting passage – that shouldn't be difficult if you read this issue! The winner will receive a £20 book token. In the case of a tie, the editor will choose the reply he deems to be the wittiest.

dju lf rdd vjfpdyj up njju eauw plv bjddpe gvmfurddphvrcwjvf jyjvm mjrv ru uwj fcvaih njjuaih pb uwj zgr. uwjvj ej fwrdd bais plu ewru ije rsyrigjf ai ripuwjv zvrigw pb uwj flztjgu nahwu wjdc up fpdyj plv cvpzdjnf, wjrv rzplu uwj npfu vjgjiu sjyjdpcnjiuf, fjj uwj drujfu rccrvrulf, ris jitpm uwj uvalncwf ris fwrvj uwj sabbaglduajf pb pds ris ije bvajisf.

LAST months guest puzzle from Howard Flack was won by Ulli Englert of Aachen, whose solution follows:

Dear Bob & Howard,

This is my attempt to answer the Dec 2006 puzzle.

a) 92 + 65 +73 = 230 (11 + 11 + 10 = 32)
92 (11) centrosymmetric space group types *(crystal classes)*

plus

65 (11) Sohnke groups = space group types without improper symmetry operations *(crystal classes)*
i.e. suitable for crystallizing an enantiopure chiral object

plus

73 (10) noncentrosymmetric space groups with improper symmetry operations *(e.g. $Pna2_1$)*

add up to a total of

230 (32) space group types (crystal classes)

b) 68 + 162 = 230 (10 + 22 = 32)
(I hope the 262 was a typo and not a trap!) (Indeed it was - sorry - Ed.)
68 (10) dipolar *(i. e. suitable for pyroelectric objects)* space group types *(crystal classes)*

plus

168 (22) non-dipolar space group types *(crystal classes)*

add up to a total of

230 (32) space group types *(crystal classes)*

c) *Was not obvious for me; the answer might be in the normalizer of the space groups.*
207 + 22 + 1 = 230
207 space groups with a centrosymmetric normalizer

plus

22 space groups with a normalizer containing no improper symmetry operations, i.e. "chiral" space groups

plus

1 space group with a normalizer containing continuous translations in all three directions (*P*1)

add up to a total of

230 space groups *(sorry - space group types!)*

I always enjoy the puzzles! Best wishes from Aachen,

Ulli

Howard Flack comments:
You win the complementary prize for puzzle no. 99 although the answer was not quite complete. Bob will publish my full explanation in due course. You get a bottle of a special Swiss wine from the Upper Rhone Valley (Wallis) called Gout du Conseil (it's a white wine). I don't have a photo of the vineyards but have a look at the ski slopes! http://www.imalp.ch/webcam.jpg
Why don't you try contributing a puzzle yourself?

Glen Smith

WE are sorry to have to report that Glen, a longstanding member of the BCA, died on 1 February. An obituary for him will appear in our June issue.

Patrick Tollin (1938-2006)

PAT TOLLIN made pioneering contributions to the development of reciprocal space Patterson Methods for solving crystal structures, in the area of computational crystallography and in the study of filamentous virus structures using fibre diffraction techniques.

Pat was a rigorous and inspirational researcher and teacher. His background was in Physics with a first degree from Glasgow, his home-town. In fact his degree was in Natural Philosophy, a fact about which he took a typically mischievous pride. This was followed by a PhD in the Cavendish Laboratory in Cambridge under the supervision of **Bill Cochran**, a sound crystallographic heritage. It was while working with Bill that Pat developed many of the ideas on using the Patterson function for determining the orientation of planar groups and of solving molecular structures containing these groups. This work was integrated with the rotation and translation functions being developed both by Pat and his collaborators and elsewhere. Among the high profile structures solved in the early days using Pat's methods was that of 2'-deoxyadenosine. His thesis "The use of a high-speed digital computer for the direct determination of crystal structures" set the scene for much of his later work.

Having turned down the opportunity to pursue a career in the Atomic Energy Authority in Dounreay, Pat was appointed Assistant Lecturer in the Department of Physics at Queen's College, Dundee (then a college of St Andrews University). By the time the University of Dundee became independent of St Andrews in 1967, Pat was Lecturer in the Carnegie Laboratory of Physics, subsequently becoming Senior Lecturer (1973) and Reader (1976).

A significant addition to Pat's research interests arose from a period spent as Visiting Associate Professor in the group of **Michael Rossmann** at Purdue in 1965. In that period, Pat worked on applications of the rotation function of Rossmann and Blow; combining these with his own translation (Q) function methods led to the determination of the position and orientation of the myoglobin molecule in the crystal structure of seal myoglobin. The Crystallography research group in the Physics Department at Dundee in those days comprised **Herbert Wilson**, Patrick, **Douglas Young** and **John Low**. This group published many crystal structures of nucleosides, nucleotides and other nucleic acid components, many of them solved using Pat's implementation of Patterson Methods. In addition, the group was heavily involved in the further exploitation of computation in crystallographic research, and in the difficult area of fibre diffraction studies of filamentous plant viruses. This work was aided by extensive use of optical diffraction, an area in which Pat had been interested since his time at Purdue, and electron micrographs. The work on plant viruses, largely in the Potex group, benefited from Pat's collaboration with Virologists at the local Scottish Crop Research Institute in Invergowrie, close to Dundee. Pat also pursued this work further as a Visiting Scientist in the Group of **John Bancroft** at Western Ontario.

Pat Tollin's published work was extensive and always beautifully argued. He produced influential publications in reciprocal space Patterson methods, both original research works and reviews, and was a contributor to texts in the areas of Patterson and Direct Methods for structure determination. In the plant virus field, he also wrote authoritative original research articles and reviews. The clarity of Pat's writing was reflected in his lecturing style, which was beautifully uncluttered and clear; he was a regular invited lecturer at conferences and at teaching schools, including the first of what are now the CCG schools at Durham.

Pat's contributions to structural science were acknowledged by his election to Fellowship of the Royal Society of Edinburgh in 1977.

It was my pleasure to be Pat's graduate student during my PhD days in Dundee in the early 1980s, and while he was by no means fully engaged in research at that point, it was clear he was an exceptionally clever and insightful man, whose questioning was always incisive and whose encouragement, delivered with a laconic wit, was heart-felt and generous. I am in his debt, for his tutoring and inspiration in crystallography and in Patterson methods, and for allowing me the opportunity to make the mistakes I did while always being on hand with sage advice on "how actually to do it properly this time, Chick". In the end I was Pat's final graduate student, but we collaborated for several years after I completed my PhD studies, in developing further Patterson Method techniques for solving molecular structures, including early attempts at structure solution from powder data, embodied in the PATMET computer program.

Pat's death in March 2006 followed several extended periods of illness, and the loss of his wife Marie in 2002. He is survived by his two sons, two daughters and two grandchildren.

Chick Wilson

BCA 2007 Spring Meeting

The Young Crystallographers' Meeting 16th - 17th April 2007 Canterbury, Kent

Monday 16th April:

1130 - 1230 Registration

1230 - 1240 Welcome: **Simon Coles** (University of Southampton).

1240 - 1510 Session 1: *Chair:* **Simon Coles**

1240 - 1310 Keynote: **Roy Copley** (GSK)
Insights into pharmaceutical small molecule crystallography.

1310 - 1325 Duncan Sneddon (University of Glasgow)
Classifying molecular geometries: Application of factor analysis to cluster formation in dSNAP.

1325 - 1340 Alexandra Ruaux (University of Southampton)
BipD - An Invasion Protein associated with the Type-III Secretion System of Burkholderia pseudomallei.

1340 - 1355 Teresa Saverese (University of Bath)
Photocrystallography: Turning a light on crystallography.

1355 - 1410 Helen Maynard (University of Edinburgh)
The High Pressure Crystallography of Methane.

1410 - 1425 Helena Shepherd (University of Durham)
Structural studies of thermally and light induced spin crossover in Iron(III) coordination polymers.

1425 - 1440 Arefeh Seyedarabi (Queen Mary, Uni. of London) *A recipe for binding and catalysis by pectate lyase.*

1440 - 1530 Tea & Coffee

1530 - 1700 Session 2: *Chair:* **Mike Probert**

1530 - 1600 Keynote: **Andres Goeta** (University of Durham) *Getting Hot Results from Cold Data.*

1600 - 1615 David Berry (University of Bradford)
Pharmaceutical Co-crystals - Screening via hot stage melts.

1615 - 1630 Liana Vella-Zarb (University of Birmingham)
Automated comparison of computational structures and experimental diffraction data.

1630 - 1645 Markus Fries (Queen Mary, Uni. Of London)
Crystallographic insights into the mechanism and specificity of pectin methylesterase.

1645 - 1700 Lars F. Lundegaard (University of Edinburgh)
Single crystal studies of pure elements at high pressure.

1700 - 1730 Tea & Coffee

1730 - 1900 Session 3: *Chair:* **Roy Copley & Mike Probert** *Flash Presentations - 1 minute presentations for Poster Contributors.*

1900 - 2100 Buffet Dinner *followed by Poster Session with wine!*

Tuesday 17th April

0900 - 1100 Session 4: *Chair:* **Alex Griffin**

0900 - 0930 Keynote: **Andrea Hadfield** (University of Bristol) *Chasing Lactate Dehydrogenase in Circles: Making Crystal Movies.*

0930 - 0945 Gemma Little (University of Birmingham)
A high pressure study of Gallosilicate Natrolite.

0945 - 1000 Robert Davies (University of Oxford)
Radioprotectant screening for cryocrystallography.

1000 - 1015 Stephen Cairns (University of Glasgow)
Synthesis and structural studies of the ettringite group of minerals.

1015 - 1030 Alexander Pohl (University of Reading)
Why couldn't Bragg solve the structure of nickel cyanide?

1030 - 1045 Gareth Lloyd (University of Durham)
Molecular Motion within Crystals.

1045 - 1100 Shu Yan (University of Oxford)
Engineering applications of X-ray Diffraction.

1100 - 1105 Closing Remarks

1105 - 1130 Tea & Coffee *Registration for main meeting.*

11:30 - 12:30 Lonsdale Lecture **Bill David** (ISIS, RAL)

Scientific Programme

Named Lectures

Lonsdale Lecture: Tuesday 11.30 - 12.30
Professor Bill David (ISIS/RAL)
Combinatorial Studies of Hydrogen Storage Materials - Playing the Odds.

Bragg Lecture: Wednesday 12.00 - 13.00
Professor Sir Roger Penrose (Oxford)
Quasi-Crystals and Non-local Assembly: A Quantum-Theory foundations issue?

Hodgkin Lecture: Wednesday 17.45 - 18.45
Professor Judith Howard (Durham)
Looking Back, Leaping Forward.

Keynote Lectures

Biological Structures Group: Wednesday 09.00 - 09.45
Professor John Moult (Maryland)
SNPs, Protein Structure and Disease.

Chemical Crystallography Group: Thursday 09.00 - 09.45
Professor Chick Wilson (Glasgow) *Beans, Sausages and Pancakes: a Recipe for understanding Thermal Motion in Crystals.*

Industrial Group: Wednesday 14.15 - 15.00
Professor R.L. Snyder (Georgia Inst. of Technology)
Nano-Materials.

Physical Crystallography Group: Tuesday 14.00 - 14.45
Professor Richard Catlow (UCL) *Modelling and Predicting the Structures of Complex Inorganic Material.*

CCDC Prize Presentation and Talk: Thursday 13.00 -13.30
Dr Andy Parkin (Glasgow University) *Disorder, similarity and probability: Improving our understanding of hydrogen bonding in the solid state.*

Parallel Sessions

Tuesday 15.15-16.45

Expression to Data Collection
Chair: **K. Brown** (Imperial)

Laurence Pearl (Cancer research UK) *Combinatorial Domain Hunting.*
Frank von Delft (SGC, Oxford) *Robotic & Protein Crystallisation: Experimental Design, Application and New Developments.*
Peter Moody (Leicester) *Automation in a Small Protein Crystallography Laboratory.*

New science from big facilities
Chair: **Jon Wright** (ERSF)

Simone Techert (Max Planck Institute, Göttingen) *Time-resolved X-ray Diffraction: Possibilities and Limitations for Studying Light-activated Matter.*
Simon Brown (ESRF, Grenoble) *Science and Instrumentation on the XMaS beamline.*
Richard Ibberson (ISIS) *Recent Highlights and Future Opportunities for Neutron Powder Diffraction at ISIS.*

Co-crystals of Pharmaceutical Materials
Chairs: **Anne Kavanagh** (AstraZeneca, Macclesfield),
Roy Copley (GSK, Harlow)

Bill Jones (Cambridge) *Strategies for Designing and Making Co-crystals.*
Keith Chadwick (Manchester) *Co-crystals - does Thermodynamics hold the Secrets of Drop Grinding?*
Chris Frampton (Pharmorphix) *Panic to Panacea: Co-crystallisation in Pharmaceutical Development.*

Wednesday 10.15 - 11.45

Complementary and Emerging Developments in SR
Chair: **Pierre Rizkallah** (CCLRC, Daresbury)

Bonnie Wallace (Birkbeck) *Synchrotron Radiation Circular Dichroism Spectroscopy: A New Tool for Structural Biology.*
Dmitri Svergun (EMBL, Hamburg) *Analysis of Biomacromolecular Solutions with Small-Angle Scattering*
So Iwata (Imperial) *Diamond Membrane Protein Laboratory.*

Solving Difficult Problems at Central Facilities
Chair: **John Warren** (CCLRC)

Bill Clegg (Newcastle) *Keeping British Chemistry at the Forefront with Synchrotron Single-Crystal Diffraction.*
Alistair Lennie (CCLRC Daresbury) *New Facilities for High Pressure at the SRS.*
Kenneth Shankland (CCLRC ISIS) *Small Molecules, Big Facilities: Some Good Reasons to write a Facility Experiment Proposal.*

XRF/XRD Joint session on thin films
Chairs: **Dave Taylor** (ICDD),
Chris Staddon (Nottingham)

Tom Ryan (Nanometrics, Oregon, USA) *Thin Films and Coatings by XRF and XRD: an Overview.*
Joachim Woitok (PANalytical) *Advanced Solid-*

state X-ray Detector for the Analysis of Thin-layered Structures.
Hugues Guerault (BrukerAXS) *Up-To-Date XRD-Techniques for investigating Ultra-thin Films and ultra-small features.*
Brian Tanner (Bede) *X-Ray Probes of the Layer and Interface Structure of Nano-Scale Films for Opto-Electronics and Spintronics.*

Disordered materials and glasses I

Chair: **Matt Tucker** (Durham)

Robert Newport (Kent) *The Use of Complementary Probes in the Study of Complex Glasses.*
Martin Wilding (Aberystwyth) *High Energy X-Ray Diffraction Studies of Refractory Oxide Liquids.*
Adrian Barnes (Bristol) *The Structure of Pure Rare Earth Aluminate Glasses, Glass Ceramics and Crystals Produced by Aerodynamic Levitation and Laser Heating.*

Wednesday 15.30 - 17.00

Computational Automation

Chair: **Vilmos Fulop** (Warwick)

Julie Wilson (York) *Alice's Adventures in Grenoble.*
Andrew Leslie (MRC, Cambridge) *Automated Diffraction Data Collection and Processing with DNA.*
Colin Nave (Daresbury) *Using the Synchrotron over the Internet via e-HTPX.*
Randy Read (Cambridge) *Likelihood and Automation in PHASER.*

Transport and Reactivity in Crystals

Chair: **Simon Parsons** (Edinburgh)

Richard Jones (Keele) *Zeolites Sorption Sites and Temperature.*
Paul Raithby (Bath) *Bright Ideas In Exciting Crystallography.*
Kenneth Harris (Cardiff) *Molecular Transport in Crystalline Tunnel Structures.*

Diffraction from Surfaces and Two Dimensional Crystallography

Chairs: **Judith Shackleton** (Manchester), **Richard Morris** (Morris Analytical X-ray)

Donna Arnold (University College Cork) *Structural Studies of Ordered Mesoporous Silica in Channelled Substrates.*
Tom Hase (Durham) *X-ray Characterisation of Nanomagnetic Materials.*
Peter Laggner (Graz) *SAXS and GI Applications Using a Novel Modular Laboratory System.*

Thursday 10.15 - 12.15

Post-phasing and Beyond

Chair: **R. Read** (Cambridge)

Tassos Perrakis (Netherlands Cancer Institute) *Algorithms and Ideas for Automated Model Completion.*
Nick Furnham (Cambridge) *RAPPER: Restraint Based Conformer Generation Using Crystallographic Data.*
Kim Watson (Reading) *GRID on the Grid: A New Workflow Environment for High-Throughput Biological Computing.*
Paul Emsley (York) *Model Building Tools in Coot NCS Tools, Helices and Strands.*

One Hundred and One Ways to Prepare an XRPD Sample

Chairs: **Jeremy Karl Cockcroft** (UCL), **Martin Gill** (Natural History Museum)

Industrial Group Young Crystallographer Prize talk

The session will continue in workshop style led by the chairs and conclude with:
Gordon Cressey (Natural History Museum) *Random Diffraction Patterns (without really trying).*

Computational methods in crystallography

Chair: **Dave Allan** (Edinburgh)

Carole Morrison (Edinburgh) *Finding the Elusive Hydrogen Atoms - how Computational Chemistry can help.*
Stewart Clark (Durham) *Density Functional Methods in Crystallography.*
Mark Johnson (ILL, Grenoble) *The Role of Total Energy Calculations in Structure Determination and Related Problems.*
Dean Sayle (Cranfield) *Ceria Nanosphere Self-assembly into Nanorods and Framework Architectures.*

Thursday 13.30 - 15.00

Dynamics in Crystals

Chair: **Chick Wilson** (Glasgow)

John Evans (Durham) *Framework Dynamics and Atomic Migrations in Inorganic Materials - Insight from Diffraction and NMR Studies.*
Stewart Parker (ISIS) *Vibrational Spectroscopy with Neutrons: Catalysts, Hydrides and Polyethylene.*
Graeme Day (Cambridge) *Dynamics in Molecular Crystals across the Crystal Packing Landscape.*

Standardless Future for Quantitative XRPD?

Chair: **Steve Norval** (ICI, Wilton)

Gordon Cressey (Natural History Museum) *Random Mounts and Reproducibility? The Key to Standardless Q.P.A.*

Christopher Gilmore et al (Glasgow) *Quantitative Analysis of Mixtures Using High Throughput Instrumentation without the Use of Standards*.

Rob Hill (BrukerAXS) *Quantitative Analysis of Cements.*

Paul O'Meara (PANalytical) *Applications of Rietveld in Aluminium Production.*

Disordered materials and glasses II

Chair: **John Loveday** (Edinburgh)

Eugene Gregoryanz (Edinburgh) *Liquid-like State of Sulphur at Megabar Pressures.*

Terry Willis (Oxford) *Local Disordered Structure in the UO_2-U_4O_9 System.*

Sylvia Mclain (ISIS) *The Structure of Biomolecules in Aqueous Solution.*

XRF Session Details

Tuesday Morning

Tutorial / Workshop Session *"XRF. Where are we now?"*
Mark Ingham is organiser and chair. We have secured two speakers of international renown to present the following sessions.

10.00 Bruno Vrebos (PANalytical) *XRF. What instruments have we got, or are likely to get soon?*

11.15 Coffee

11.45 Rene Van Grieken (Antwerp) *XRF. What can we do with them?*

Tuesday Afternoon

14.00 - 15.00 Semi-quantitative
Ros Schwarz is organiser and chair.

14.00 M N Ingham, H M Harrison or N D Eatherington (British Geological Survey, Keyworth)
What on earth is this?

14.30 Belen Morales, Paul Hurditch (London and Scandinavian Ltd) *When to use XRF-Semi-quantitative analysis. Case Studies.*

15.30 - 16.45 Calibration Samples
Ros Schwarz is organiser and chair.

15.30 David Beveridge (ILFORD Photo) *No standards? No blanks? No standardless software? No problem!*

15.55 Phil Russell (PANalytical) *Normative Committees.*

16.20 M N Ingham, N D Eatherington or C J B Gowing (British Geological Survey, Keyworth)
Wide Range Oxide fused bead standards.

16.45 Break

17.00 - 18.30 XRF Exhibitors' Forum
Dave Taylor is organiser and chair. Exhibitors will be allowed to give commercial talks aimed at encouraging delegates to visit their exhibition stand for further information. Exhibitors will be required to register in advance to give a presentation and the available time of 90 minutes will be divided equally to fit in all the talks.

Tuesday Evening

Posters and Exhibition with buffet and wine.

Wednesday Morning

10.15 - 12.00 XRF / XRD Joint session on thin films
Dave Taylor & Chris Staddon are the organisers.

10.15 Tom Ryan (Nanometrics, Oregon, USA) *Thin Films and Coatings by XRF and XRD. an Overview.*

11.00 Joachim Woitok (PANalytical, Almelo) *Advanced solid-state X-ray detector for the analysis of thin layered structures.*

11.20 Hugues Guerault (BrukerAXS)
Up-To-Date XRD-Techniques for investigating ultra-thin films and ultra-small features.

11.40 Brian Tanner (Bede) *X-ray probes of the layer and interface structure of nano-scale films for opto-electronics and spintronics.*

Wednesday Afternoon

13.30 - 15.00 and 15.30 - 17.00 XRF Applications - including Cultural Heritage
David Beveridge is organiser and chair.

13.30 Luisa Carvalho (Lisbon) *X-Ray Fluorescence Analysis on paper characterization.*

14.00 Clair Collins (Oxford Instruments) *Analysis of archaeological artefacts by handheld XRF.*

14.30 Malcolm Haigh (Spectro) *Analysis of Geological Samples using a Polarised-Beam Benchtop XRF Spectrometer.*

15.00 Tea

15.30 M N Ingham, L D Grimsley, S J Carter or H M Harrison (British Geological Survey, Keyworth) *Mobile XRF and MCERTS analysis of soils.*

16.00 Jean-Philippe Gagnon (Claisse) *Volatiles management in XRF analysis.*

16.30 Margaret West (West X-ray Solutions) & **D Jefferson** (Jefferson Consulting) *Conservation and Restoration - XRF brings the past into our future.*

Thursday Morning

Margaret West is organiser and chair.

10.00 XRF Foundation Lecture
Rene Van Grieken(Antwerp) *Environmental Issues.*

11.00 - 12.30 Presentations on Environmental issues

11.00 Nick Marsh (Leicester) *Climate records - lurking in the small print? What's at the bottom of your lake?*

11.25 Chris Vanhoof (VITO, Belgium) *Development and validation results of a new European Standard prEN 15309 for the determination of the elemental composition of waste and soil by XRF.*

11.50 Stan Piorek (Niton) *Screening of electronic products with a "small-spot" hand-held XRF analyser for compliance with RoHS Directive.*

12.10 Ros Schwarz (Oxford Instruments) *Micro-spot XRF in RoHS compliance testing performance and pitfalls.*

12.30 Closing Remarks

CCDC Prize Lecture

THE CCDC prize is awarded annually to a scientist nominated by the CCG who is under 35 years of age on 1st January of the award year.

The award is for excellence in original research in the field of chemical crystallography or the application of crystallographic information to structural chemistry. This includes advances in instrumental, experimental, theoretical or computational techniques that contribute to this field.

This year's winner is **Dr Andy Parkin** (Glasgow University) who will receive the award at 13.00 on Thursday and will present a talk: *Disorder, similarity and probability: Improving our understanding of hydrogen bonding in the solid state.*

Sam Motherwell Symposium

Thursday 19 April (pm) - Friday 20 April (am)

SAM Motherwell retired from his position as CCDC Research Manager on 31 December 2006. Sam obtained a BSc (chemistry) and a PhD (crystallography - with John Iball) from Dundee/St Andrews and joined the embryo CCDC in 1968. Sam's scientific interests have been wide ranging. He was one of the pioneers of molecular graphics software through the Pluto program, was involved in the early development of direct methods, and played a major role in the very first releases of the Cambridge Structural Database. For the CSD, he wrote the original 2D substructure search code (CONNSER) and extended this to 3D substructure searching and data analysis in the GEOM program. Many of these fundamental ideas (and even some code) have contributed to the more recent CSD programs QUEST and ConQuest.

In 1978, Sam moved to the University Library in Cambridge as Head of Automation, rejoining the CCDC in January 1992. Since that time, his research career has moved towards applications of CSD information in crystal engineering and pharmaceutical materials development, including work in crystal structure prediction, where he has organised three well-known 'blind tests' of developing CSP methodologies. Since 2002, he has been an Associate Director of the Cambridge-based Pfizer Institute for Pharmaceutical Materials Science, and has worked closely with scientists from the University Departments of Chemistry and Materials Science, and with Pfizer scientists worldwide.

Sam has published more than 110 papers (and rising), and has been responsible for originating software and ideas that have been used by generations of crystallographers and chemists.

The speakers detailed below demonstrate the scientific range of Sam's unique contribution. The Symposium comprises talks by both established and younger scientists. There will be a banquet in honour of Sam

Motherwell on the evening of Thursday 19 April. The Symposium will be chaired by **Frank Allen** (CCDC) and **Graeme Day** (University of Cambridge).

Frank Allen (CCDC, Cambridge, UK)
Introduction: Sam Motherwell's science at the CCDC.

Robin Taylor (CCDC, Cambridge, UK)
Using small-molecule crystal-structure data to validate protein-ligand structures.

Neil Feeder (Pfizer Research, Sandwich, UK)
The Pfizer Institute for Pharmaceutical Materials Science (PIPMS) - Towards Predictive Pharmaceutical Solid Form Selection.

Carol Brock (University of Kentucky, Lexington, USA)
Phase Sequences in Some Crystals Containing M(NO3)2, water, and 15 - Crown - 5.

Sally Price (University College London, UK)
The CCDC International Blind Tests of Crystal Structure Prediction - what have we learnt?

Clare Macrae (CCDC, Cambridge, UK)
Crystal structure visualisation at the CCDC: Past, Present and Future.

James Chisholm (CCDC, Cambridge, UK)
Searching the CSD for extended motifs and other challenging queries.

Aurora Cruz Cabeza (PIPMS, University of Cambridge, UK)
A comparative study of carbamazepine and its dihydro derivative: prediction and observation of polymorphs and solvates.

Elna Pidcock (CCDC, Cambridge, UK)
Symmetry, space groups, molecular packing and chirality.

Peter Wood (University of Edinburgh, UK)
Understanding High - Pressure Phase Transitions with Pixel Calculations.

Jack Dunitz (ETH, Zurich, Switzerland)
Fluorine - the odd man out.

Sam Motherwell (CCDC, Cambridge, UK)
The CSD - 400,000 answers .... but what are the questions.

Commercial Exhibition

THE exhibition, which will be in the Rutherford Hall is sold out this year! The popular Exhibitors' Forum will be at 17.00-18.30 on Tuesday.

Westminster Fellowship Scheme Seeks Candidates

Deadline: Friday 30 March 2007

http://www.rsc.org/ScienceAndTechnology/Parliament/

WestminsterFellowshipScheme2007.asp

THE RSC in collaboration with the Parliamentary Office of Science and Technology (POST), are delighted to offer this great opportunity to spend 3 months working at the Parliamentary Office of Science and Technology in Westminster, gaining real life experience of science research and writing for government and the general public.

Contact: Julie Smart smartj@rsc.org

Web Course on Basic Crystallography

GERVAIS CHAPUIS (Lausanne) wrote to say: I would be pleased if you could advertise the new web based course on basic crystallography. The course can be directly and freely accessed at http://escher.epfl.ch/eCrystallography

With kind regards

Gervais Chapuis
http://lcr.epfl.ch

From the Secretary

Announcement of elections to Council

AT the 2006 Annual Meeting in Canterbury we will elect a new Vice-President and Secretary of Council as the present incumbents of these positions have reached the end of their terms. We will also be electing the new Education Co-ordinator. There are no other vacancies on Council this year. Nominations for all three posts are invited. Each nomination requires a proposer and seconder, and, should you wish to nominate someone, please obtain their consent first.

Properly seconded nominations will be received up till two weeks before the date of the AGM which is on 18th April 2007. They may be sent by email to secretary@crystallography.org.uk

Christine Cardin
Secretary to Council

Agenda

THE Annual General Meeting of the British Crystallographic Association will be held on Wednesday 18th April 2007 at 4.30 p.m. in the University of Kent at Canterbury.

At this meeting we will elect a new Vice-President and Secretary.

Draft Agenda

1. Approval of Agenda.
2. Apologies for absence.
3. Minutes of the last AGM (published in Crystallography News).
4. President's Report.
5. Secretary's Annual Report.
6. Northern Networking's Report.
7. Report of the Treasurer to include Presentation of the Accounts for 2006 and the Examining Accountant's Report.
8. Acceptance of the Accounts.
9. Elections to Council.
10. Appointment of Examining Accountant for 2007.
11. Any other business.

Christine Cardin (Hon Secretary)

Minutes of AGM

Held on Wednesday, 5th April 2006 at 16.35 p.m. in The University of Lancaster

THE President (Chick Wilson) in the Chair.
115 voting members were present.

1. Approval of agenda. The agenda was approved

2. Apologies for absence. There were no apologies for absence.

3. Minutes of the previous AGM. These had been published in the March 2006 issue of Crystallography News. They were approved as a correct record of the meeting. Proposer: **Harry Powell**. Seconder: **Sheila Gould**

4. President's Report. The President reported that 360 delegates were present at this Spring Meeting, an encouraging number. He was however disappointed that the proposal to hold the European Crystallographic Meeting in Edinburgh in 2009 had not been accepted by the European Crystallographic Association. He thanked everyone concerned for the smooth running of the Spring Meeting, particularly **Paul Raithby** for acting as the Programme Chair for the meeting. He was particularly gratified at the success of the Young Crystallographers' meeting, which had attracted over 90 delegates, following on from the inaugural meeting of this group in UMIST in 2004.

The President noted with sadness the passing of **Robin Shirley**, **Robert Evans**, **Uli Arndt** and **Patrick Tollin**. These included two former Honorary Members.

The President announced that **Peter Main** and **Chris Gilmore** had been elected as new Honorary Members. The President thanked the members for their staunch support during his term of office.

5. Secretary's Report. The secretary, **Christine Cardin**, presented her report, which has since been published in Crystallography News.

6. Elections.

6.1 President of Council

There were two candidates for President. **Paul Raithby** (nom: **John Helliwell**; sec: **Sandy Blake**) **Garry Taylor** (nom: **Richard Pauptit**; sec: **Elspeth Garman**) The election was by secret ballot (tellers **John Finney** and **Bob Gould**) and **Paul Raithby** was declared elected. In his acceptance speech, Paul said that his priorities would be to stabilise the financial situation, to develop an inclusive organisation and forge links with other societies, and to extend even further the BCA's educational role, to include, for example, final year project students.

6.2. Ordinary Members of Council

There were five candidates for three places on Council.
Graham Bushnell-Wye (nom: John Finney; sec: **Paul Barnes**)
Bill Clegg (nom: **Jeremy Cockcroft**; sec: **Mike Glazer**)
Richard Cooper (nom: **Simon Parsons**; sec: **Andy Parkin**)

Elspeth Garman (nom: Christine Cardin; sec: Sheila Gould)
Andrea Hadfield (nom: Richard Pauptit; sec: Sheila Gover).

The election was by single transferable vote, and the tellers were **Jeremy Cockcroft** and **John Evans**). The electorate was 115, so the quota was 38. **Bill Clegg**, **Elspeth Garman** and **Richard Cooper** were duly declared elected, following elimination of the lowest ranked candidate and redistribution of the second preference votes.

7. Northern Networking report. This report was presented orally. **Gill Moore** said that there are now 17 companies as Corporate members and 689 paid up members on the database. She reported that Crystallography News flourishes, and that the Spring Meeting was the largest ever, with 360 registered participants. There were six new exhibitors. The Young Crystallographers sessions had been a great success with over 90 at the sessions. There have been 123 posters, and Douglas Moore is thanked for his help in rearranging them. Elaine has made a good job of running her first BCA conference. The 2007 meeting has been booked for Kent for the 17-19th April 2007. It is expected that the 2008 meeting will be held in Swansea from 8-10th April 2008.

8. Treasurer's report. The Treasurer, **Sheila Gould**, presented a detailed report, subsequently published in Crystallography News. Crystallography News has broken even, and the advertisers are thanked for their continuing support. Membership subscriptions are however down and a review is in process. Investments did well and the bursary fund was well used. There is an overall deficit over the year of £3172. One tangible asset has been written off - the computer previously used to produce Crystallography News. The Spring Meeting has made a surplus of about £3500 in line with the past three years. The margin of error here is quite small, so Gill and Elaine should be congratulated on their good management.

Mike Glazer proposed that the accounts be accepted, seconded by **Chris Gilmore**. The reappointment of the accountant was also approved. **Sheila Gould** recommended that the Young Company be reappointed. **Paul Raithby** proposed that the meeting accept this, seconded **Christine Cardin**. The meeting voted with one abstention and no votes against to raise the membership subscription to £20, with a corporate fee of £750 and a student fee of £20 for the three year term. This will be implemented with the 2007 membership renewals.

9. AOB The incoming President, **Paul Raithby**, asked **Garry Taylor** if he would agree to being co-opted to Council, and he accepted. He was pleased to announce that **Lindsay Sawyer** had agreed to be next year's Programme Chairman. Finally, Paul thanked **Chick Wilson**, as outgoing President, for his leadership, this commonsense, his calmness and his overwhelming enthusiasm.

There being no further business the meeting closed at 1730.

Christine Cardin
Secretary to Council

Bursary Report 2006 - from the Treasurer

THE BCA is always pleased to fulfil its duties to further the education of crystallographers by supporting them financially to attend meetings relevant to their research activities, and we do appreciate the generous donations to the Arnold Beevers Bursary Fund which enable these bursaries to be awarded. This year the BSG donated £768.13, the interest from its reserves, to the fund and the Gift Aid refund of £845.59 on the membership subscriptions was also placed in the fund. Other membership donations amounted to £231.50.

The number of applications for bursaries increased this year, mainly due to the Young Crystallographers sessions at the Spring Meeting in Lancaster. There were 47 bursaries worth £175 awarded to students attending the Spring meeting. 8 of these Bursaries had commercial sponsors, and we are very grateful to ICDD (2), PANalytical (4) and Rigaku (2) for this valuable support.

During the rest of the year, there were 8 Arnold Beevers Bursaries awarded, totalling £1,600. Many of the bursars' reports of these meetings have been incorporated into the articles which have been printed in Crystallography News.

ECM-23, Leuven
Noelia Sanchez Ballester University of Loughborough
Kathy Guille University of Newcastle-Uupon-Tyne
Ross Harrington University of Newcastle-upon-Tyne

Higher European Research Course for Users of Large Experimental Systems, Grenoble
Shu Yan Zhang University of Oxford

American Crystallographic Association, Honolulu
Rebecca Conners University of Bristol

Synchrotron Radiation Summer School, Daresbury
Suzanne Harte University of Glasgow

International Intensive Course on Structure Determination, Siena
Kennedy Abuga Birkbeck College

MRS Fall Meeting 2006, Boston
Dave Aldous University of St. Andrews

The BCA also donated £1000 to enable students to attend the Sagamore Conference held this year at the University of Warwick.

IUCr Congress Bursary Fund

The BCA Council has offered the money in this fund on loan to the organising committee of the XXI Congress in Osaka, Japan in 2008.

Sheila Gould

BCA 2007 Spring Meeting -

<table>
<tr><th></th><th colspan="2">Monday 16th April</th><th colspan="3">Tuesday 17th April</th></tr>
<tr><td></td><td colspan="2">Satellite Mtg</td><td colspan="3"></td></tr>
<tr><td>0900</td><td colspan="2" rowspan="10"></td><td rowspan="4">YC Session 4

09.00 to 11.00</td><td colspan="2" rowspan="4">Possible Workshop?</td></tr>
<tr><td>0915</td></tr>
<tr><td>0930</td></tr>
<tr><td>0945</td></tr>
<tr><td>1000</td><td colspan="3"></td></tr>
<tr><td>1015</td><td colspan="3"></td></tr>
<tr><td>1030</td><td colspan="3"></td></tr>
<tr><td>1045</td><td colspan="3"></td></tr>
<tr><td>1100</td><td colspan="3" rowspan="2">Coffee & Registration
1100 to 1130</td></tr>
<tr><td>1115</td></tr>
<tr><td>1130</td><td rowspan="6">Young Crystallographers
Registration

11.30 to 13.00</td><td rowspan="12"></td><td colspan="3" rowspan="3">Lonsdale Lecture

11.30 to 12.30
Professor William David (ISIS)</td></tr>
<tr><td>1145</td></tr>
<tr><td>1200</td></tr>
<tr><td>1215</td><td colspan="3" rowspan="4">Lunch, Exhibition &
Registration

12.30 to 14.00</td></tr>
<tr><td>1230</td></tr>
<tr><td>1245</td></tr>
<tr><td>1300</td><td rowspan="6">Young Crystallographers
Session 1

13.00 to 15.00</td></tr>
<tr><td>1315</td><td colspan="3" rowspan="3">Keynote PCG
Richard Catlow (London)
14.00 to 14.45</td></tr>
<tr><td>1330</td></tr>
<tr><td>1345</td></tr>
<tr><td>1400</td><td colspan="3" rowspan="2">Tea & Coffee
1445 to 1515</td></tr>
<tr><td>1415</td></tr>
<tr><td>1430</td><td colspan="3" rowspan="2"></td></tr>
<tr><td>1445</td></tr>
<tr><td>1500</td><td colspan="2" rowspan="2">Tea & Coffee 15.00 to 15.30</td><td rowspan="2">BSG
Session 1
Expression

1515 to
1645</td><td rowspan="2">CCG/PCG
Session 1
New Science

1515 to
1645</td><td rowspan="2">IG
Session 1
Co-crystals

1515 to 1645</td></tr>
<tr><td>1515</td></tr>
<tr><td>1530</td><td rowspan="6">YC Session 2

1530 to 1700</td><td rowspan="14">Possible Workshop
or special interest
groups</td><td colspan="3" rowspan="2">Break 15 mins</td></tr>
<tr><td>1545</td></tr>
<tr><td>1600</td><td colspan="3" rowspan="4">Exhibitors' Forum

17.00 to 18.30</td></tr>
<tr><td>1615</td></tr>
<tr><td>1630</td></tr>
<tr><td>1645</td></tr>
<tr><td>1700</td><td rowspan="2"></td></tr>
<tr><td>1715</td></tr>
<tr><td>1730</td><td rowspan="6">YC Session 3
17.30 to 19.00</td><td colspan="3" rowspan="4">Poster Exhibition
Buffet Dinner
18.30</td></tr>
<tr><td>1745</td></tr>
<tr><td>1800</td></tr>
<tr><td>1815</td></tr>
<tr><td>1830</td><td colspan="3" rowspan="2"></td></tr>
<tr><td>1845</td></tr>
<tr><td>1900</td><td>YC Dinner
19.00</td><td></td><td colspan="3"></td></tr>
</table>

Timetable

	Wednesday 18th April				Thursday 19th April			
XRF Regist	Keynote BSG John Moult (CARB) 09.00 to 09.45				Teaching Keynote (CCG) Chick Wilson (Glasgow) 09.00 to 09.45			Coffee
	Tea & Coffee 0945 to 1015				Tea & Coffee 0945 to 1015			XRF 5 Keynote
XRF 1A	BSG Session 2 Synchrotron 1015 to 1145	CCG Session 2 Problems 1015 to 1145	PCG Session 2 Glasses 1 1015 to 1145	XRF 3 & XRD Thin Films	BSG Session 4 Postphasing 1015 to 1215	PCG Session 3 Computation 1015 to 1215	PCG Session 2 10.15 to 12.15	Break
Coffee Regist								XRF 5
	Break 11.45 to 12.00							
XRF 1B	Bragg Lecture 12.00 to 13:00 Professor Sir Roger Penrose (Oxford)			Lunch & Exhib	Lunch & Exhibition 1215 to 1330			Lunch & Exhib
Lunch	Lunch & Exhibition 13.00 to 14.15		PCG AGM	IG AGM				
		BSG AGM	CGG AGM	XRF 4A	CCG Session 4 Dynamics 1330 to 1500	IG Session 4 Standardless 1330 to 1500	PCG Session 4 Glasses 2 1330 to 1500	
XRF 2A	Keynote Lecture IG R L Snyder (Georgia) 14.15 to 15.00							
Tea	Tea & Coffee 15.00 to 15.30				Tea & Coffee 1500 to 1530			
XRF 2B	BSG Session 3 Computation 1530 to 1700	CCG Session 3 Transport 1530 to 1700	IG Session 2 Surfaces 1530 to 1700	XRF 4B	Sam Motherwell Event Talks Dinner Talks on Friday			
XRF Exhib Forum	BCA AGM 17.00 to 17.45							
	Hodgkin Lecture 17.45 to 18.45 Professor Judith Howard (Durham)							
	Dinner 19.15 for 19.45							

The Z' > 1 Phenomenon

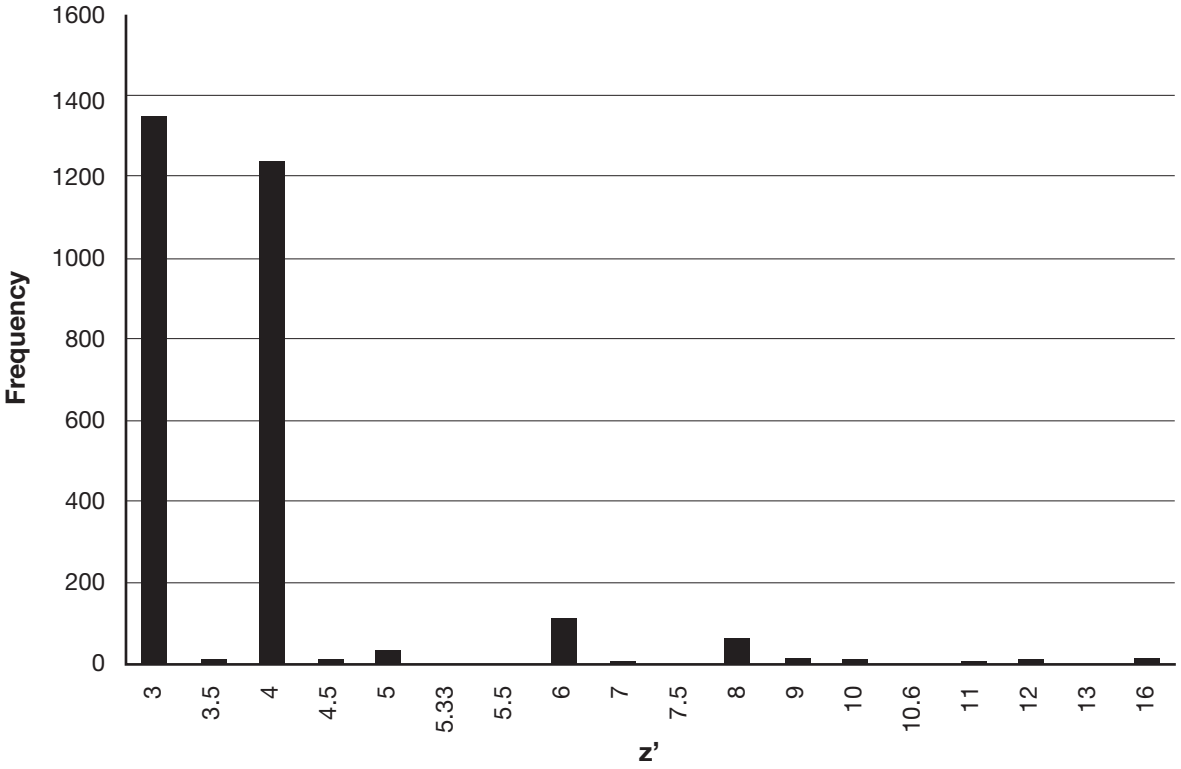

Fig.1: Frequency table for structures with Z' > 2.

THE parameter Z' is conventionally used to denote the number of molecules in the asymmetric unit. Of course, Z' is therefore crucially dependent on the somewhat subjective definition of what constitutes the 'molecule', or more properly the 'formula unit'. Strictly Z' is defined as the number of formula units in the unit cell divided by the number of independent general positions. The complexity of the asymmetric unit derives from the fact that the molecules within the asymmetric unit are free to associate themselves in three-dimensional space, unlike the asymmetric units themselves which are compelled to tessellate via particular symmetry operators (to form one of the 230 space groups).

Around 8.8%[1] of structures in the Cambridge Structural Database (CSD)[2] crystallise with more than one molecule in the asymmetric unit (i.e. Z' > 1) with values ranging from 1 $^{1}/_{12}$ to 32. Even numbers of Z' are more common than odd numbers and the number of structures with Z' > 4 is very small (Figure 1). Certain classes of compound such as nucleosides, nucleotides, steroids and other natural products[3] show a greater tendency to form high Z' structures. Strong intermolecular interactions such as the highly directional O-H···O interaction have been implicated in the formation of high Z' structures, although there are also many high Z' structures known which arise from only weak interactions (e.g. the rhenium(I) complex $[Re(MeCN)Cl_2(NO)(PMe_3)_2]$ (WODCOH), Z' = 11 (Figure 2)[4] which is held together predominantly by C-H···O and C-H···Cl hydrogen bonds):

www.dur.ac.uk/zprime/structures.html - WODCOH

In the past, refinement and solution of high Z' structures was often problematic due to large unit cells containing a sizeable number of non-hydrogen atoms. However, since the advent of CCD and area detector systems as well as enhanced computer capability these problems are now much reduced and the Z' phenomenon is enjoying intense current interest.5

Broadly, our research is based on our belief that high Z' structures can arise from frustration between two or more competing interactions (e.g. optimisation of hydrogen bonds vs. optimal shape packing) either during the nucleation process or as a dominant contribution to the bulk structure. We have explicitly probed this frustration concept through a database and experimental study combining centrosymmetric synthons and resolved chiral compounds which demonstrates an overwhelming tendency towards Z' > 1.[6]

The observation of Z' > 1 may also be regarded as a special case of co-crystallisation where the two components are the same as one another. Thus research on high Z' structures is closely related to co-crystals, solvates, hydrates etc. Reported high Z' structures may also be approximations to modulated structures that might be better handled by superspace refinement methods.[7]

The nucleation process may also be a good source of information on high Z' structures as it has been postulated that many high Z' structures are "fossil relics" of the fastest growing crystal nucleus[8] or metastable polymorphs. Techniques such as Differential Scanning Calorimetry (DSC) or variable temperature X-ray crystallography can be used to probe high Z' structures for polymorphic behaviour.

In view of the current interest in these fascinating systems, and as part of an EPSRC funded project, the Durham University Supramolecular Chemistry Group, run by **Jonathan Steed**, have developed a web site dedicated to bringing together all the information and publications known about these fascinating systems The main feature of the website is an annotated database of structures with Z' > 4, which is updated regularly (Figure 3). Each entry contains the name, chemical formula, journal reference and Cambridge Structural Database Refcode (where applicable) in addition to a "Notes" section reporting anything of interest about the packing or composition of the asymmetric unit, as well as links to polymorphs, redeterminations or similar structures. Possible errors in Z' or space group assignment are also highlighted. The structures included in the database are mainly drawn from the CSD; however, readers with unpublished high Z' structures are also invited to submit their structures for inclusion in the database.

The website also contains a general introduction to the Z' phenomenon as well as a list of useful references concerning all aspects of high Z' structures.

For further information please visit **www.durham.ac.uk/zprime** or email **zprime@durham.ac.uk**

Kirsty Anderson
University of Durham

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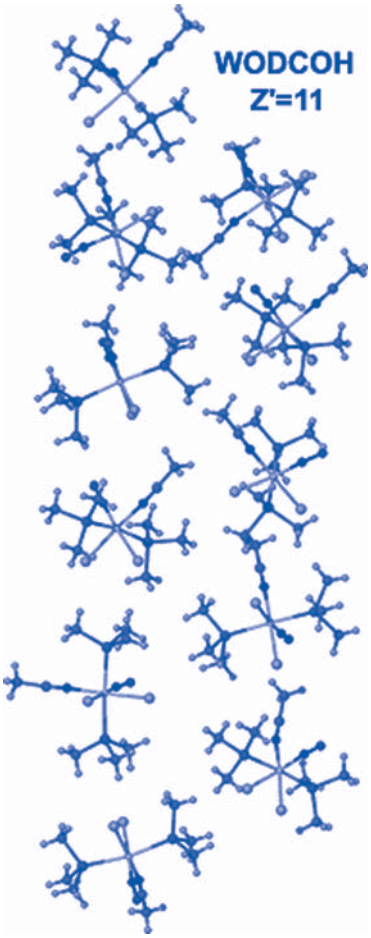


Fig. 2: Packing in WODCOH with Z' = 11.

Z' = 11				
Z' = 11	$C_9 H_{10}$ Poly(m-methylstyrene)	Organic polymer, space group identification ambiguous. The Z' value relates to covalent monomers within a repeat of the covalent polymer strand.	P. Corradini, P. Ganis, *J. Polym. Sci.*, 1960, **43**, 311	WIMTOB
Z' = 11	$C_8 H_{21} Cl_2 N_2 O P_2 Re$ (Acetonitrile)-dichloro-(nitrosyl)-bis(trimethylphosphine)-rhenium	Some disorder in molecules. Structure held together by C-H···O and C-H···Cl hydrogen bonds	H. Jacobsen, H. W. Schmalle, A. Messmer, H. Berke, *Inorg. Chim. Acta*, 2000, **306**, 153	WODCOH

Fig. 3: Section of database of structures with Z' > 4.

IUCr Computing Commission

THE November 2006 Seventh issue of the IUCr Computing Commission newsletter is available as an Adobe Acrobat PDF file via:

www.iucr.org/iucr-top/comm/ccom/newsletters/2006nov/

Besides having articles of general interest, this edition has the theme "Understanding Crystal Structures", edited by **Lachlan Cranswick** and **Simon Parsons**.

Understanding Crystal Structures:

- Multipurpose crystallochemical analysis with the program package TOPOS - **Vladislav A. Blatov**
- The XPac Program for Comparing Molecular Packings - **Thomas Gelbrich**
- The Pixel module of the OPiX computer program package: affordable calculation of intermolecular interaction energies for large organic molecules and crystals - **Angelo Gavezzotti**
- Quantifying the Similarity of Crystal Structures - **Rene de Gelder**
- Topological analysis of crystal structures - Oleg V. Dolomanov
- On the Detection of Solvent Accessible Voids in Crystal Structures with PLATON/SOLV - **Anthony L. (Ton) Spek**

Other Articles :

- The charge flipping algorithm: a powerful and universal tool for the a priori solution of crystal structures in any dimension - **Gervais Chapuis** and **Lukas Palatinus**
- cctbx news - **Ralf W. Grosse-Kunstleve**, **Peter H. Zwart**, **Pavel V. Afonine**, **Thomas R. Ioerge**r and **Paul D. Adams**
- An integrated three-dimensional visualization system VESTA using wxWidgets - **Koichi Momma** and **Fujio Izumi**
- Visual Graphic Library VGLIB5 for Crystallographic Programs on Windows PCs - **Kenji Okada**, **Ploenpit Boochatum**, **Keiichi Noguch**i and **Kenji Okuyama**
- Notes on the calculation of the derivatives for least-squares crystal structure refinement - **Riccardo Spagna**

Call for Contributions to the Next CompComm Newsletter:

The eighth issue of the Compcomm Newsletter is expected to appear around November of 2007 with the primary theme to be determined. If no-one is else is co-opted, the newsletter will be edited by **Lachlan Cranswick**.

Contributions would be also greatly appreciated on matters of general interest to the crystallographic computing community, e.g. meeting reports, future meetings, developments in software, algorithms, coding, historical articles, programming languages, techniques and other news.

www.iucr.org/iucr-top/comm/ccom/newsletters/

Lachlan Cranswick

Blind Test of Structure Prediction - can you help?

I am organising a blind test of crystal structure prediction for the Cambridge Crystallographic Data Centre. The purpose of this exercise is to evaluate current computational methodologies for ab initio crystal structure prediction of molecular crystals. Previous such "blind tests" have been extremely valuable in gauging the reliability of current methods.

A fourth blind test of crystal structure prediction is being organised to evaluate current methodologies in ab initio crystal structure prediction. Previous blind tests (the latest was published in Acta Cryst B, 2005, vol 61, 511-527) have been a useful exercise in gauging the reliability of computational methods. The upcoming blind test, whose "targets" will be announced mid-January 2007 and will run until July 2007, is open to participation from any research group involved in developing new methods for crystal structure prediction. Anyone interested in participating should contact **Graeme Day**, University of Cambridge (gmd27@cam.ac.uk) for details.

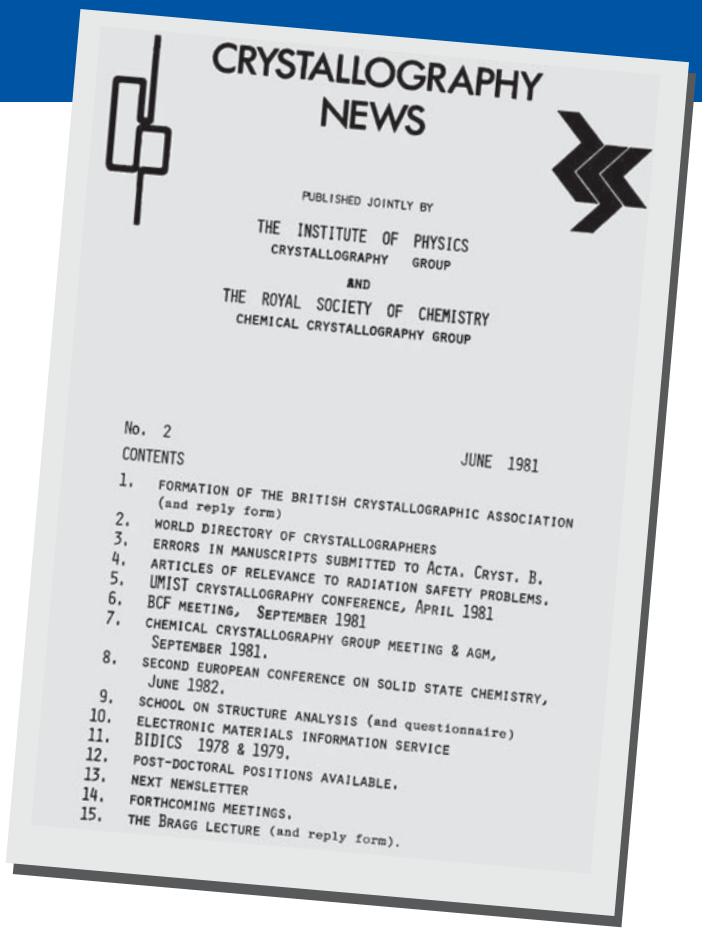
Graeme Day

History

Off the Shelf - Some Articles out of our History

CRYSTALLOGRAPHY NEWS sprang to life in June, 1982, under the editorship of Moreton Moore, following the inception of the BCA earlier that year. It was, in fact, barely distinguishable from its predecessor, also called Crystallography News, the joint Newsletter of the Crystallography Group of the Institute of Physics and the Chemical Crystallography Group of the Royal Society of Chemistry.

It was 24 pages long, and was cyclostyled on A4 paper with a green page 1, all held together by three staples along the edge. It soon reduced itself to A5, with proper stapling on a spine, and slowly improved with the technology of the time until it returned to its present A4 format at issue 76 in 2000. An illustration of improvements in technology is given by the fact that the article below was scanned from its duplicated sheet with hardly an error. It is very good that we can see that **David Phillips**' hopes from then have largely been fulfilled or are at least our objectives now!



CRYSTALLOGRAPHY NEWS

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AND
THE ROYAL SOCIETY OF CHEMISTRY
CHEMICAL CRYSTALLOGRAPHY GROUP

No. 2

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15. THE BRAGG LECTURE (and reply form).

The first "From the President" - issue 1, June, 1982

***THE** British Crystallographic Association*

*X-ray crystallography began just seventy years ago, at this time of year in 1912, when Friedrich and Knipping first observed the diffraction of X-rays by a crystal. The results were announced by von Laue on 8 June 1912 and we all know that within a year **W.L. Bragg** had exploited the new phenomenon to solve the first crystal structure. The record since then has been one of continuous expansion into new fields so that crystallography and the study of diffraction effects have transformed physics, chemistry, mineralogy, metallurgy and, most recently, biology.*

During these developments crystallographers were drawn together by their use of common methods and formed a closely integrated community, internationally as well as in this country. In recent years, however, we have tended increasingly to think of ourselves as physicists, chemists, mineralogists, metallurgists, biochemists, and so on, who happen to use crystallographic and diffraction methods in our researches, and many of us have concentrated on our contributions to these sciences and neglected our continuing common interest in crystallography. In part this is surely a natural and a healthy development, but we neglect our base in crystallography at our peril. Hence the need for the BCA.

The enthusiasm with which the formation of a British Crystallographic Association was welcomed at the Durham meeting in April shows that many of us see the need to renew and extend our contacts with our fellow crystallographers in all branches of science. We are united in the belief that the BCA will provide a framework within which that will be possible without disturbing the existing groupings of like-minded crystallographers that have flourished for so many years in association with the Institute of Physics and the Royal Society of Chemistry. Indeed these groups, and new ones helping to focus other interests, have important parts to play in the BCA and we must all work together to develop the activities of the new association.

Let us all resolve to meet with our fellow crystallographers every year at the Spring Meeting of the BCA. There we shall find out what new advances in another branch of the subject might help to solve our problems, hear about the most recent developments, see the latest apparatus, and enjoy the triumphs and share the difficulties of old and new friends. I shall look forward to seeing you at Royal Holloway College, 28-31 March, 1983.

D. C. Phillips

That LOGO

ALMOST as old as the BCA is our "child's brick" Logo, which resulted from a competition in 1982. The following is the announcement of the result of the competition in issue 5 for June, 1983. Reproduced here is the logo as it appeared in that issue. It has been the subject of much debate since - mainly about whether the perspective is right or not. The form currently in use does have a great deal more tapering, but possibly, at its lower end, tapers in the wrong direction. Please don't hesitate to keep this debate alive!

BCA Logo

***I** hope you will have noticed our brand new logo on the front cover. The design is based on a primitive Bravais lattice, which is something fundamental to all areas of crystallography, and was adopted as the official BCA Logo at the Council meeting held on 31st March, 1983.*

By the end of the Logo Competition at the Spring Meeting, I had 30 entries (one arrived on the first day of the meeting from Teheran). My thanks to all those who sent in their designs.

The logos were on display throughout the meeting, and judging was entrusted to our President. He in turn convened an ad hoc panel of 6 members, representing different areas of crystallography, to help resolve this weighty matter.

There were two similar designs which were particularly liked, and the decision of the panel was that the BCA Logo should lie somewhere between these two entries, and that the bottle of Lagavulin should go to our Editor, ***Moreton Moore****. It was with great pleasure that I was able to present Moreton with his prize at the Conference Dinner.*

Andrzej Skapski

Divorce!

BY the mid-1990s, relationships between the CCG and the RSC had become strained. Organising meetings with the RSC was often expensive and inconvenient, and the financial constraints of being an RSC subject group led to a separation. The item below appeared in issue 56 for March, 1996. Fortunately, the case was not seriously contested, and the decree absolute was indeed reached on 1 January 1997. As in all divorces, not everyone was happy, and some members left the BCA as a matter of principle. Since then, most would agree that it was a wise move. The CCG is very healthy, attracting non-crystallographers to its meetings, and most of its members attend meetings organized by the RSC.

Chemical Crystallography Group

IMPORTANT !!

***BELOW** are the texts of three resolutions for voting on at the CCG AGM in Cambridge, on 2nd April 1996. They pertain to the mechanics of the Group's severance of formal links with the RSC, and becoming a fully-fledged BCA subject group. Please come along to the AGM prepared to vote on these.*

Resolution 1:

" ... that the Chemical Crystallography Subject Group of The Royal Society of Chemistry recommends to the Council of the Society that it, the CCSG, be formally dissolved with effect from 31st December 1996."

Resolution 2:

"... that the Chemical Crystallography Group be reconstituted as a full subject group of the British Crystallographic Association, as of 1st January 1997, subject to approval by the AGM of the British Crystallographic Association."

Resolution 3:

"... that the Chemical Crystallography Group petitions The Royal Society of Chemistry for the transfer of all the assets of the Chemical Crystallography Group Trust at the time of its dissolution (i.e. one NSB account of approx. £700, one Coutts current account of approx. £200) to the new Chemical Crystallography subject group of the British Crystallographic Association."

The Last day

MOST people would agree that the highpoint of activity in the BCA was the hosting of the IUCr in 1999. This was the work of many years, and although very many people worked very hard for it, the key figure was our former president, the indefatigable **Chris Gilmore.** It is hard to select from the many things written about it, but outstanding is the following from the issue 70 of September 1999. The poem was a composition of that much loved and much missed member of the BCA, **Robin Shirley,** who sadly died in 2005.

The very last day....

***I** found **Justin Wark's** lecture in the last plenary session, 'Picosecond X-ray diffraction', to be the most exciting, with its prospect of much cheaper, faster X-ray sources using lasers.*

*The Closing Ceremony was held in the Barony Hall of Strathclyde University, adjacent to the Hall of Residence where many of us were staying. **Judith Howard** thanked everyone who had helped to make this Congress such a success before inviting **Steve Maginn** to present the CCDC prizes for the best posters by young scientists. Judged by a panel of distinguished crystallographers, four prizes were awarded. They were (in no particular order):*

*- P08.06.010: **Peter Müller**, Göttingen University, Germany; "Holes in Crystals?"*
*- P11.0D.001: **Alicia Beatty** & **Christer Aakeroy**, Kansas State University, USA;*
"Beyond the first dimension: organic/inorganic hybrid materials assembled via H-bonds".
*- P09.09.008: **C. Baehtz** & **H. Fuess**, Darmstadt University, Germany;*
"Tetrathiafulvalene and tetracyano-p-quinodimethane in faujasite".
*- P13.22.003: **S. Leoni** & **R. Nesper**; "Tilings on hyperbolic surfaces as representatives of chemical networks".*

*The Oxford Cryosystems prize for the best poster associated with cryogenics was awarded to **F.Wien** for poster P08.01.003 "A portable Cryostream to transfer crystals" The outgoing IUCr President, **Ted Baker**, explained he had known this would be a wonderful Congress, years ago, when he had heard **Chris Gilmore** et al. explaining how to translate Glaswegian. He handed over to the new President, **Henk Schenk**, who recalled his first visit to an IUCr Congress in Stonybrook, USA, thanked Ted for preparing the IUCr so well for the new century and looked forward to working with us all for the next 3 years.*

Kate Crennell

Poem for IUCrXVIII

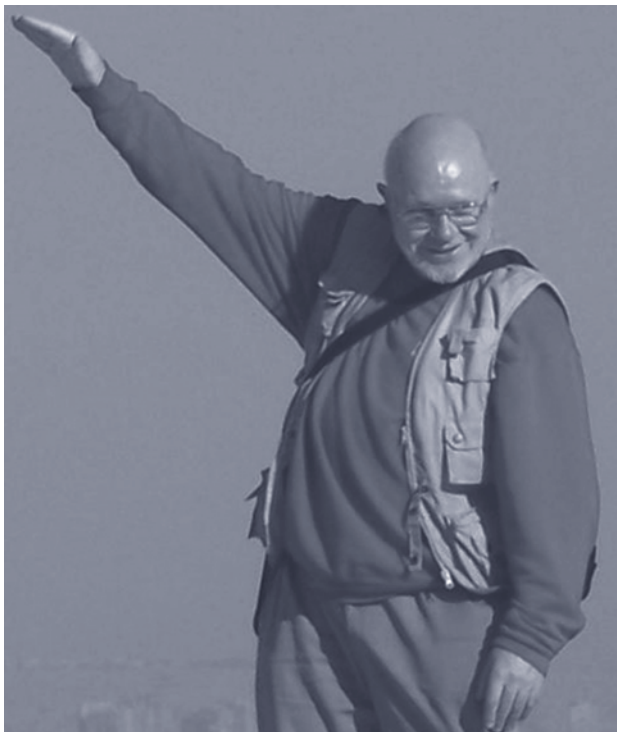
***THE** poem below was written for the IUCr Glasgow Congress. Part of his "Zen" series, the poet tries to capture the vast scope of crystallography, extending from our macroscopic world to the inner structure of (biological) tissues and finally to a nano-universe in which the atoms themselves loom like giant planets...*

The Zen of Scale

Launched on a journey
across the void of dimensions

from the intricate tapestry of tissues
to the rhythms encoded in atoms

arriving at last
to orbit electron-gas giants.



Robin Shirley is an English poet, crystallographer and computer scientist who was brought up in an artistic milieu, his family traditions being split equally between art and sciences. (A software article by him appeared later in the same issue.)

News from the Groups

The attendees enjoying January sunshine

PCG School on Rietveld Refinement

THE third PCG training course on practical aspects of Rietveld refinement was held in Trevelyan College and Department of Chemistry at Durham University, from 7-11th January 2007. It was attended by 60 students from 23 UK Universities, 6 foreign academic and research institutions and 2 industrial companies. The academic background of the participants was extremely diverse and included students and post-docs from chemistry, physics, materials, crystallography, geology and engineering departments. The international flavour was provided by participants travelling from France, Belgium, Slovenia, Greece, India and the USA.

Lectures on topics including the basics of powder diffraction and data collection, symmetry, peak shape analysis, structure factors, peak intensities and agreement factors in Rietveld refinement, restraints, constraints and rigid bodies were given by **Jeremy Cockcroft**, **John Evans** and **Ivana Evans**. Hands-on problem solving sessions illustrated these topics, but also covered powder pattern indexing and unit cell refinements; Rietveld refinements of extended, molecular and nanomaterials and combined use of X-ray and neutron diffraction data. Examples of structure solution of different types of systems were also provided. During the final morning, students were set the challenge of spotting the mistakes in eight different "badly recorded" data sets. First prize and a bottle of bubbly went to **Lee Gerrard** and **Shirley Fong**. With sixty students working on around fifty different problems using four different main software packages, the smooth running of the tutorial sessions was only possible thanks to the hard work of expert tutors: **Sarah Lister**, **Will Bisson**, **Lars Peters** and **Graham Stinton**. Their help is gratefully acknowledged.

We also thank those who generously supported the course: The Physical Crystallography Group of the BCA, The Structural Condensed Matter Physics Group of the Institute of Physics, The Centre for Molecular Structure and Dynamics, CCP14, AWE and Durham University Chemistry Department.

Ivana Evans

Hard at work

Industrial Group Meetings in 2007/8

CALL FOR PAPERS: **The Industrial Group have a further three meetings planned for 2007 and two in 2008 so please help us to fill the programmes by offering a talk. The autumn meeting is preceded by a pharmaceutical SIG, both at AstraZeneca, Alderley Park. Expect more on our 14th May 2008 XRF meeting and 15th May 2008 "XRD and Minerals" (both at British Geological Survey, Keyworth) in future editions and all these meetings on our web pages. To offer a talk please contact a session organiser.**

Small Angle Scattering Special Interest Group -

July 2007 ILL, Grenoble
Planning is under way for a two day Small Angle Scattering meeting at ILL Grenoble to be held early July 2007.
Organisers: Richard Morris and **Jeremy Cockcroft**
Delegate numbers will be limited.

Pharmaceutical Special Interest Group

7th November 2007, AstraZeneca, Alderley Park, Cheshire
Morning session:
General pharmaceutical applications
Organisers: Anne Kavanagh & **Roy Copley**
Afternoon session:
Structure solution from powder data, Microstructural applications and Rietveld quantification
Organisers: Anne Kavanagh & **Roy Copley**

Autumn Meeting

8th November 2007, AstraZeneca, Alderley Park, Cheshire
Morning session:
Rietveld applications.
Organisers: Steve Norval & **Jeremy Cockcroft**
Afternoon session:
Crystallography in Industry - a varied mix of short talks of interest to a wide audience
Organiser: Judith Shackleton

Local organiser:
Dr Anne Kavanagh PAR&D AstraZeneca,
Silk Road Business Park, Macclesfield, Cheshire
SK10 2NA Tel:01625 517454
Email: anne.kavanagh@astrazeneca.com

The Impact of Crystallography in an Industrial Environment

Photograph of Speakers. Insets: Ivan Parkin (left), Andrew Hodge (right). From Left to Right: Graham Smith, Chris Staddon, Richard Morris, Mark Farnworth, Gordon Barr, Peter Stacy and Ian Ferguson.

The meeting, held on November 9 at the Pilkington European Technical Centre, began with an introduction by Jeremy Cockcroft, the Industrial Group Chair, who thanked Pilkington for hosting the meeting and providing lunch. He commented that it was good to see the meeting return to the site of an industrial company. The sessions started with an introduction to Pilkington by Mary Ormsby, a senior manager on site. Fairly recently, Pilkington was taken over by the Japanese glass company NSG - half its size - and the two organisations are slowly merging. Whereas Pilkington had in recent years majored on building and automotive products, NSG has a lot of hi-tech applications. The next few months will be an interesting time as the cultures merge.

The first scientific talk of the day was by **Gordon Barr** (U. of Glasgow), who spoke about high throughput screening with XRPD and Raman. In both cases, full profile patterns are compared, using both parametric and nonparametric statistics. Correlation coefficients are calculated from which a distance matrix is set up. Finally various techniques for cluster analysis are applied. The result is a robust and rapid method of grouping data on large groups of samples.

The next speaker was an old friend, **Ian Ferguson**, who described the characterisation of SiC coatings on nuclear reactor fuel pellets. This amounted to an interesting reminder of the value of relatively simple approaches to strain analysis. Some of this work went back a long way - how many of us remember computer data entry on 5-hole punch tape? - but it is still relevant.

The last speaker in the morning session was **Ivan Parkin** (UCL) who talked about XRPD mapping of CVD coatings on glass. WO_3 coatings are always the same polymorph, but crystallite morphology and orientation vary with the reagent used to hydrolyse WCl_6. The surfaces can be highly hydrophilic: on the other hand, if the coating is of WSe_2, then the surface will be very hydrophobic. This comparison led on to a discussion of different models for the hydrophilic/hydrophobic nature of surfaces, and a comparison with various TiO_2 - based films.

During the lunch break, we enjoyed a tour of the exhibition area - so interesting did we find it that two of the three parties were late back, and the afternoon session got under way a little behind schedule. **Mark Farnworth** (Pilkington) led with a description of how XRPD and X-ray reflectivity can be used in the glass industry. Estimation

of the proportion of amorphous material is important but because it is always compositionally similar, a simple method can be used. Silver in coatings on glass shows marked preferred orientation, which can be seen by XRD at different angles of incidence.

Andrew Hodge (BP) spoke next, describing some of the varied work he carries out on a wide range of samples associated with chemicals, oils and their applications. He compared the use of XRD in its 80's heyday of seven instruments and 9 staff to today's two instruments and one staff. Recent modernisation and migration to new instruments includes an old high temperature 30 bar pressure + temperature chamber with a sophisticated reactive gas flow system used for catalyst studies.

Richard Morris (Morris Analytical X-Ray) had chosen the title "Dog Food 'n Diffraction" for an interesting talk; the various reactions of members of the audience made an amusing study in human nature. Polyphosphates find a lot of uses in meat products, but some of them have undesirable properties. Trisodium hydrogen pyrophosphate is useful but not easily prepared, and Richard had been involved with a project that found a route to a crystalline form of it. The product is analysed by XRPD, the results from which agree well with ^{31}P NMR.

Chris Staddon (U. of Nottingham) had a similarish title, "XRD 'n Chips" - silicon chips to be precise, and other semiconductors, particularly III-V's but especially Ga(As,N). This occurs in the two ZnS structures and, with doping, atoms on unexpected lattice or interstitial sites and so on, form a complex group of species. The determination of Mn, and of where in the lattice it is to be found in GaMnAs, is a complex task for which a combination of XRF and XRD has proved reasonably successful.

Graham Smith (Shell, Thornton) told us about some of the work he has done over the years on samples associated with the application of oil products. Pitting of a valve from an aero-engine was found to be associated with a deposit of Pb_2CrO_5, a high-temperature oxidation product of the valve material, whose presence indicated excessive engine temperatures. Fuel starvation in a petrol engine was found to be due to a blocked filter in the petrol tank. The blockage was shown by XRPD to contain Fe_3O_4, Cu, CuO and graphite. The first was rust, but the others derived from wear of the (totally immersed) electric fuel pump's commutator and brushgear. These and other examples made this a fascinating talk. Another old technique which had come in handy was a Debye-Scherrer camera, useful with very small samples.

The last talk was by **Peter Stacey** (HSL, Buxton) who also talked about his work. The main topic of his talk was the quantification of crystalline SiO_2 in air samples. The recently-reduced WEL is now 0.1 mg m^{-3}; while there are calls for lower limits, the difficulty of analysis would make them hard to enforce. At the proposed level of 0.04 mg m^{-3}, the interlaboratory uncertainty would lead to relative 95 % confidence limits around ± 50 % for 4 hours measurement. Large samples require corrections for absorption of X-rays, which would be an added complication. He concluded with further examples relating to asbestos and calcium phosphates.

All in all, it was an interesting meeting in an excellent venue, and the thirty-odd participants went home well satisfied.

David Beveridge

Chemical Crystallography Group Autumn Meeting

Speakers at the CCG Autumn Meeting: Back row: Andy Parkin, Andy Burrows, Matteo Lusi, Junhua Jia. Front row: Philip Gale, Lee Brammer, Nick Blagden , Dario Braga

THIS years autumn meeting was held at Glasgow University on 15 November, with the subject of Crystal Engineering. I was really looking forward to the event anticipating finding out new secrets to help me with my own research until such time as our esteemed editor caught my eye and 'persuaded me' to write a summary of the meeting. With a little trepidation I accepted his 'invitation' and became the willing victim. I just hope that I can do justice to what turned out be, an excellent meeting.

A healthy turnout of crystallographers from throughout the world were present at the meeting. Some, admittedly, were on other duties in the UK but nevertheless took advantage of their situation to come along and listen/contribute to the event. To start the meeting **Prof Dario Braga** of the University of Bologna took us through his investigation of solvent-free solid-solid and solid-gas reactions. He showed that by combining solids in this manner a new range of cocrystals, polymorphs and solvates could be found and used as seeds in solution based reactions.

Junhua Jia (PhD student, University of Nottingham) followed presenting her work on porous metal-organic frameworks for hydrogen storage. Much of this was based around pyridine dicarboxylic acids. These compunds are able to withstand the loss of the solvent found in the pores, enabling the addition of hydrogen to the structure. She found that trinuclear complexes had the highest percentage hydrogen storage.

Lee Brammer (Univeristy of Sheffield) took us into the world of halogen bonding. He highlighted the various networks that could be formed using halogen bonds. He showed that with the addition/removal of HCl from a system he was able to reversibly form new compounds that retained the halogen bonds.

Andy Parkin (University of Glasgow) took a slightly different view and discussed a novel method for the analysis of many crystal structures to try and quantify any similarities or differences within a set.

Philip Gale (University of Southampton) discussed the importance of anion receptors and sensors. He discussed many different types of molecules (calix-(4)-pyrroles, amidopyrroles) and their affinities for binding specific anions, even using nature's binders to help direct his research.

Matteo Lusi (PhD student, University of Bristol) continued, to show how various organometallics could be synthesised by solid state reactions, and how by subjecting the solid to varying conditions one could perform solid state interconversions of hydrogen-bonded salts.

Andy Burrows (University of Bath) is looking into coordination networks using diketonate ligands. He found that solvent quality plays a large part in the formation of these coordination networks. He investigated this by conducting the same reactions with solvents of various qualities. He started to look at dicarboxylates because of their high thermal stability and their low ability to form penetrated coordination complexes. Many different networks could be formed from similar reaction conditions, but with a variation of reaction time.

The last talk of the day was presented by **Nick Blagden** (University of Bradford) who was looking at the very heart of crystallisation and the nucleation of crystals. He studied the effect of different solvents on the crystallisation of molecular crystals by both experimental and theoretical simulations. He finished by discussing the possibility of growing crystals on crystals and the interface between the two.

Thanks go to the organisers of the meeting for what was a very successful meeting. I am sure there were many ideas generated from the day's presentations.

Iain Oswald
Edinburgh University

Biological Structures Group

Winter Meeting 2006
Structural Biology of Pathogens

THE Winter Meeting of the British Crystallographic Association, Biological Structures Group was held on Monday 18 December 2006 at the University of Birmingham. The meeting was got off the ground with a plenary lecture by David Stuart (Oxford), Virus Identity Crises - Can crystallography help? (it seems it can!) with Rolf Hilgenfeld from Lübeck describing progress in understanding and fighting SARS, and Stephen Fuller (Oxford) giving us a tour around the latest cryo-electron microscopy of HIV.

After coffee, the session focussed on Parasites and Bacteria. **Bill Hunter** (Dundee) started the session with an excellent talk about using crystallography in drug discovery in an academic context: *Picking pockets to feed drug discovery*. **Del Besra** (Birmingham) and **Kate Brown** (ICL) spoke about different targets in *Mycobacterium tuberculosis* and **Karthik Rajesekar** (Birmingham) talked about KorA, a repressor for the IncP-1 plasmid, associated with antibiotic resistance.

The afternoon focused on bacterial secretion systems with **Susan Lea** (Oxford) describing fascinating work about a type three secretion system and **Gabriel Waksman** (Birkbeck) talking about structural biology of *Pilus biogenesis* and bacterial attachment. The session concluded with talks from **Rebecca Conners** (Bristol) about cell recognition by *Moraxella* pathogens and from **Thomas Wollert** (Braunschweig) on Structure based Pathogen Design.

Sessions at BCA Spring Meeting

A strong Biological programme has been coordinated by Dr. Kate Brown and Prof. Randy Read, with Prof. Lindsay Sawyer taking overall charge of this special 25th BCA spring meeting. See the programme in this edition for full details.

AGM

THIS was held at the BSG Winter meeting. The full minutes will be published elsewhere. Elections were held for the posts of Chairman, Vice-chairman and two vacant committee member positions. The current committee comprises:

Chairman:	**Andrea Hadfield** (University of Bristol)
Vice-chairman:	**Vilmos Fulop** (University of Warwick)
Treasurer:	**Nick Keep** (Birkbeck College)
Secretary :	**Sheila Gover**
Webmaster:	**Jon Cooper** (Southampton University)
	Neera Borkakoti (Medevir UK)
	Kate Brown (Imperial College)
	Pierre Rizkallah (Daresbury Laboratory)
	Darren Thompson (University of Sussex).

Winter Meeting 2007

THE BSG winter meeting will be held at Birkbeck in 2007, and will be organised by Snezana Djordjevic and Gary Parkinson.

Andrea Hadfield

Meetings

2006 Materials Research Society Fall Meeting Boston, Massachusetts

George Washington in Boston Common

THANKS to the BCA, I was able to attend the 2006 Materials Research Society Fall Meeting in Boston. The conference was attended by over 4,500 delegates and split into 43 separate symposia.

The symposium of main interest to me was the Solid-State Chemistry of Inorganic Materials VI, which covered topics from Polar and Optical Materials to Electronic Solids to Porous and Nanostructured Materials.

The first session was Polar and Optical Materials with the plenary speaker being **Peter Davies** and his talk on *"Structure Control in Perovskites: Bi Ferroelectrics and Li Checkerboards"*. The session lasted all day but was joined with Solid State Chemistry of Ionic Conductors in the afternoon and featured excellent talks such as *"New Insights into the formation of Organically Templated Vandium Oxides"* by **Arunachalam Ramanan**.

The second session was on Porous and Nanostructured Materials. This session strongly featured the link between nanomaterials and their change in properties from bulk materials. This was typified by the talk by **Wolfgang Tremmel** on *"From Single Molecules to Nanoscopically Structured Functional Materials"*. The plenary lecture was by **Christopher Murray** of IBM on *"Routes to Multifunctional Nanocomposites"*. A talk of particular interest to me and my research was the lecture by **Stanley Whittingham** et al on *"How Molecules Turn into Solids"*. This talk highlighted the use of pressure, water content and pH on the formation of 1-D to 3-D structures and how each of these factors plays a role in synthesis.

The final session was comprised of two parts; Electronic Solids and Synthesis and Structure. The plenary lecture for the Electronic Solids was by **Zenji Hiroi** on *"The Superconductivity in the Pyrochlore Oxides"*. The session also featured a talk by **Hans-Conrad Zur Loye** on *"Materials Discovery by Crystal Growth"* which was very interesting. The final afternoon session was on Synthesis and Structure and was chaired by **David Mitzi** and featured a fascinating plenary lecture by **Tina Nenoff** on the *"Structure/Property of Water in Nanoporous Spaces: Characterisation of Zeolites"*.

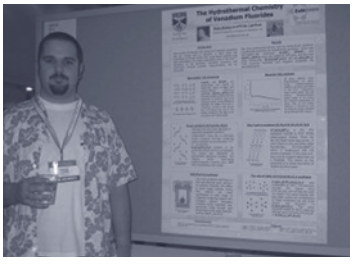
After each session in the evening there would be the poster session of all symposia, which took place in one large hall. This allowed for a real fusion of scientific ideas and allowed material researchers to see different work to which they would normally never come across. The cross-fertilisation of ideas certainly increased as the free bar became more popular! This meant some of the questions asked of the posters were certainly different to the usual ones!

The 2006 Materials Research Society Fall Meeting in Boston also marked the 30th Anniversary of the Scientific Basis for Nuclear Waste Management meeting. This included a special evening session of talks on *"Historical Perspectives and Future Trends"* which was led by the plenary lecture *"What Has Changed in Thirty Years"* given by **Rodney Ewing**.

Solid-State Chemistry of Inorganic Materials VI was only one of 43 multiple symposia that I attended. I also attended talks given in several of the other sessions including: Hydrogen Storage Technologies, Solid State Ionics, Ferroelectrics and Multiferroics and Materials Research at High Pressure which were all excellent. Throughout the conference during every lunch hour, a 1 hour symposium called Frontiers of Materials Research took place. This featured talks from the *"Developments of OLED Display Technology"* by Ching Tang to the *"The X-Files of Material Science"* by **Dierk Raabe**. The personal highlight for me was the Acta Materialia Gold Award presentation by **Subra Suresh** on *"Cell and Molecular Mechanics at the Crossroads of Nanotechnology, Life Sciences and Medicine"*. The work they had done on cell mechanics and the durability of red bloods cells with very simple techniques was really inspiring.

As this was my first international conference it allowed me to see the diversity of materials research being carried out all over the world. It allowed me to view my research from a different angle, enabling me to see how it fits into the wider field of solid state chemistry and material science.

Dave Aldous
St Andrews



The Author with his poster

CCP4 at Reading

THE annual Collaborative Computational Project in Macromolecular Crystallography (CCP4) Study Weekend returned to the University of Reading this year for a thought provoking meeting on January 5-6, 2006. The meeting, "Molecular Replacement", was highly focused on the range of current and emerging computational methods used to phase protein structures with this technique. The scientific programme was organised by Frank von Delft (Structural Genomics Consortium, University of Oxford, UK) and Garib Murshudov (University of York, UK). This popular meeting was attended by 375 delegates from both academia and industry, with representation from Europe, the United States and China.

The chairman of CCP4 Working Group 1, **Jim Naismith** (St Andrews University) opened the workshop by reminding everyone that CCP4 is a COLLABORATIVE project. He addressed a plea to all interested people to contribute with their discussions, ideas and programs. Jorge Navaza (IBS, Grenoble, France), chairing this session, remarked about the increasing importance of Molecular Replacement as a structure determination method. PDB depositions in the early 1990s had a very small fraction solved with MR. The fraction rose to 50% by the turn of the century, and is currently running at around 75% of all deposited models.

Phil Evans (MRC-LMB Cambridge) revisited the 'Basics of MR'. The requirement of a model is that it should be sufficiently similar to the unknown in conformation or fold, not just sequence. A 6D search can be performed with such a model, moving it in set steps in 3D and performing a rotation search at each point. A scoring function determines the peaks of agreement between model and observed structure factors. But this 'brute force' approach is computationally expensive, although many programs can perform such a search. More efficiently, the search can be split into two 3D searches. The first determines the best orientation that would match the model to the observation, by rotating the Patterson map in 3 angular directions. This relies on the fact that the molecular vector map represented by the Patterson function would be the same for the observed and the rotated models. A convolution of the two would give peaks where they are well matched. The second 3D search is a convolution of the observed Patterson and the Patterson of the rotated model as it is translated systematically through the asymmetric unit, subtracting the self vectors and taking into account symmetry equivalents and applying error ellipsoids. Finally, the best peak undergoes a random walk in rotation and translation space to maximise the likelihood of F_c given F_o. An apparently successful result still needs to be verified by testing the packing of the solution in the unit cell, and obtaining reasonable agreement between F_o and F_c.

Stefano Trapani (IBS, Grenoble, France) described the latest developments in the AMORE Package. Rotation searches use Patterson overlap convolutions, which are now searched with a 3D FFT, accelerating both the speed and accuracy of the results. Structural genomics exercises are heavily dependent on screening a large number of models to get a reasonable match. The new AMORE has incorporated some automatic procedures to perform this function. Also ensembles of models can be used as a search object, via super-positioning the electron density maps, implicitly down-weighting regions of flexibility. A graphical interface has been developed to allow inspection of the results interactively, enabling the positioning of small size components or extra copies in the cell given the current solution.

Eleanor Dodson (University of York) underlined the aim of the crystallography exercise as obtaining biological knowledge of the system being studied. This can be used in reverse, by using models not closely related to the experiment for structure determination with MR. The MSD Target database is a good repository for representative models, which can be used in the automatic fashion described in AMORE. Knowledge of the oligomeric state of the molecule could accelerate successful searches, particularly when there might be translational NCS in the crystal. Diffraction data at higher resolution is important for refinement, but a lower resolution data set could be sufficient for structure solution, provided the low resolution shell completeness is reasonably high, the quality of the data is adequate, and the twinning status of the data is clear. The final check for a successful MR result always relies on satisfactory electron density maps upon refinement of the resultant model. However, earlier indicators of success might come from the successful identification of heavy atom sites or anomalous scattering elements from MR solutions based phases.

The second session was entitled "Model Generation". **Geoff Barton** (University of Dundee) discussed how to use available sequence and structure data to get the best possible probe model for MR. He explained the difference between structural alignment (what we want) and sequence alignment (what we can get). He showed how powerful multiple sequence alignment can be and the value of Z-scores over simple percentage identity. He showed how to avoid being misled, and why inspection and review of models was essential. **Andrey Lebedev** (University of York) then took us through the ways the model is improved within the program MOLREP; he described how surface regions and variable regions are down-weighted, and how the choice of monomer or oligomer may influence results. He also discussed the merits of leaving out incorrect or doubtful parts of the model and the use of identified

domains separately. Of course, the inherent flexibility of the model also needs to be considered, and **Marc Delarue** (CNRS Institute Pasteur, Paris, France) showed how normal models can be used to allow for conformational changes in the experimental model, as the simple division into domains is often not straightforward. Normal mode algorithms allow the prediction of low frequency harmonic models, thus allowing the construction of more, possible search models. He went on to describe how a normal model can be used to predict boundaries for rigid body-like refinement of an MR solution.

Gerald Bricogne (Global Phasing Limited, Cambridge) started the 'Structure Validation and Model Completion' session with a humorous description of the crystallographic phase problem: if you take the amplitudes from Brigitte Bardot and combine them with the phases from John Major, then unfortunately you still will get the latter image back. Gerald described the latest developments in BUSTER including dihedral parameterisation at low-medium resolution with a few molecular replacement examples. **Serge Cohen** (NKI, Amsterdam, Holland) demonstrated with three examples the use of ARP/WARP to complete a structure from a partial model, a poor starting phase set and the help of non-crystallographic density averaging. The final speaker of the day, **Paul Adams** (Lawrence Berkeley Laboratory, USA) introduced the PHENIX package for molecular replacement, which uses PHASER for maximum likelihood molecular replacement, RESOLVE for statistical density modification and automated model (re)building, and automated structure refinement (phenix.refine). Some results were also presented.

The meeting opened the following day with **Jorge Navaza** (IBC Grenoble, France) who discussed how data from X-ray crystallography and electron microscopy (EM) can be combined in complementary ways. In one example, he showed how the crystal structure of major capsid protein VP6 of a rotavirus could be docked into an EM image, using techniques very similar to molecular replacement by treating each molecule as a rigid body - although he pointed out that normal mode methods can be also be used as necessary. Alternatively, he explained how a low resolution EM reconstruction could be used as a search initial model for phasing X-ray diffraction data using molecular replacement methods and described related work on the VP7 protein from Blue Tongue virus. The utility of his methods were illustrated with other examples including docking of molecules into negatively-stained EM images and correct assemblage of oligomeric assemblies. A complementary talk by **Yong Xiong** (Yale University, USA) then followed which provided a critical assessment of the how EM images can be used in the solution of crystal structures by molecular replacement. Using, for example, EM and X-ray diffraction data obtained yeast fatty acid synthase. he critically compared current software packages. He demonstrated how EM image manipulation and magnification errors, along with the quality and completeness of X-ray diffraction data had different effects upon the success of different packages to obtain a correct solution. It was apparent that combined expertise in understanding the quality and limitations of data arising from both methods can prove hugely advantageous in tackling challenging problems of phasing large proteins and complexes.

This session was rounded out by **Kevin Cowtan** (University of York) who showed, using attractive and informative graphics images, how small fragments of a protein structure can be fitted into electron density maps using various combinations of rotation and translation searches with programmes such as CAPRA and FFFear. He also discussed applications to classification of fragments, with reference to the problem of matching residue types to the initial chain trace in his protein model building software Buccaneer. Buccaneer has been successful at providing some traces of electron density maps even at resolutions of 3.5 Ångstroms, which may give hope to those of us struggling with poor maps where even a partial structure may accelerate our ability to improve phases and ultimately lead to a reasonable structure solution. An example of the problem of classifying side chain types is shown on our front cover, where mean (blue) and variance (red) electron density is shown averaged over threonine side chains, along with the two most common rotamers. Note that the electron density is conserved only in places where the atoms cannot be, thus these 'empty' places provide the strongest indication of a threonine.

Session 5 dealt with complicated cases and molecular replacement. **Randy Read** (CIMR, Cambridge) opened the session with a clear explanation of how the likelihood function in Phaser has been modified to deal with the case of translational non-crystallographic symmetry. tNCS leads to a break down of the default assumptions about the distribution of structure factor intensities. It is necessary to refine the non-crystallographic translation, any small rotation between copies and the non-isomorphism between copies. Doing this has made the likelihood function more accurate when there is tNCS and has allowed some test cases to be solved. The community is hoping that when this version is released many more of their backlog of unsolved structures will be solved, as happened when Phaser first came out. **Mischa Isupov** (Exeter) then gave an excellent set of examples of tricky cases where examination of the self rotation function had restricted the search to one or two dimensions (a list of candidate rotations) and had allowed difficult cases to be solved. Knowledge of the biological oligomer and aligning this with the crystallographic and non-crystallographic symmetry was superior to brute force approaches. In one case, only the dimer was known and so 3600 possible trial models in point group 52 were made by constructing physically sensible oligomers (those where the dimers touched but did not overlap excessively). **Peter Zwar**t (Lawrence Berkeley Labs) then discussed the idea of crystallographic subgroups and showed how wrong space group assignment can arise from the combinations of crystallographic and non-crystallographic symmetry interacting to suggest a false space group. He strongly recommended analysing structure factors with programs such as pointless, xtriage, xprep, sfcheck and dtcell. **Judit Debreczeni** (SGC, Oxford) then gave an excellent explanation for twinning, which, as she said, is still not dealt with as well in protein crystallography as it is in small molecule crystallography. We are promised that more of the refinement programs will handle it properly soon. At the moment SHELXL is the main program for twinned data. Only 0.3% of structures in the PDB are twinned compared to 4% at the SGC. Molecular replacement is least sensitive to twinning.

She showed an example of how a non-merohedrally twinned crystal which typically would have been thrown away as 'split' by protein crystallographers could be fully solved using data processed with EVALCCD. Finally **Adrian Lapthorn** (Glasgow) gave a light-hearted pre-lunch presentation of what actually was a serious and formidable piece of work, where there was excellent resolution, but this *P*1 structure has 192 monomers of 150 residues, arranged in 16 dodecamers within the unit cell! As they could use a dodecamer PDB 1GU1 as their search model, the classic AMoRe software could place all 16 dodecamer copies well enough to refine the ligand in the active site, which was their aim. The structure is a superlattice of type II dehydroquinase from *Streptomyces coelicolor* with both translational and rotational NCS, and is illustrated on our front cover, in glorious colour!

The final session of the meeting concerned MR pipelines. **Martyn Wynn** (CCP4, Daresbury) described MrBUMP, which, starting with structure factors and amino acid sequence, aims to deliver a positioned and partly refined model. There is emphasis on discovery and editing of a large number of search models (templates) to feed to the molecular replacement core programs, possibly more rigorously than a user might hence increasing the likelihood of success for difficult cases. JALVIEW is used for sequence editing and CHAINSAW is used in the preparation of templates. **Fei Long** (York) discussed BALBES (Baysian ALgorithm….?), which has a Python manager to minimise user intervention (two files are supplied, sequence and reflection data). The PDB is reorganised into a non-redundant set (knowledge-base) including domain and oligomeric structure to speed up similarity searching (<10 s). The PyMOL manager makes decisions on resolution, presence of pseudo-translation, etc., and search models are fed into MOLREP, REFMAC and SFCHECK with several protocols addressing possible domain models. The PDB reports that 67% of structures were solved by molecular replacement: using BALBES, 75% of the non-redundant knowledge-base can be re-solved - this suggests the PDB contains structures that could have been solved by MR, and BALBES might have been an appropriate tool to achieve this. **Lucas Jaroszewski** (Burnham Institute) discussed the MR pipeline used at the JCSG (Joint Consortium for Structural Genomics), with special emphasis on use of multiple sequence alignments. By using fold recognition algorithms (see **FFAS03** server), potentially successful trial models with low sequence homology might be recognised. Use of multiple parallel alignment and WHATIF creates a pool of models. Lucas suggested that about half of the recognisable homologues in the traditional twilight zone (less than 30% sequence identity) are solvable. The meeting concluded with a presentation by one of the organisers, **Frank von Delft** (SGC). Frank spectacularly condensed his talk so as to have the meeting finish at the scheduled time. He discussed the experiences of solving structures rapidly at the SGC with some interesting philosophical observations. The key was to be ruthless in abandoning dead ends, freeing up time for successful work. Is the initial map bad enough (*sic*) to suggest it isn't biased, and is genuine new information observed? Whereas initially the psychology of failure might encourage an individual to persist, this would not improve overall success. Thus, if a first data set is bad news (*sic*), it is thrown away and different constructs or crystal forms are pursued. Internal "structure proofreading" by colleagues enables a two-week refinement turnaround. The refiner is not plagued by the psychology of wanting to fix every problem, knowing the proofreaders (who flag, not fix) will trap problems. Validation uses COOT, MolProbity, and Frank mentioned he misses the peptide flip functionality in O and Whatcheck. This was a suitably impressive conclusion to a great session in a wonderful meeting. Finally, a meeting of this size and scope demands an excellent support team and in this regard we are truly indebted to the great work of the CCP4 organisation (Daresbury) which includes the Administrative Organiser **Maeri Howard** and her colleagues **Shirley Miller**, **Damian James** and **Nina Woodall**. Special thanks are also due to **Stuart Eyres** for all the audio and visual technical expertise including production the meeting photos (see **http://www.ccp4.ac.uk/courses/stwk07/**).

Kate Brown

2006 IUCr School on Basic Crystallography, Siena

FIRSTLY, my thanks to the BCA for awarding me a bursary towards my participation in the IUCr school on basic crystallography at the Certosa di Pontignano, Siena, Italy. It gave me an excellent chance to acquire the basic knowledge on crystallographic techniques. Prior to coming to the UK from the University of Nairobi, Kenya, I had had no training in this field.

The lectures were well organised and time was faithfully adhered to. I found the lecturers clear in their presentations and especially helpful during the tutorial sessions. The learners had the opportunity to get individual attention, which was very informative.

The programme started with a stimulating maths refresher by **Peter Main** and an introduction to diffraction. **Bob Gould** made the exercises on symmetry and Patterson and direct methods especially interesting by involving all participants in the accompanying calculations. In addition the lectures on data acquisition addressed everyday problems encountered during diffractometry experiments. For me, the sessions on structure refinement formed the climax of the school. The demonstrations by **David Watkin** were particularly enlightening.

The venue was very appropriate for such an intensive training programme. In its isolated location and serene surroundings the Certosa was a superb place to hold the event. I would recommend that the IUCr organises similar schools regularly to provide a training opportunity for non-crystallographers involved in crystallographically supported research.

Kennedy Abuga
Birkbeck College

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, gould@ed.ac.uk. The help of **Dr Simon Parsons** and the IUCr listing is gratefully acknowledged.

1 - 4 March 2007
The 5th Workshop on Structural Analysis of Aperiodic Crystals. Bayreuth, Germany.
www.crystal.uni-bayreuth.de/inc_workshop2007/index.html

5 - 9 March 2007
Annual meeting of the Deutsche Gesellschaft für Kristallographie, Bremen, Germany
www.dgk-dgkk-2007.uni-bremen.de/

21 - 22 March 2007
Polymorphism & Crystallisation 2007. London
www.iqpc.co.uk/cgi-bin/templates/singlecell.html?topic=237&event=12028

22 - 23 March 2007
Molsoft ICM Workshop: Protein Structure and Drug Discovery. La Jolla, CA, USA
www.molsoft.com/training.html

24 March - 2 April 2007
11th BCA/CCG Intensive Course in X-ray Structural Analysis, Durham
www.crystallography.co.uk/ccg/ccg.html

2 - 6 April 2007
Latin American Workshop on Applications of Powder Diffraction and Satellite Workshop - Methods of Powder Diffraction. Laboratório Nacional de Luz Síncrotron (LNLS) Campinas, SP, Brazil
http://www.lnls.br

9 - 13 April 2007
Materials Research Society Spring Meeting, San Francisco CA USA
www.mrs.org/spring2007

15 - 20 April 2007
LDSD2007: the Sixth International Conference on Low-Dimensional Structures and Devices, San Andres, Colombia
www.fis.cinvestav.mx/ldsd2007

16 - 19 April 2007
BCA Spring Meeting, University of Kent, Canterbury
www.crystallography.org/

16 - 20 April 2007
Latin American Workshop on Applications of Powder Diffraction and satellite mini-course "Methods of Powder Diffraction", Campinas, Brazil
www.lnls.br/lawpd

22 - 27 April 2007
Rapid Data Collection and Structure Solving at the NSLS: A Practical Course in Macromolecular X-Ray Diffraction Measurement. Brookhaven National Laboratory, NY, USA
www.px.nsls.bnl.gov RapiData2007/

9 - 11 May 2007
GISAXS - an advanced scattering "method", HASYLAB@DESY, Hamburg, Germany
https://indico.desy.de/conferenceDisplay.py?confId=111

16 - 18 May 2007
Seventh Canadian Powder Diffraction Workshop, Université du Québec à Trois-Rivières, Québec, Canada
www.cins.ca/cpdw/

23 - 25 May 2007
14th BENSC Users' Meeting, Hahn-Meitner-Institute, Berlin, Germany
www.hmi.de/bensc

3 - 10 June2007
Sixth European Workshop in Drug Design, Certosa di Pontignano, Siena (Italy)
ewdd@unisi.it

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

11 - 13 June 2007
2nd TOPAS Users' Meeting. Karlsruhe, Germany
www.bruker-axs.de/

11 - 17 June 2007
First school and workshop on X-ray micro and nanoprobes: instruments, methodologies and applications. Erice, Italy
www.ifn.cnr.it/XMNP2007/home.htm

15 - 29 June 2007
Nanoscaled Magnetism, ICNM-2007. Istanbul,Turkey
http://web.gyte.edu.tr/ICNM/2007

17 - 22 June 2007
16th International Conference on Dynamical Processes in Excited States of Solids. Segovia, Spain
www.dpc07.org/

24 - 29 June 2007
9th International Workshop on Physical Characterization of Pharmaceutical Solids. Natick, Boston, USA
www.assainternational.com/

25 - 29 June, 2007
The 4th European Conference on Neutron Scattering. Lund, Sweden
www.ecns2007.org/

1 - 6 July 2007
"School on Materials Applications of the Organic Solid State" (SMAOSS), Mérida, Venezuela
www.ula.ve/eventos/iccoss

8 - 13 July 2007
XVIII International Conference on the Chemistry of the Organic Solid State (XVIII-ICCOSS), Mérida, Venezuela
www.ula.ve/eventos/iccoss

9 - 13 July 2007
9th Annual Inter/Micro 2007 Conference. Chicago, IL, USA
www.mcri.org/IM_info_page.html

11 - 13 July 2007
Neutrons in Biology, ISIS, RAL
www.isis.rl.ac.uk/conferences/nib2007/

15 - 20 July 2007
International School on Mathematical and Theoretical Crystallography. The University of Havana, Cuba
www.cristalografia.net/havana2007/

21 - 26 July 2007
ACA Annual Meeting - Salt Lake City, UT, USA
www.hwi.buffalo.edu/ACA/

23 - 31 July 2007
ICNX 2007 (the International Conference on Neutron and X-Ray Scattering 2007), Indonesia
http://centrin.net.id/~nslbatan/icnx

29 July - 3 August 2007
15th International Conference on Vacuum Ultraviolet Radiation Physics, Berlin, Germany
www.bessy.de/VUVXV/front_content.php.

29 July - 8 August 2007
Small-Molecule Crystallography Summer School. San Diego, USA
http://chem-tech.ucsd.edu/Recharges/SMXF/crystalschool.html

12 - 17 August 2007
ICCG-15 / ICVGE-13 / OMVPE-13: International Conference on Crystal Growth, Salt Lake City UT USA
www.crystalgraowth.org/conferences/iccg15/index.php

13 - 17 August 2007
BSR2007 - Ninth International Conference on Biology and Synchrotron Radiation. Manchester, UK
www.srs.ac.uk/bsr2007/

20 - 22 August
ECM-23 Satellite Meeting "The enchanting beauty of Moroccan Ornaments" Marrakech, Morocco
www.lcm3b.uhpnancy.fr/mathcryst/marrakech2007.htm

22 - 27 August 2007
ECM-24, European Crystallographic Meeting, Marrakech, Morocco
www.ucam.ac.ma/fssm/ecm24>

2 - 5 September 2007
9th European Conference on Surface Crystallography and Dynamics. Vienna, Austria
www.iap.tuwien.ac.at/www/ECSCD9/

3 - 6 September 2007
Advanced Methods in X-Ray Charge Density Analysis: Extracting Properties from a Multipole Refinement. Martina Franca, Italy
http://dcssi.istm.cnr.it/XD-Workshop/home.htm

10 - 11 September 2007
Annual Meeting of the SGK/SSCr. Villigen, Switzerland
http://diffraction.web.psi.ch/sgk-sscr-2007.htm

10 - 13 September 2007
Euromat 2007: Advanced Materials and Processes. Nürnberg, Germany
http://euromat2007.fems.org

11 - 12 September 2007
User Meeting of the Swiss Light Source. Villigen, Switzerland
www.psi.ch/sls

26 - 28 September 2007
Non-ambient X-ray powder diffraction workshop, Max-Planck-Institut für Kohlenforschung Mülheim, Germany
www.mpi-muelheim.mpg.de/xray/

7 - 9 October 2007
Size-Strain - Diffraction Analysis of the Microstructure of Materials Garmisch-Partenkirchen Germany
www.mf.mpg.de/ss-v

28 October - 1 November 2007
XIVth International Workshop on Quantum Atomic and Molecular Tunneling in Solids and other Condensed Phases. Houston, TX, USA
www.iucr.ac.uk/cww-top/mtg.anc5.html

8 - 10 April 2008
BCA Spring Meeting, Swansea
www.crystallography .org

27 April - 3 May 2008
Summer School on Mathematical and Theoretical Crystallography. Gargnano, Garda Lake, Italy
www.lcm3b.uhp-nancy.fr/mathcryst/gargnano2008.htm

31 May - 5 June 2008
ACA Annual Meeting - Knoxville
www.hwi.buffalo.edu/ACA/

9 - 14 June 2008
ICQ10 - 10th International Conference on Quasicrystals, Zurich, Switzerland
http://icq10.ethz.ch/

23 - 31 August 2008
21st Congress of the International Union of Crystallography 2008. Osaka, Japan
www.congre.co.jp/iucr2008/greeting.html

25 - 30 July 2009
Annual Meeting of the American Crystallographic Association 2009. Toronto, ON, Canada
www.amercrystalassn.org/meetingspg_list/futuremeetings.html