Crystallography News

British Crystallographic Association

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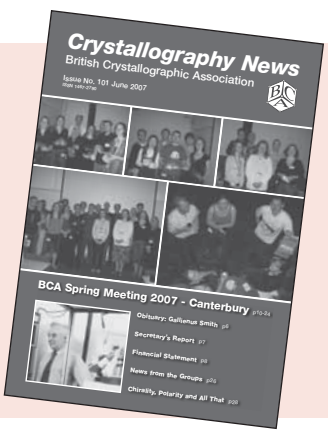
BCA Spring Meeting 2007 - Canterbury p10-24

Contents

This month's cover:

Welcome to the great group of Young Crystallographers (and their friends) who joined us at Canterbury (p.22)! Sadly, we also say farewell to a much loved BCA person in Glen Smith (p.6).



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From the President

I am writing this column on the way back from the 25th Anniversary Spring Meeting, at Canterbury. I am pleased to say that the sun shone throughout the Meeting and I think that it is fair to say that everyone enjoyed the scientific programme immensely. I would like to pass my thanks on to **Lindsay Sawyer**, the programme chair, and the whole programme committee for doing such an excellent job.

As this was the Silver Jubilee Meeting many of the sessions reflected the developments in crystallography over the last 25 years and, perhaps more importantly, looked forward to the next twenty five. The tone was very much set by the "named" lecturers. **Judith Howard**, the Hodgkin Lecturer, mapped out **Dorothy Hodgkin's** achievements and gave an insight as to how her own career had developed including her latest studies on spin crossover systems, solid state organic reactions and the development of instrumentation capable of cooling crystals to very low temperatures. She concluded by speculating on future developments and showing that the future of crystallography is very bright indeed. **Bill David**, the Lonsdale Lecturer, described some structural studies in the "hot" area of hydrogen storage materials. This is an area that will certainly be at the forefront of scientific research in the coming decades. **Sir Roger Penrose**, the Bragg Lecturer, captivated the audience with his description of Penrose surfaces and quasi-crystals that led on to a discussion of quantum entanglement.

This year, it was also a particular pleasure to welcome the XRF community who ran their meeting in parallel to the main sessions. We look forward to another joint meeting in 2009.

In addition to the programme committee there are many people who work extremely hard to make our Spring Meetings successful. This year we attracted over 370 registered delegates and particular thanks go to **Gill Moore** and **Elaine Fulton** of Northern Networking Events for their tireless effort throughout the year and at the conference. We would not be able to run the meeting without the generous contributions from the sponsors and exhibitors. This year we had a record number of over thirty who were: Analysco Ltd, Anton Paar Ltd, Bruker AXS Ltd, CCDC, CrystalMaker Software Ltd, Fluidigm, Genomic Solutions Ltd, Horiba Jobin Yvon Ltd, ICDD, Incoatec GmbH, IUCr, Korima Inc, Marresearch GmbH, Molecular Dimensions, Thermo Fisher Scientific (Nitron Analyzers Europe), Oxford Cryosystems, Oxford Diffraction, Oxford University Press, PANalytical, Pfizer Ltd, React Array, Rigaku, the RSC, Sci-Lab Analytical Ltd, Socachim-XRF Scientific, Spec AC Ltd, SpectroAnalytical, Spex Certiprep Ltd, Taylor & Francis, Thermo Fisher Scientific, Wyatt Technology and Xenocs SA.

Most of all, I would like to thank all the delegates for coming and look forward to seeing you next year in Swansea. You will be pleased to know that the programme chairs for next year, **John** and **Ivana Evans**, already have the planning well underway and details of the Meeting will appear in future issues of Crystallography News.

There have been a number of changes on the BCA Council this year. **John Finney** and **Christine Cardin** have retired as Vice President and Secretary, respectively, and I am most grateful to them for all their hard work throughout their terms of office. It is also a great pleasure to welcome onto council **Sandy Blake** and **Georgina Rosair** as the new Vice President and Secretary, respectively, **Chick Wilson** as the new Education Co-ordinator and **Jon 'Charlie' Charmant** as the new CCG Representative (replacing Georgina).

It is with great sadness that I have to report the death of **Glen Smith**, a distinguished member of the BCA. He will be sadly missed. An obituary appears later in this issue.

Finally, our thoughts turn to the Summer. The focus is the 24th ECM Meeting in Marrakech between 22-27 August and I should also flag up the Synchrotron Radiation Users Meeting at Diamond on 13-14 September where many issues relating to crystallography will be discussed. The first beamlines are operational and the day-2 beamlines will be operational during 2008, so there will be plenty of new science to plan.

Paul Raithby

BCA Council 2006-07

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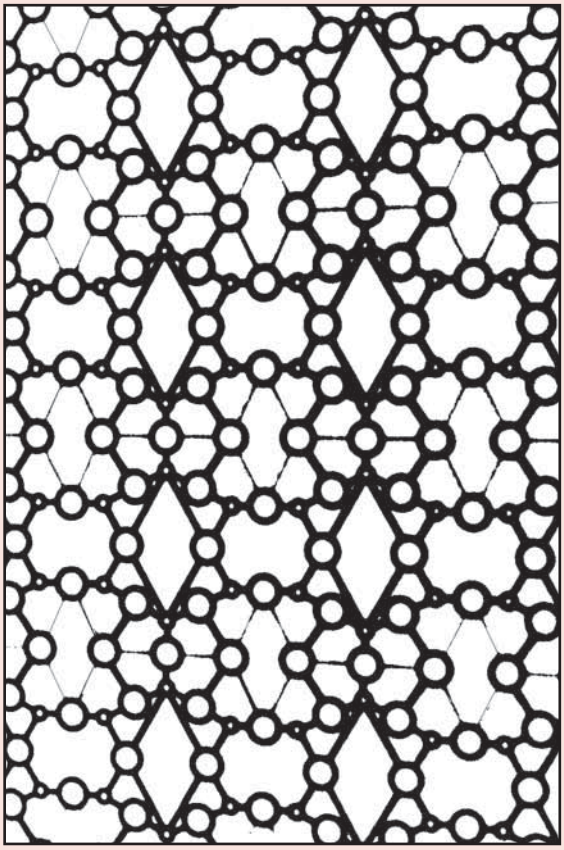
Full committee details on the BCA website **www.crystallography.org.uk**

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

Puzzle Corner

LETTER from Peter Morris of the Science Museum

This letter and the accompanying picture were received by Kate Crennell. Can anyone help? We are using it as a puzzle this time, and the prize will go to the most ingenious (in the opinion of the Editor, of course) identification, true or false!



Dear Kate,

We are trying to catalogue our Festival of Britain patterns and we are not sure what some of them are (i.e. what diffraction pattern they represent). Could you or another BCA member help with this? I would e-mail jpegs to you one by one and you could then tell me what they are. I attach a sample one (which would help to fill two gaps actually). Think it might be hydragillite, but it is different from the usual pattern

Best wishes and thanks,

Peter

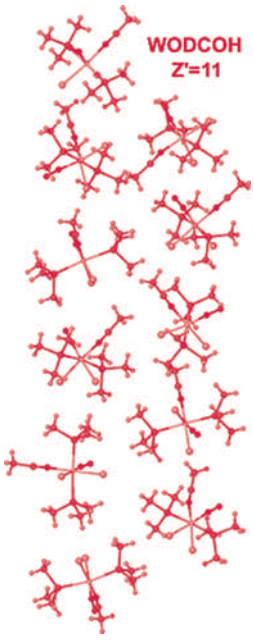
LAST month's puzzle was answered correctly by several people. This time, I really must give the prize to Tim Weakley, who again answered before my CN had arrived! It was, of course, the sentiments expressed by our first President, and on page 22 of the March issue:

"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."

A Letter to the Editor From Kirsty Anderson

DEAR BOB,

Il just wanted to say a very big thank you for publishing our article on Z' > 1 in the latest BCA news, I was particularly pleased with the high visibility the article received (with a mention on the cover as well as in the editorial!). In the 10 days or so since the newsletter was sent out we have seen an increase in the number of visitors to the site and have also received several interesting emails and offers of unpublished high Z' structures as a direct result of the article - thus achieving our objective of raising awareness of the Z' phenomenon as we had hoped would be the case.



Many thanks again,

Best wishes,

Kirsty

From the Editor

THE Spring Meeting in Canterbury was certainly memorable for many things. Our very capable Gill Moore of Northern Networking had to handle the usual complaints, but even she had difficulty helping someone who thought that the weather was *far* too good, and no one was taking things seriously. I certainly can't remember a warmer, sunnier, Spring Meeting, and that seemed suitable for our silver jubilee. The relatively long walks between the lectures and the exhibition were a real pleasure!

This issue is mainly devoted to the meeting, some of which, including the Motherwell Symposium, will, however, spill over into the September issue. As usual, we have had a very good return from our bursars. The "prize-winners" for coverage of the whole meeting are Gary Nichol, now of the University of Arizona, and Gareth Lloyd, whose "Canterbury Tales" appear on page 9. Special thanks also to Martin Adam of Glasgow for his excellent coverage of the entire Young Crystallographers' Meeting. Others have contributed to coverage of various individual sessions, and will, I hope, pardon my contractions and splicings!

The Secretary's Report is the last one to be submitted by Christine Cardin, who has now retired from the post. I'd like to record my thanks to her for her friendliness and support over the years I have been Editor of *Crystallography News*.

It is a particular, but sad, honour to remember Glen Smith in this issue. He was a regular attender of the BCA, always with a huge grin. There can be few people who enjoyed solving structures more than he did, and it is very fitting that his photograph shows him with his trusty CAD4.

The indomitable Howard Flack has been good as his word and supplied us with a full explanation of the background to his puzzle in Issue 99. Comments, particularly on the last sentence, would be most welcome!

One thing that has certainly been growing in recent years has been the number of meetings that we record on our *Meetings of Interest* list. Even so, I am aware that this is by no means complete. I make use of the list which Simon Parsons edits on the IUCr website, and I do receive some which are not listed there. I shall shortly be taking over that listing, and would appreciate anyone who is organising a meeting which is even marginally of interest to crystallographers getting in touch about it. The E-mail for the IUCr listing is: news.online@iucr.org

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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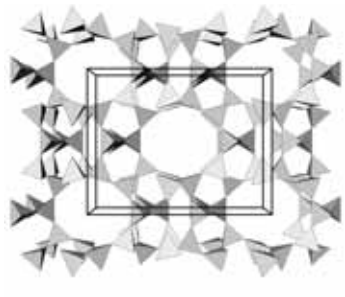
Thermo Fisher Scientific

Gallienus (Glen) W Smith 1924 - 2007

GALLIENUS SMITH better known to family, friends and colleagues as Glen, was born in 1924 in Battersea. Early recognition of his mathematical abilities led to Glen winning a scholarship to a local public school, Emmanuel School in Wandsworth, from where he matriculated in 1940. After two years working as a clerk Glen was called up and served in the Navy. He spent his early war years on aircraft carriers in the North Sea, Mediterranean and Pacific working in meteorology, using the limited number of weather reports to draw maps of isobars. After surviving a torpedo hit, he was transferred to Greenwich for officer training. He spent the remainder of the war in the Admiralty and whilst working in the forecasting division he met Eva whom he married in 1953.

After the war Glen studied Physics at Kings College London. His first job was working for the British Coal Utilisation Research Association where he published his first paper in 1949 on the design of a laboratory de-airing extrusion apparatus. Shortly after this paper was published he changed jobs moving to BICC and at once found his métier, X-ray diffraction, working on its application to metallurgical problems in wires. After work he cycled from White City to Birkbeck College to study for his MSc in Crystallography and then cycled from central London to his home in Stoneleigh, Surrey.

The majority of his career was spent at the BP Research Centre at Sunbury on Thames. He found the routine phase identification of catalysts, corrosion products and the analytical work in support of the business units not to his taste and his passion was in crystal structure determination. In the 60s and 70s there was much interest in the biological origin and formation of petroleum. New compounds were separated and identified by chromatography, mass spectrometry and NMR but for a full structure determination it was necessary to carry out single crystal X-ray investigations. Data for the first triterpanes to be extracted from crude oil were obtained photographically and the structures solved by painstaking Patterson and trial and error methods and at the weekends he used the only computer available in BP. Glen attended the early conferences on direct methods which he subsequently used to solve other triterpane structures. Later he obtained diffractometer data from a number of universities solving and refining structures in-house. Eventually BP purchased a CAD4, which became Glen's favourite toy. He was delighted at last to be able to collect his own digital data and used it to solve several structures, mostly minerals or materials related to catalysis.



As he approached retirement, he succeeded in solving the structure of the novel zeolite, Theta-1, from laboratory powder diffraction data, a major tour-de-force for the early 1980s, and arguably one of his most notable achievements. An approximate unit cell and 3 possible space groups were obtained from an analysis of electron diffraction patterns. Intensities were extracted manually from the powder diffraction pattern and as the c axis was only 5Å he decided to solve the crystal structure in projection. Fixing the sign of *110* the next strongest 6 *hk0*s were syste matically varied and used to compute 2^6 Fourier projections. The two most promising maps were used as a starting point for another 2^4 Fourier calculations. As Glen drew the contours by hand, slowly a plausible framework emerged and the structure was refined using all the data available (~200 reflections). The first choice of $Cmc2_1$ was later confirmed when attempted solutions in the other possible space groups failed. Later work at the SRS at Daresbury on submicron crystals and Rietveld refinement of neutron data collected at ISIS were in agreement with the original work. This zeolite, with its channel structure, has use as a catalyst and for hydrocarbon separation. It was the subject of patent disputes between BP, ICI and Mobil. BP won in Europe and drew in the US.

Glen was a member of the IoP X-ray Analysis Group, becoming a founder member of the BCA and serving as the first vice-chairman of the Industrial Group.

After retirement from BP, Glen worked for several days a week with Dave Povey in the Department of Chemistry at University of Surrey, delighting to tackle the structures that others had failed, or were too busy, to solve. Thus many students benefited from his past experiences and anecdotes. The bulk of his publications are from his 'retirement time' working in academia. Apart from crystallography, Glen's interests fell into 3 categories: sport, culture and making things. As well as cycling to work & college, Glen went on several lengthy cycle tours. He swam quite seriously, continuing to swim whenever a good opportunity arose (ie in the sea). He and Eva enjoyed long distance walks staying in B&Bs and until recently they were out walking in Surrey. They were both keen on opera and ballet, Glen having a soft spot for Viennese music and still buying tickets for Covent Garden in his last few months. He was good with his hands, keeping an A30 car running for ~20 years and making many toys such as the train set in his loft. He leaves his wife Eva and son Roger.

Kevin Knight, Mary Vickers and **Roger Smith**

Main refs: Triterapane: Nature (1968) **219**,243 ; Acta Crystall. (1970) **B26**, 1746
Theta-1: Acta Crystall. (1985) **C41**, 1391

Secretary's Annual Report

COUNCIL has had another busy year, culminating in this highly successful Spring meeting, which has over 370 registered participants. We would like to thank Professor Lindsay Sawyer for agreeing to take on the role of Programme Chair and for arranging such an excellent and wide-ranging programme.

At the present AGM, we have elections for a new Vice-President and Secretary. Council has approved the creation of an Education Coordinator in recognition of the importance of the educational role of the BCA, underpinning its charitable status. Council will ask the AGM to vote for the person who will be co-opted to Council to fill this role for a three year term.

Council met twice, before this meeting and in University College (London) in September 2006. Issues which continue to concern Council include the long-term financial viability, and the membership numbers. These issues are obviously related.

Two years ago now, **Elaine Fulton** joined Northern Networking Events Ltd. as our main contact person, and you will have all had a chance to meet her during this meeting. She and our Treasurer, **Sheila Gould** have now undertaken a review of the membership database, which had become very difficult to maintain. This is an important task: We now have 743 paid-up members, which is an increase on the 704 (paid-up) members this time last year, and compared with 705 in November 2005, whereas we have been talking about a target of 1000 members for the last few years. This number breaks down as follows (last year's figures in brackets) : Corporate 101 (98), Ordinary 462 (413), Retired 44 (39), Student 83 (140), Unemployed 4 (5), Honorary 16 (13), life/Term 33(30). Membership by groups is as follows (last year's figures in brackets): the Biological Structures Group have 210 (178) members, the Chemical Crystallography Group 249(190) members, the Industrial Group 78 (126) members, and the Physical Cystallography Group 92(114) members, with 114(81) members having no stated group affiliation. It may well be that your records are out of date as regards your group affiliations in the membership database. You can check your entry with Elaine Fulton, and you are encouraged to do so.

We have recently awarded Northern Networking Events Ltd a further five-year contract to continue as our professional administrators, and we would like to thank them for their competent and cheerful handling of our rather complex requirements.

Since the last AGM, **Glen Smith**, one of our Founder Members, has sadly died. An obituary appears in this issue of Crystallography News. We have one new Honorary life Member, **Professor Mike Hursthouse**. We welcome nominations for more. Constitutionally, we are allowed to have 20 such members, and we have 16 currently. All the groups have organised meetings during the year. The Biological Structures Group organised a successful Winter Meeting in Birmingham which attracted 71 participants, and hosted a Summer School in Oxford. This year, the Winter Meeting will be held in Birkbeck College, organised by **Snezana Djordevic** and **Gary Parkinson**. The Chemical Crystallography Group held their Autumn Meeting in Glasgow on 'Crystal engineering - the secrets revealed' which attracted over 80 attendees. Their next Autumn Meeting will be at Diamond, on a synchrotron-related theme. They have just hosted the Chemical Crystallography School again in Durham. The Industrial Group held an Autumn meeting on the Impact of Crystallography in an Industrial Environment at Pilkingtons with 30 delegates, and an XRF meeting at the British Geological Survey, Keyworth in May 2006. The latter was run jointly with the RSC. The Physical Crystallography Group held an Autumn Meeting with the title 'A Snapshot of Physical Crystallography in the UK', and ran a three day Rietveld refinement workshop in January 2007.

We are very happy to see the flourishing activities of the Young Crystallographers, who now have their own separate Group within the BCA, and have again organised a very professional Young Crystallographers meeting as part of the Spring Meeting.

The new Conference website was launched in time for the current Spring Meeting, and has greatly simplified the process of registering for the Meeting and providing up to date information for participants. Credit card on-line payments have also been implemented.

Our Crystallography News editor, the immensely capable **Bob Gould**, has just completed work on his 21st issue of this extremely professional publication, whose length averages at 32 pages. This is a landmark edition, as it is the 100th issue, and it is encouraging to note that Editorship is a life-enhancing activity as all the Editors since the inception are alive and well. As we will shortly be seeking a new Editor, this is a plus point to record. Council has previously been concerned that this publication was a drain on funds, but this year it has broken even financially. We are all very appreciative of the work involved. Bob always welcomes contributions, especially those with high-quality pictures attached – and *not* buried in the text!

Finally, as always, we are a voluntary organisation and could not exist without enthusiastic new people being willing to take over the various roles within it. Every year I have thanked our retiring members of Council for their services over the last year. This year, **John Finney** is retiring as vice-president, and I am retiring as secretary. I strongly recommend younger people to become involved in the BCA Groups or with Council - you will make many new friends. You will also be able to contribute to the further development of the BCA. I wish my successor a very productive term of office; it has been a pleasure to work with you all.

Christine Cardin Secretary to Council

Financial Statement 31/12/06

The British Crystallographic Association

Summary Financial Statements for year ended 31 December 2006

Examining Accountant: R A Young, BSc. FCA
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These are consolidated accounts and include the BCA, BSG, IG, CCG and CCG School funds, expressed in pounds sterling (£)

INCOMING RESOURCES:

	2006	2005
Grants and sponsorship	425	7,548
Donations	1,905	1,986
Annual Conference(5)	90,951	74,977
Meetings of groups	3,783	2,287
Crystallography News	17,773	24,802
Membership Subscriptions	19,702	12,636
Course fees	-	10,261
Net Income from trading	13	115
Investment income	6,027	6,180
Interest received	2,341	2,877
IUCr Bursary	23,780	-
Sundry Income	-	71
TOTAL INCOME	**166,700**	**143,740**

EXPENSES:

	2006	2005
Direct Charitable expenditure(2)	119,957	129,460
Management & administration(3)	27,827	24,321
TOTAL EXPENDITURE	**147,784**	**153,781**

	2006	2005
NET INCOME:	18,916	(10,041)
Unrealised gains on investment assets	4,896	6,869
NET MOVEMENT IN FUNDS	**23,812**	**(3,172)**
Balances brought forward at 1 January	193,954	197,126
Balances carried forward at 31 December	217,766	193,954

ASSETS:

Fixed assets	**2006**	**2005**
Tangible assets	5	32
Investments	93,145	99,109
Total	93,150	99,141
Current assets		
Stock	493	520
Debtors	2,850	375
Cash at Bank	138,891	99,355
Total	142,234	100,250
LIABILITIES: amounts falling due within one year	(16,386)	(3,764)
LIABILITIES: amounts falling due after more than one year	(1,232)	(1,673)
NET ASSETS	**217,766**	**193,954**

INCOME FUNDS:

	2006	2005
Restricted funds (4)	85,413	64,393
Unrestricted funds (4)	132,353	129,561
Total	**217,766**	**193,954**

NOTES TO THE SUMMARY FINANCIAL STATEMENTS

1. ACCOUNTING POLICIES.

These summary statements are based on financial statements which have been prepared under the historical cost convention, with the exception of investments which are included at market value. The financial statements have been prepared in accordance with the Statement of Recommended Practice, "Accounting and Reporting by Charities" published in March 2005 and applicable accounting standards.

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

Tangible fixed assets are stated at cost less depreciation. Depreciation is provided at rates calculated to write off the cost of fixed assets, less their estimated residual value, over their expected useful lives.

2. DIRECT CHARITABLE EXPENDITURE

	2006	2005
Subscription to International bodies	4,032	3,363
Annual conference (5)	87,860	71,493
Meetings of groups	5,281	1,503
Crystallography News + Newsletters	18,367	24,491
Course fees and accommodation	1,615	20,000
Grants and sponsorship	1,202	1,000
Prizes	-	50
Crystallography Reviews	-	4,000
Arnold Beevers Bursary Fund	1,600	3,560
Total	**119,957**	**129,460**

3. MANAGEMENT AND ADMINISTRATION

General expenses		
Depreciation	27	335
Administration fee	22,066	16,420
Accounting fee	3,819	3,316
Insurance	378	378
Bank and security charges	134	298
Special Interest Group Administration	108	2,684
Administration		
Council Members' expenses	1,295	504
Officers	-	324
Other Council expenditure	-	62
Total	**27,827**	**24,321**

The full BCA accounts for 2006 are available as an e-mail attached file from the BCA administrative office.

The British Crystallographic Association

Summary Financial Statements for year ended 31 December 2006

4. STATEMENT OF FUNDS	Brought Forward	Incoming Resources	Resources Expended	Transfers in/(out)	Gains (Losses)	Carried Forward
UNRESTRICTED FUNDS						
General Fund	**129,561**	**135,757**	**(137,861)**	**-**	**4,896**	**132,353**
RESTRICTED FUNDS						
IUCr bursary fund	1	23,780	-	-	-	23,781
Arnold Beevers bursary fund	16,083	1,177	(1600)	738	-	16,398
Dorothy Hodgkin prize fund	7,810	728	-	-	-	8,538
Chemical group teaching school	7,545	-	(500)	-	-	7,045
Chemical group fund	6,491	661	(2,097)	-	-	5,055
Industrial group fund	6,954	3,669	(3,839)	-	-	6,784
Biological Structures group fund	19,509	928	(1,887)	(738)	-	17,812
Subtotal	**64,393**	**30,943**	**(9,923)**	**-**	**-**	**85,413**
Total of Funds	**193,954**	**166,700**	**(147,784)**	**-**	**4,896**	**217,766**

5. Spring Meeting 2006 Lancaster	
INCOME	
Sponsorship	10,178
Registration	60,741
Exhibition	18,632
Bursaries	1,400
Total	**90,951**
EXPENDITURE	
Accommodation & Meals	21,120
Facilities	4,874
Catering	15,400
Social Event	5,200
BCA Speakers Expenses	7,105
Refunds	1,998
Abstract Book	2,513
NNE Fee	15,983
Administration	5,704
Printing & Stationery	1,538
Bursaries	6,425
Total	**87,860**
TOTAL INCOME	**90,951**
TOTAL EXPENDITURE	**87,860**
MEETING SURPLUS	**3,091**

Treasurer's Report 2006

The Association had an overall surplus of £23,812 during the year ended 31 December 2006. The principal part of this surplus is the return of the bursary fund of £23,780 by the organisers of the XX IUCr Congress in Florence in 2005. This fund exists to help to fund bursaries at the triennial IUCr meetings and is restricted to that purpose. So the 2006 surplus apart from this fund is £32.

The Association has no material guarantees or commitments which could affect its future solvency. The income from our investments was down this year in line with the general movement of the Stock Exchange but it still brought in an income of £8,368 this year.

Council members have conducted a review of the major risks to which the Association is exposed. The only consideration is with regard to its major reserves, namely its investments, and to mitigate those risks the Association has all its investments placed with an independent professional management company. These investments, valued at £93,145, also provide useful but fluctuating income for sustaining the Association's objectives, which are to advance the education of the public in the sciences of crystallography, and to promote its teaching and applications in academia and industry. The Council's review of the reserves indicates that we should always be striving to generate more income to enable us to plan and encourage even higher levels of educational and scientific activity.

One of our activities in 2006 was to set up the Young Crystallographers Group within the BCA. The Young Crystallographers symposium before the Spring Meeting in Lancaster was well attended and appreciated, and sponsors were generous in their support too. In response to this symposium, we awarded 47 bursaries to the Spring Meeting, eight of which were commercially sponsored. Otherwise, we awarded bursaries totalling £1,600 from the Arnold Beevers Bursary Fund to 8 people attending meetings on a wide variety of crystallographic topics. The bursary fund for the IUCr has been offered to the organisers of the meeting in Osaka, Japan in 2008, but our offer was not taken up by the end of 2006.

There was no Crystallography School this year.

Crystallography News has almost broken even this year on a turnover of £17,773. The BCA owes a debt of gratitude to its advertisers and sponsors who generously support our activities. We are also very grateful to all who gave sponsorship to the Spring Meeting. The surplus from the Spring Meeting is a welcome addition to our income.

Subscriptions to international bodies were £4,032, covering our membership of the IUCr at the five-vote level and of the European Crystallographic Association. Administration costs, including all fees and expenses including setting up the interactive conference website, are £22,066. The contract with Northern Networking Events had run its course and we have negotiated a new five-year administration contract with Northern Networking Events to run until the end of March 2012. Their expertise and hard work is very much appreciated .

Membership income is up by £7066 with the number of Corporate Members rising from 13 to 17 during the year. From the total membership we were able to claim £846.00 Gift Aid from the Inland Revenue. These monies were allocated to the Arnold Beevers Bursary Fund, and this Fund was also boosted by a transfer of £738 bank interest income from the BSG, for which the BCA is very grateful. After the decision taken at the AGM to increase the annual subscription, Northern Networking Events have circulated everyone with the new rates and we are looking forward to the resulting increase in revenue coming through in 2007.

As ever, I rely heavily on the goodwill, patience and understanding of many people, and I would like to thank everyone, in particular Paul Raithby, members of Council, Gill and Elaine at Northern Networking Events, and our accountant Bob Young for all their help throughout the year.

Sheila Gould
Hon Treasurer

The full BCA accounts for 2006 are available as an e-mail attached file from the BCA administrative office.

BCA Spring Meeting Canterbury

Two Canterbury Tales

THE following accounts of the entire meeting were, we thought, worthy of publication in full!

Ed

1. The Jetsetter's Tale

SITTING in one of Continental Airlines' big iron birds on the tarmac of Tucson airport on a Sunday morning, watching my fellow passengers struggle with their outsized 'hand luggage' and seeing the baggage handlers load our suitcases into the hold with carefree abandon, it struck me that crystallographers make excellent travellers. Patience when dealing with disorder keeps us calm in the chaos of modern airports, experience in close-packing makes the Tetris-like arranging and re-arranging of bags in the overhead lockers (and my goodness do Americans carry a lot on board!) a breeze and, perhaps most elegantly, the sandals-and-socks combo is ideal for sailing through security checkpoints and the over-zealous X-raying of shoes.

A fortunate string of events at the end of April meant that I would be around to attend the BCA Spring Meeting, my fifth so far. The effects of jet-lag sadly took hold so that I spent most of the Young Crystallographers' Meeting quietly snoozing (not actually in the lecture theatres I must add!), although I did manage to hear **Roy Copley** discuss how crystallography is used in the pharmaceutical industry, aided by some flying index cards. On Tuesday, **Andrés Goeta** discussed exactly why it is we do routine crystallography at low temperatures (and not because someone else left the Cryostream turned on) and then discussed the facilities at Durham which are designed for ultra low-temperature experiments. The first big lecture of the main meeting, acting as a link between the YC and BCA proper, was given by **Bill David**. He discussed some of the politics and science behind the use of hydrogen as a fuel, and some of the current developments on hydrogen storage. The challenge is huge and may well be unachievable unless there are some significant, and probably painful, changes in society's attitudes to fuel and fuel consumption too since technology may well not solve this problem.

The afternoon session contained a mix of parallel sessions, and I attended the Industrial Group session on co-crystallisation, although it could easily have been sponsored by the CCG too. **Bill Jones** compared and contrasted different methods of growing co-crystals with respect to caffeine and theophylline co-crystallised with carboxylic acid compounds. He reported that co-crystals with different stoichiometries and also polymorphs can be obtained by simple variation of the method employed (solution growth vs. solid state grinding etc). Second up was **Keith Chadwick**, discussing different approaches to the co-crystallisation of benzophenone with diphenylamine. He showed how a phase diagram can be constructed to permit understanding of the crystallization conditions needed to obtain crystals of a metastable phase of benzophenone-diphenylamine. Finally **Chris Frampton** examined co-crystallisation from a pharmaceutical perspective. Co-crystallisation changes the properties of pharmaceutical compounds, making them more (or less) soluble in water, affecting stability and crystallinity etc. However, caution is also needed to ensure that the 'other' compound in the crystal is non-toxic too. Powder diffraction is often used for rapid co-crystal screening. However, Chris gave examples of powders assumed to be co-crystals which were in fact new chemical compounds, something identifiable only by single-crystal studies. All speakers touched on the various definitions of a co-crystal and it seems that it's something we all recognise when we see it, but putting that recognition into words which meet with universal approval is rather more difficult than it seems.

The evening's exhibition and poster session proved lively as usual, but the location – a ten minute walk from the lecture rooms – could have been much improved. I remember previous meetings at York and Manchester where everything took place in one building, and the lecture theatres spilled out into the exhibition. We need to return to places with such large facilities and not the smaller venues with separate buildings.

On Wednesday I heard **Bill Clegg** discuss access to synchrotron facilities via the EPSRC National Crystallography Service. Bill gave examples of work which would have been impossible to do using even very 'bright' laboratory sources (including one of my own!) and discussed some new chemistry resulting from this service. I then moved to the

Thin Films session to hear **Joachim Woitik** and **H. Roland**, respectively of PANalytical and Bruker discuss some of their new technological developments in the field of thin film analysis. Before lunch, **Sir Roger Penrose** gave the Bragg Lecture on some of the mathematical (and rather visually appealing) underlyings of quasi-crystals and even some possible relationships between Islamic tiling patterns, quasi-symmetry and quasi-crystals.

Following the CCG AGM I attended the session on Transport and Reactivity in Crystals. **Richard Jones** discussed some further advances in the use of zeolite compounds in sorption studies whilst **Paul Raithby** discussed two different aspects of photocrystallography: solid-state [2+2] cycloaddition reactions monitored by X-ray powder diffraction and also laser-induced metastable structures as determined by single-crystal diffraction using synchrotron radiation. The final speaker was **Kenneth Harris**, discussing the formation of unusual urea 'tunnel' crystal structures containing guest molecules. These tunnels collapse when the guest compound is removed and so methods for guest-exchange were discussed. Changing the guest molecules can make the 'tunnels' more stable.

Giving the 2007 Hodgkin Lecture, and following in the not inconsiderable shoes of George Sheldrick (the previous Hodgkin Lecturer), and with an eye on the BCA's 25th anniversary year, **Judith Howard** presented a timeline of sorts, discussing the career of **Dorothy Hodgkin**, some of the major crystallographic advances made during that time, and also the more contemporary changes in crystallography, giving some food for thought as to future developments in the science.

Chick Wilson was charged with delivering the lecture on 'the morning after the night before'. To a fairly large audience, he delivered an entertaining lecture giving thoughts on the causes and effects of thermal motion in crystals. Giving his CCDC CCG Prize Lecture, **Andy Parkin** also picked up on the topic of thermal motion whilst discussing hydrogen bonding in small organic compounds.

As I left Canterbury to drive to Gatwick airport, I realised that the Spring Meeting locations seem to be increasingly in extreme parts of the country. This year Canterbury, next year Swansea, one wonders if the 2009 meeting will be in the Channel Isles. Whilst it's nice to visit different parts of the country, the location of most university campuses is outside the city proper and we really don't get to see much more than lecture theatres and halls of residence. Thought should be given to holding the meetings in one of just a handful of good, central locations with plentiful transport links and satisfactory conference facilities. Sacrificing variety for reliability would be of immense benefit to the meeting.

I thank the International Centre for Diffraction Data for sponsoring a bursary to permit my attendance at this meeting.

Gary S Nichol
The University of Arizona

2. The Durham Traveller's Tale

A foreign student experiencing a new, exciting, first world conference known as the BCA Spring meeting arrives in Canterbury on a Sunday night with expectations high. The first order of business is the finding of some much needed food after a rather long trip from the dark, wet regions of the north. The incidents of the peculiar one way road system with the city centre resulted in the use of a rather shady kebab take away. Would our intrepid explorer end up regretting that decision?

The first day! With the sun blazing, shorts were worn proudly as the temperature finally seemed to creep above acceptable temperatures. Further good news from the excitable and keen young crystallographers organizing committee resulted in some stress being released through the squashing of some balls. The first talk of the day was from the ever enthusiastic **Roy Copley** who gave us insights into the world of pharmaceuticals. Unfortunately, or is that fortunately, none were supplied. The young crystallographers then followed bravely after that. Snapping quickly into line they showed excellent skills in presentation and the work presented was fascinating. One crazy soul even presented using a mac! After tea, **Andrés Goeta** showed us some hot work, or is that cold work? Once again a strong showing by the young crystallographers ensued with even a biological lecture on some protein-ase being well accepted.

The exciting evening sessions then followed after a short respite where copious amounts of caffeine were consumed. The dreaded one minute presentations of posters were a total success and full of fun. Even the cow managed to make an appearance in the form of two crazy Scotsmen. After a short nap overnight following the festivities such as the poster session which included a buffet supper on trays, the first proper morning of lectures were presented. Even

with sagging eyelids and bold statements like "Why couldn't Bragg solve the structure of ….?", the audience managed to soak up the new lectures with gay abandon. Talking about abandoning, one unfortunate incident involving the previous night's supper did occur.

It must be mentioned that the young crystallographers presented some of the best lectures ever to be given at the BCA Spring meeting, maybe even at any conference. You should all give yourselves a good pat on the back.

So that was the end of the young crystallographers' meeting. Such a pity, but we had so much more to look forward to. First and certainly not least, was the Lonsdale Lecture by **Prof. David**. His views on the design of chemical hydrogen storage materials revealed the close relationship between the crystallography and chemical synthesis of materials.

The need to learn some new techniques using crystallography led to the choice of listening to what must be the most complex and mind destroying lecture ever. **Simone Techert's** talk on time-resolved X-ray diffraction was so complex the question everyone had to ask afterwards was, did you understand that? She did show, however, that is a powerful technique to use, if you are clever enough to be able to actually understand it. Moving onto to something a little less disturbing, the co-crystal session illustrated how the phenomenon of co-crystals has had an effect on the pharmaceutical industry.

A release from the lecture hall resulted in some poster-revealing (for the second time) and exhibitors showing their items of interest. A full day of lectures loomed dark and moody for the next day, resulting in another long evening for most.

So moving on to the next named lecture, the Bragg Lecture by **Professor Sir Roger Penrose** , revealed how much you can do without Powerpoint. He showed eloquently that you do not need modern computers to explain a complex topic, just a fine hand for art work. He also gave us a glimpse into the most extra-ordinarily intricate subject of quantum theory. However, the world is very complicated and we all have lots of choices to make and that is why Schrödinger's cat was shot.

After such non-chemical ideas, it was time to move onto a subject that is more, how does one say it, easy to understand. Transport and reactivity in crystals. These three lectures were full of interesting ideas on how to move, locate and even change chemical entities within a crystal.

A short break after these lecture lead to the most anticipated talk for the day, the Hodgkin Lecture by **Professor Judith Howard**. Her aptly titled "looking back, leaping forward" talk illustrated the long history behind and the bright future still awaiting British crystallography.

The highlight of the entire BCA spring meeting has to always be the dinner, where all the "speeches" are given and prizes handed out. A few other things tend to be consumed in large quantities as well. Many happy and proud people received their much deserved prizes. The festivities continued well into the night, as of course they should. So it was impressive that **Chick Wilson** could give a rather intriguing teaching keynote lecture the next morning to a surprisingly large audience.

That is nearly the full story of the BCA Spring meeting at the University of Kent at Canterbury. The organization and professionalism of the lecturers must be commended and all were sad to leave this event and are all keenly look forward to the next one.

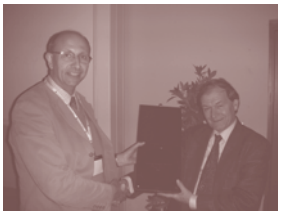
Gareth Lloyd
University of Durham

The Main Speakers at Canterbury

LONSDALE LECTURE: Combinatorial Studies of Hydrogen Storage Materials

In the Lonsdale lecture **Bill David** (ISIS) introduced his research into materials able to store hydrogen at low pressure and room temperature, which would enable hydrogen to be used safely as a fuel in motor vehicles. The background to this is, of course, the need to find a fuel source which is less polluting than that based on petrochemicals. This is essential in respect of the alarming scenarios of global climate change which have emerged and at last seem to be getting a public airing. The crystalline structure of metallic hydrides is able to absorb and store hydrogen and subsequently release it on heating. The search continues for the most appropriate material for this use.

BRAGG LECTURE: Quasi Crystals and Non-local Assembly: A Quantum-Theory Foundations Issue



Sir Roger Penrose gave the Bragg Lecture. The starting point of this fascinating talk was a description of the tilling pattern which bears his name, "Penrose tiling". This seems, at fist glance, to exhibit five fold symmetry. As crystallographers we know that this cannot be true, but these quasi-crystalline symmetries do have some amazing properties. When two examples of the densely drawn patterns were superimposed, swirling patterns and lines appeared as if by magic. The idea of carrying out this type of construction in 8 or 12 fold quasisymmetry or in 3 dimensions was quite mind blowing. If the pattern is

incorrectly built at one location, it may be impossible to complete it at some distance from the error and Penrose suggests a relationship with superposition and quantum mechanics, an intriguing subject but quite beyond my understanding. His carefully hand crafted drawings of Schrödinger's cat only succeeded in confusing me further while the illustration for the book "The Emperor's New Mind" was deceptively simple.

HODGKIN LECTURE: Looking Back, Leaping Forward

Judith Howard talked about **Dorothy Hodgkin's** life both personal and professional. She gave some of the highlights of Dorothy's career including solving the structure of insulin and of course her Nobel Prize. Judith then continued on to talk about her own work which itself began doing her PhD with Dorothy. A large amount of her research has been instrument development, particularly low temperature devices. Her current research interests involve high pressure research at low temperatures and perhaps more notable the 'Age Concern' project which is aimed at keeping computational crystallography alive. A demonstration of the new Olex2 software was given near the end of the lecture.

CCG PLENARY: Beans, Sausages and Pancakes: A recipe for understanding thermal motion in crystals

Despite the conference dinner having been the night before, **Chick Wilson's** talk was one of the most animated at the conference. The unusual title and the talk more than lived up to expectation. The term "lively" is often used to describe a lecture but rarely more appropriately than on this occasion. The food items in the title refer to the possible shape of thermal ellipsoids and the talk was about the information that can be derived from these. He demonstrated various motions by jumping around – an activity I doubt many delegates would have been willing to perform given the time of morning! He covered the basics of thermal motion in crystals and cited a few examples along the way. A great deal of thermal motion and energy were expended by the speaker and audience participation was encouraged.

BSG PLENARY: SNPs, Protein Structure and Disease

The Biological Structures Group Keynote Lecture was given by **John Moult**. He explained that many human diseases are caused by a single nucleotide polymorphism (SNP) leading to an amino acid substitution. The result of this is to destabilize the protein molecule encoded by that gene; modelling can be used to assess the effect. He proposed that it may be possible to use computational virtual docking to identify small molecules able to stabilize such mutant molecules by binding at a site other than the active site.

PCG PLENARY: Structure Prediction of Complex Materials and Nano-Particles

Richard Catlow presented his work in the field of crystal structure prediction. He began by giving an outline of the reasons, challenges and methods for crystal structure prediction. The application of such methods evidently provides elegant answers to both previously answered questions and those which are either unanswerable or at the least difficult to answer. Particularly interesting was the study on MnO_2 nanoparticles which gave insight into the formation of defects and crystallisation processes via simulated melting and recrystallisation using high and low T molecular dynamics.

Jenny Patterson, University of Keele
Fraser White, University of Edinburgh

Prizes Presented at the Dinner in Canterbury

BIOLOGICAL: **Andrea Habgood** presents the bluejohn to **Ivan Iaponogov**

CHEMICAL: **Richard Cooper** presents the Poster prize to **Andrew Bond**

THESIS: **Reg Nicoll** presents the PANalytical prize to **Lynne Thomas**

Symposia - Canterbury

Expression to Data Collection

LAURENCE PEARL (Cancer Research UK) spoke on ***Combinational Domain Hunting – A High-Throughput Approach to Identification of Soluble Protein Constructs*.** He talked about the difficulty of finding the best construct to express protein in *E coli* for subsequent structure determination by crystallization. The underlying aim of this talk was to present an automated approach to replace the current "Postdoc-soul-destroying" manual methods. The method has formatted the basis or a company called Domainex and involves encoding the entire gene and creating a fragment library containing all possible fragments. The library is then used to select the soluble genes. He described how this technique has enabled expression of soluble domains needed for crystallization but doesn't solve all the problems. The aphorism "must not make the perfect the enemy of the good" could apply to many aspects of life as well as protein expression.

The second talk, by **Gabor Bunkoczi** (Structural Genomics Consortium, Oxford), was entitled *Big-Budget High-Throughput Crystallization at the SGC*. High-throughput has required the development of an information management system for data storage and many structures have been solved from ligand bound proteins since this binding appears to stabilize the protein.

The idea of trying to replicate big-budget processes with only limited funds seemed an interesting task. The project focussed on modifying off the shelf equipment instead of investing in expensive larger equipment. The firm were able to exceed their starting remit and it was interesting to see how these methods could be applied to smaller labs.

Peter Moody (Leicester) gave an entertaining introduction to Leicester and his new lab in his talk entitled *Automation in a Small Protein Crystallography Laboratory.* He based the talk on his experience of automating his small-scale academic protein crystallography unit. Various pieces of equipment were reviewed in the context of the task-in-hand and explanations behind the various decisions that were made given. He described the decision making processes he went through in selecting equipment most appropriate to a lab the size of his; the robot for setting up plates and that for adding protein and the two imaging systems, one in the cold room so that it is not necessary to sit in there for hours hunched over a microscope. His motorbike certainly added to the attraction of the sculpture which had apparently been rejected by a large organisation and is now situated outside the new lab!

Peter Moody, Lawrence Pearl and Gabor Bunkoczi

Graham Findlay, University of Glasgow
Jenny Patterson, University of Keele

Complementary and Emerging Developments in Synchrotron Radiation

Dmitri Svergun, Liz Carpenter, Bonnie Wallace,and Pierre Rizkallah

THIS session by Dr Pierre Rizkallah (CCLRC, Daresbury). The first speaker was Professor Bonnie Wallace (Birkbeck, University of London) who talked about the use of Circular Dichroism (CD) spectroscopy as a method for identifying secondary structural features, conformational changes and

molecular interactions in proteins. This is of great use in complementing the data available from protein crystals since it can be carried out under more physiological conditions than those required for crystallization. She focused on the use of CD spectroscopy at Synchrotron Radiation facilities, and explained that laboratory sources usually run to a minimum wavelength of about 180nm, while SR facilities allowed access to wavelengths much lower than this (down to about 120nm), allowing collection of higher resolution data. Bonnie also detailed how the use of SR allows a significantly higher signal to noise ratio, collection of time-resolved data and allowed collection of data in solvents and crystallisation conditions. Of particular interest was the ability to assign secondary structure unambiguously with the use of SRCD compared with that of a lab source.

Our second speaker of the morning was **Dr Dmitri Svergun** (EMBL, Hamburg) who provided an entertaining insight into the use of small angle scattering with biomacromolecular solutions. He described how small-angle scattering can give a low resolution structure of a protein that cannot be crystallized, or can complement knowledge of a crystallographic structure. The many amusing cartoons and video clips helped those who were feeling a little swamped by information at this stage in the proceedings to concentrate a little longer. He first showed us the results from a data collection experiment conducted over 30 years ago on the T7 virus, and then showed how they are able to identify some basic structure of the virus using a 30A electron density map. EM experiments in 2005 confirmed that many of their assignments had been correct. He explained the problems of solution scattering i.e. the low resolution data obtained and its interpretation, but showed that it does provide useful information. One of his case studies was the fibrillation of insulin. Insulin forms fibrils over time by some process of aggregation. Small angle scattering allowed the identification of a third component; this third component was the precursor to the fibrils and showed how the fibrils were not formed directly from single insulin molecules.

Our final speaker of the session was **Dr Liz Carpenter** (Imperial College London) who filled in for **Professor So Iwata** who could not be present. Liz detailed the setup for the new Membrane Protein Laboratory (MPL) at the diamond facility in Oxford. She emphasised the need for concentrated effort in structure solution of membrane proteins by pointing out that while 30% of proteins and 60% of drug targets are membrane proteins, only 125 of the 45,000 structures in the PDB are membrane proteins. The aim of the lab is to develop methods of working with these proteins, train others in these methods provide facilities for visiting workers. She highlighted the difficulties of working with these proteins due to their contrasting hydrophobic and hydrophilic ends, which make them difficult to express, purify and crystallise. She explained how a high throughput system is being developed to screen pH, concentration and other variables. Their robotics systems consist of a Thermofisher Opus, 2 Rhombix machines running at 4°C and 30°C and a liquid handler which can handle 30 x 96 well crystallisation plates. Liz detailed how they also have a PX scanner to enable screening of the crystallisation plates online, using a microfocus beamline. Liz also explained the open application process for using the MPL and how they are hoping to have grant applications by October and receive their first visitors by January 2008.

Stuart Fisher, University of Manchester
Jenny Paterson, University of Keele

Post Phasing and Beyond

THIS session was chaired by Professor Randy Read (Cambridge University) who introduced the first speaker Dr Tassos Perrakis (Netherlands Cancer Institute). Tassos described a series of new tools in the ARP/wARP package for automated model building. One such tool was for the identification of side-chains from electron density maps. pyWARP was also mentioned, a control system for ARP/wARP written in modular PYTHON designed for automating decisions for partial model building and molecular replacement. A variety of test cases involving successfully built models at ever coarser diffraction resolutions was described. He also described a loop building tool that has been developed based on torsion angles using results from the protein data bank. This attempts to build disordered regions between known fragments on the main chain, using electron density only as one criterion and as such is able to suggest possible loop structures in areas of weak density.

The second speaker was **Dr Nick Furnham** (Cambridge University) who discussed the use of RAPPER, a new tool in the CCP4 project, for restraint-based conformer generation. RAPPER uses the major degrees of freedom ψ, φ, and ω, (with ω restrained to 0º or 180º) in order to explore a potential gradient, identifying local and global minima. He described how RAPPER has been tested using Lif1 and Lig4 crystals to 3.9Å and heavy atom derivatives to 4.5Å resolution giving satisfactory results. RAPPER has been specifically designed to work with low-resolution data. Nick described how it can take input ranging from information on primary and secondary structure and poor electron density maps and identify general features. RAPPER has been used to investigate dimer and tetramer regions where there are multiple conformers at the interface region. RAPPER also allows for multiple fragment searches (i.e. for pharmaceuticals) and allows for identification of residues conflicting with binding sites. Validation is conducted using RAMPAGE, another CCP4 package.

The third speaker of the session was **Dr Kim Watson** (Reading University) who gave a talk on using the GRID program on a grid computing infrastructure to assess the function and binding sites of unknown proteins. The GRID program and its current weaknesses were discussed, i.e. its execution time and its user interface. It is hoped to update the grid program by speeding up its execution time using grid computing, and to make the interface more user-friendly

Continued on page 18

Exhibitors BCA 2007 Sprin

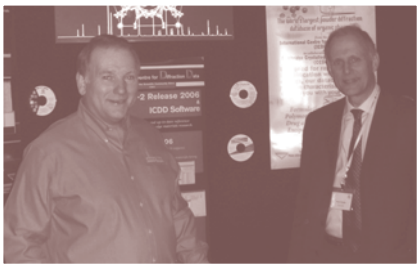
Analysco Ltd

Bruker AXS Ltd

CCDC

Crystalmaker Software Ltd

Genomic Solutions Ltd



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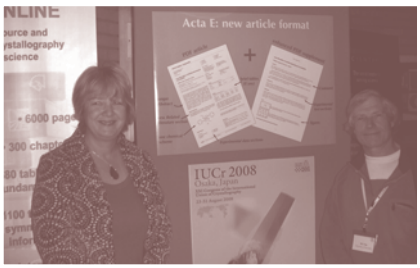
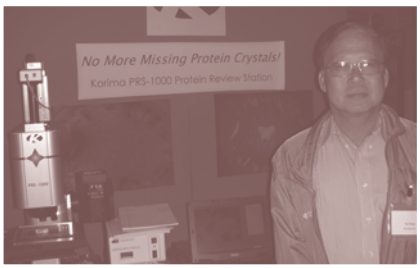
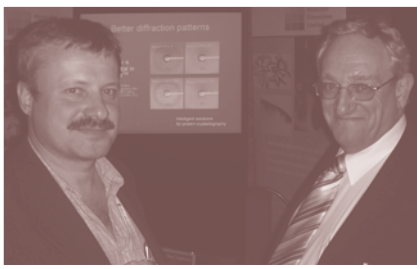


IUCr



Korima Inc

Marresearch GmbH



Molecular Dimensions

Niton Analysers Europe

Oxford University Press

Oxford Cryosystems

Oxford Diffraction

PANalytical

ng Meeting, Canterbury

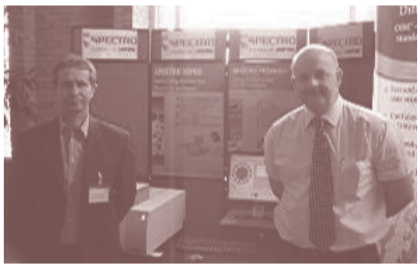
React Array

Rigaku

Royal Society of Chemistry

Socachim-XRF Scientific

Spec AC Ltd



Spectro Analytical

Spex Certiprep Ltd

ThermoFisher

Wyatt Technology

Xenocs SA

and accessible through a web interface. allowing queuing of jobs and access from offsite. How the GRID program currently works was explained, using molecular interaction fields from which binding sites can be determined. Current probes include charged metal species, water, H donors (N), H acceptors (O). The discussion after the talk explored the very positive aspects of widening of access via this web interface to a much broader community but specifically where there is then the risk of relatively inexperienced users of structural data making incorrect predictions. It was agreed that such risks would need to be managed e.g. via a 'level of confidence' alerting to users.

The final speaker of the session was **Dr Paul Emsley** (York University) who discussed some useful new tools he has been developing for the model building program COOT to enable the automatic building of helices, beta sheets and loops from electron density maps at low resolution. Paul detailed how COOT can automatically fit helices based on a cylinder which can be used as a search model. A 2-D molecular replacement style technique is used based on this search model, and then the C-beta positions are used to locate the direction of the helix. The situation for strands is more complex as strands are not standardised between proteins, taking a strand from one protein and placing into electron density of another and refining with least squares does not give a good starting model. Paul described using 'N' segments for a translational and rotational search instead.

Stuart Fisher
University of Manchester

Tassos Perrakis, Nick Furnham, Paul Emsley, Randy Read and Kim Watson

New Science from Big Facilities

TIME resolved XRD is an emerging field which is allowing the study of reaction processes via monitoring structural changes evidenced in the diffraction pattern. Simone Techert has been striving to improve the resolution of these experiments using state of the art techniques. Currently studies on femtosecond timescales have been achieved using laser pulse-probe techniques on light induced reactions e.g. isomerisation or dissociation.

At the ESRF there is a beamline set up for the study of magnetic scattering of x-rays, the XMaS beamline. **Simon Brown** came along to advertise the versatility of this UK funded beamline and the equipment available there. The beamline has many capabilities ranging from harmonic rejection mirrors, focussing mirrors, magnetic fields of up to 4 Tesla and temperatures as low as 0.95 K. This allows the ability to freeze magnetic states allowing the removal of the field.

Of the three speakers **Richard Ibberson** presented the most accessible talk. He outlined some of the recent work undertaken at HRPD, OSIRIS and GEM and also gave us insights into future possibilities available in each of the stations at ISIS as well as the planned upgrades during the shutdown. Impressively, the addition of elliptical supermirrors to the HRPD guide is expected to provide 40x increase in flux at short wavelengths and 10x overall allowing collection of usable data to 0.35 Å in *d*-spacing. This will be greatly beneficial to research where very small changes in structure result in small changes to the diffraction patterns, changes that may remain unresolved on lower resolution instruments. Current work has involved the determination of the phase diagram of cyclohexane, in-situ H_2 cycling in Mg hydride and simultaneous measurement of diffraction and physical characteristics such as mass.

Fraser White, University of Edinburgh
Sarah Lister, University of Durham

Solving Difficult Problems at Central Facilities

THE first speaker was Bill Clegg (Newcastle University), *Keeping British chemistry at the forefront with synchrotron single crystal diffraction.* The talk covered the Daresbury Laboratory Synchrotron Radiation Source (SRS) single crystal facilities, their use and method of function. The benefits of synchrotron radiation are unlikely to be a mystery to most, except those newly introduced to crystallography, but that is not to say that reminders of the specifics are not always welcomed! **Bill Clegg** did precisely that, not only reminding us why we should use a synchrotron but also why we should use Daresbury in particular. Daresbury, at the age of 25, may be about to retire, but is still a source of world class science and a lot of it too!

He began by explaining that a synchrotron works by accelerating a stream of electrons around a ring. To keep the electrons contained within the ring a series of magnets is used to continually change the direction of travel. Every time the direction of travel is changed, a burst of X-ray

radiation is emitted. The X-rays can then be used for a variety of different experiments. The X-rays emitted are of a much higher intensity than those from a standard x-ray tube. He went onto talk about how the higher intensity X-rays produced are useful in diffraction experiments with materials which are poorly crystalline. The service has successfully resolved structures for materials that cannot be solved elsewhere (e.g distorted, twisted or poorly crystalline samples). Only a small number of samples (which aren't crystalline) cannot be solved. Given the quality of the samples that make it through to the Daresbury side of the National Crystallography Service, it is quite impressive to think that data can be collected on two thirds of them. With Diamond coming online next year this situation can only get better. The success of Daresbury is attributed to its specialist beamlines rather than multipurpose multimode beamlines at other facilities allowing higher throughput. The resulting datasets from these samples can contain as many as half a million reflections. He finished by explaining that funding is secure until 2009 and that, by submitting samples to the SRS at Southampton, the samples can be analysed rapidly by a professional and skilled on-site team which can either collect the data or give a full structural determination.

The second speaker was **Alistair Lennie** (Daresbury Laboratory) on *New facilities for high pressure* at the SRS. He also gave us reasons to be cheerful about Daresbury, and it would be right to assume that he wasn't talking about the food! He was in fact talking about station 9.5, a station configured primarily for high pressure powder diffraction experiments.This talk covered the development process to convert station 9.5 to a dedicated diamond anvil cell powder diffraction station. The diamond windows absorb and scatter the beam so an increase in X-ray intensity is required to ensure that rapid collection of data is still possible. A Laue monochromator was developed in house which increases both flux and bandwidth, fixing these problems and allowing high pressure powder diffraction experiments to be carried out.

Gordon Cunningham, University of Glasgow
Fraser White, University of Edinburgh

Transport and Reactivity in Crystals

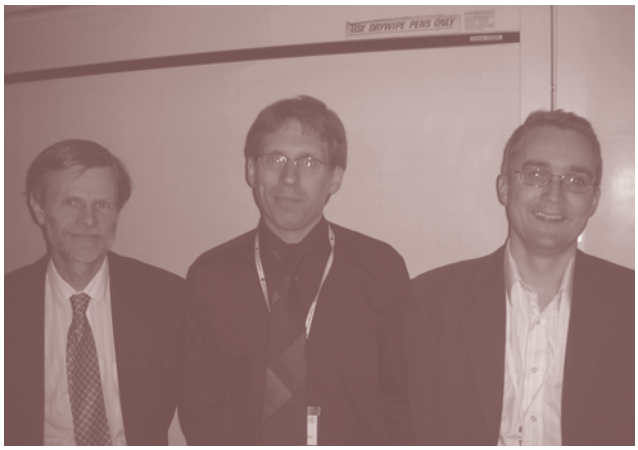
THE Wednesday afternoon session, chaired by Simon Parsons, started with a very enlightening talk by Richard Jones on *The Location of Guest Species in Microporous Materials*. This presentation started with a nice overview of zeolites for those of us who are generally baffled by the topic, explaining that they are crystalline microporous aluminosilicate materials with 3D frameworks built up from TO_4 tetrahedra. These materials contain channels and cages of molecular size, but are particularly stable to heat and radiation. This means that zeolites are useful as potential catalysts in terms of both activity and selectivity. The various types of zeolites were shown to be able to host various compounds within their channels or cages, as well as being effective for shape selectivity of molecules by only allowing certain shapes through the pores. Some of their current uses include ion exchange, catalysis, water treatment, detergent builders and molecular sieves. His studies included Xe in zeolite Rho using neutron diffraction and a lab x-ray source and Kr in chabazite.

On a similar theme to **Simone Techert** in the big facilities session, **Paul Raithby** talked about photoreactivity in crystals in a talk entitled Bright Ideas in Exciting Crystallography. Pump-probe techniques were also employed in this work involving 2+2 cycloaddition reactions in the solid state. One of these techniques involves studying crystalline excited states by using synchrotron x-ray diffraction for structural determination both with and without laser excitation. He outlined the types of systems which can potentially undergo such reactions and provided rough guidelines. He also highlighted the fact that these were only guidelines as many factors are at play and, most notably, strong hydrogen bonded networks rarely worked despite the reactive double bonds being close enough. Excited state structures can be investigated in this way by finding the difference between the ground state model and the excited crystal diffraction data, because only a percentage of the crystal is in the excited state at any time. An example of this work is in linkage isomerism in transition metal complexes, where irradiation can modify the binding of sulphur dioxide to Ru. The coordination is seen to change upon excitation from the ground state η^1-S-planar binding to a first excited state with η^2-S,*O*-side bound coordination and then to a further η^1-*O*-bent coordinated metastable state.

The final presentation in this session was by **Kenneth Harris** on *Molecular Transport in Crystalline Tunnel Systems*. This talk focussed on the structural forms of urea inclusion compounds which crystallise in the chiral, hexagonal space groups (e.g. $P6_122$). These are interesting materials with pores running through them parallel to c capable of taking up e.g. n-alkanes. His studies focus on the replacement of the guests with more energetically favourable guests in these pores, and the processes which can occur within them. It is found that these structures are unstable and will collapse under normal conditions into the structure of pure urea, but if the channels are filled with a guest molecule then the structure becomes stable. Studies have been done on these inclusion systems using incoherent quasi-elastic neutron scattering and solid state proton NMR to probe the dynamics of the guest molecules. Results show that the guest molecules could be displaced by dipping one end of the crystal into a liquid of a potentially better inclusion compound and effectively sucking up the new guest molecules like a straw without leaving the channels empty.

Fraser White University of Edinburgh
Peter Wood, University of Edinburgh

Dynamics in Crystals



Stewart Parker, Greame Day and John Evans

THE final CCG session was chaired by Chick Wilson and kicked off with a talk from John Evans (Durham) on *Framework Dynamics and Atomic Migrations in Inorganic Materials – Insight from Diffraction and NMR Studies*. John discussed a number of examples in which the movement of atoms within the crystal structure had fundamental importance in the understanding of its behaviour. The compound zirconium tungstate (ZrW_2O_5) is seen to have negative thermal expansion (NTE), which is very unusual and difficult to explain simply by looking at the basic structure. It is necessary in this case to analyse the total scattering of the material in order to learn about the dynamic effects. Study of the structural dynamics showed that the NTE is due to the oxygen atoms within the structure, which are bonded (on average) linearly between the W and Zr atoms, vibrating more in the direction perpendicular to the bonds as temperature is increased and thus pulling the W and Zr atoms closer together.

Stewart Parker (ISIS) next spoke about his research into *Vibrational Spectroscopy with Neutrons: Catalysts, Hydrides and Polyethylene*. Using neutrons for vibrational spectroscopy is a technique that is complementary to IR and Raman spectroscopy as there are no selection rules because the interaction is with nuclei rather than electrons, and it is also relatively simple to calculate the intensities. A particularly important use of this method is for materials containing hydrogen as neutrons are more sensitive to hydrogen than other probes. Examples of compounds studied are ternary metal hydrides, which are potential hydrogen storage materials, and hydrogen-adsorbed fuel cell catalysts.

The last talk of the session was then presented by **Graeme Day** (Cambridge) on *Dynamics in Molecular Crystals across the Crystal Packing Landscape*. The motivation for performing lattice dynamics calculations included the determination of the dynamic energy contribution to free energies for lattices and the ability to calculate terahertz spectra, which covers the region of lattice vibrational modes. Analysis of crystal structure prediction results has shown that the dynamic energy term is very important, with the ranking of predicted structures being completely changed in some systems. The terahertz spectra have proved to be very informative as well because these can act as a structural 'fingerprint' and can also be used to compare and contrast different polymorphs of the same compound.

Peter Wood
University of Edinburgh

Co-Crystals of Pharmaceutical Materials

THE session started with Bill Jones (University of Cambridge) giving his talk *Strategies for Designing and Making Co-crystals*. He started giving the "alphabet" and the "grammar" to understand what co-crystals are and how they are synthesized. With various examples he provided us knowledge about a broad range of different methods to obtain these materials in different stoichiometric and polymorphic formations involving just different solvents and physical states. To explain some of the interesting properties that co-crystals can have he gave us the example of caffeine that can circumvent the hydration difficulties. His main technique involved solid-state grinding for producing co-crystals, rather than putting samples into solution. This seemed too simplistic but he backed it up very well with experimental results he has produced via this method, although unfortunately for those of us who don't have a robot, this does seem an awfully energy-consuming process!

The second speaker was **Keith Chadwick** (University of Manchester), whose talk *Nucleation and Phase Relationships for a Cocrystal* focussed on a particularly "old" co-crystal: the benzophenone-diphenylamine system which is known since the "prehistory" of this kind of materials, 1933. Two different polymorphs of this co-crystal are known: the stable and metastable forms. Using thermodynamics and variable temperature microscopy Keith proposed a mechanism for the solid state reaction between the two components of the co-crystal. In the second part of his talk he presented a phase diagram for a more complicated system formed by benzophenone-diphenylamine-methanol. The diagram has also been used as guide for the preparation of crystals of co-crystal from methanol. He indicated the importance of in-situ XRPD. This is a very worthwhile technique as it enables even small changes in conditions to be noted as soon as they occur, and the formation of co-crystals can be noticed easily.

Last but not least in this session, **Chris Frampton**

(Pharmorphix) gave the industrial view on co-crystals: their benefits and also the fact that sometimes they are more hassle than they are worth. He was also the only speaker brave enough to try and put up a definition of a co-crystal, though he put up more than one to be on the safe side! He mentioned the opportunity that co-crystals can bring to pharmaceutical development in general. He could give us a broad presentation of many aspects about the creation and engineering of new co-crystals including definition, design, preparation, analysis and characterisation. From an industrial point of view the problem of the intellectual property with its regulatory issues was covered.

The session was most enjoyable and set the tone for a highly entertaining and scientifically beneficial BCA spring meeting.

Alessandro Prescimone, University of Edinburgh
Andrew O'Neill, University of Glasgow

Chris Frampton, Keith Chadwick, Bill Jones, Anne Kavanagh and Roy Copley

Computational Methods in Crystallography

Dave Allan, Carole Morrison, Mark Johnson and Dean Sayle

THIS Physical group session was chaired by **Dave Allan. Carole Morrison** started the session with ***"Finding the Elusive Hydrogen Atoms – How Computational Chemistry can help".*** The computational chemist can indeed help the crystallographer to complete/confirm crystal structures derived from poor experimental datasets. In high pressure and high temperature studies the positioning of the hydrogen atoms can be particularly difficult due to a lack of data or larger thermal motion of the hydrogens. She presented a couple of high pressure datasets of molecular crystals, which usually are neither of good quality nor complete due to experimental limitations. The experimental information she was provided with were lattice parameters and coordinates of the heavy atoms (C, N, O), but not their assignments. The procedure to complete those structures by computational methods are Monte Carlo simulations to give a set of starting geometries, subsequent geometry optimisations and energy minimisations. The lowest reasonable looking energy structures are then tested by molecular dynamic simulations to check if they behave at finite temperatures. Finally, the results are verified by computed and experimental spectroscopic data, or information originating from for example powder neutron diffraction. Examples of the use of this method were shown for nitric acid dihydrate, in which molecular dynamics calculations were also used to determine the correct structure, and a new high pressure phase of hydroxylamine, for which the x-ray data could not even discriminate between the N and O atoms.

Unfortunately **Stewart Clark**, one of the CASTEP coders, wasn't able to attend the meeting and we missed a potentially very interesting lecture. **Mark Johnson** from the ILL in Grenoble continued the session on *The Role of Total Energy Calculations in Structure Determination and Related Problems*. The uses of total energy calculations are varied and include situations where powder data has been collected, but a Rietveld refinement cannot be started due to a lack of a good model or for the purpose of supporting relatively inaccurate experimental results. There are also a number of options for the computational technique used depending on the precision of calculation required and the amount of computer time for use. Empirical force fields, for example, are often used for studying large molecules or nanoparticles whereas DFT has been seen to be very useful for detailed investigating structural investigation and even magnetic structure.

Dean Sayle concluded the session with his work on *Ceria Nanosphere Self-Assembly into Nanorods and Framework Architectures*. These were indeed true nanomaterials. In times when everything less than the 10Å mark is labelled "nano" for fashion and funding, it is nice to see the word being used in context of cerium oxide clusters comprised of tens of thousands of atoms. He melted and recrystallised these clusters and studied the effect of doping the same with titanium, all by computer simulations. The simulated morphologies of the "recrystallised" clusters were all in very good agreement with the experimental. He then took it one step further and positioned "melted" clusters in a regular periodic arrangement before letting them crystallise to form regular porous frameworks and tubes.

Marc Schmidtmann, University of Glasgow
Peter Wood, University of Edinburgh

The Young Crystallographers

THE Young Crystallographers meeting is a brilliant way to kick start the BCA. The range of research presented stretches across all facets of crystallography, and the fun, laid-back atmosphere is ideal for all to get to know each other even before the alcohol starts to flow.

It is important to not only know what is going on in crystallography in academia but also industry. **Roy Copley** from GlaxoSmithKline was able to address this in his keynote *Insight into pharmaceutical small molecule crystallography*. Powder diffraction is extensively used in industry, testing for purity and for polymorphs, and sometimes for structure determination, but the single crystal still plays an important role. Roy gave some examples of some problems that he had overcome, highlighting the extra detail that can be gained with small molecule single crystal diffraction.

Duncan Sneddon was the first student up, giving a talk entitled *Classifying molecular geometries: Application of biplots to cluster formation in dSNAP*. dSNAP can cluster structures from the CCDC in terms of their similarity, allowing you to group together molecules that you are interested in or even see how your product compares to what is already in the data-base. Duncan's talk revolved around visualising multidimensional data in a 2D plot, and then being able to pick out the variables that are important in the definition of the cluster. Biplots are one way in which this could be possible, producing easily understood and elegant pictures to represent the information.

Alexandra Ruaux BipD – *An invasion Protein associated with the type-III Secretion System of Burkholderia pseudomallei*. The interest in BipD comes from its use by bacteria to attack and enter cells, as well as its threat as a weapon used by bio-terrorists. With no bio-terrorists on site, Alexandra was able to describe the way in which BipD acts similarly to a big syringe. So far, she has determined a structure from X-ray diffraction, which to a small molecule crystallographer like myself looks like the streamers from a party popper. Beam time for an experiment at Grenoble will allow the structure to be improved.

Computers are constantly getting smaller and new ways to aid this are of great interest. **Teresa Savarese**'s talk *Photocrystallography: Turning light on crystallography* focused on single molecule electronic switches which are seen as the future of computers. A linkage isomerism shown as an example was observed when it was illuminated by a bright light. This resulted in change from yellow to red. The practicalities of doing experiments on this compound caused a few problems. The structure change can cause strain and destroy crystals, and the laser only excites 20% of the molecules at any one time, making it extremely difficult to get good data. As well as the experimental work she is making use of DFT studies.

The noise that you normally associate with methane is farting cows but according to **Helen Maynard**'s enthusiastic talk *The High Pressure Crystallography of Methane*; apparently you can also make very loud bangs! The phase diagram of methane is complex with lots of different phases, several of which occur under high pressure. In the study presented, it was phases A & B that were of interest. A very small amount of sample was loaded into a Merrill-Basset high-pressure cell that was then tightened by hand to immense pressure (she must have a strong hand shake). The small sample and the fact that it is a weak diffractor meant there were only 17 unique data points. This is also when she found out that squeezing methane can make loud bangs!

Helena Shepherd's title was *Structural studies of spin crossover in Iron(III)* coordination polymers and looked at changing from a high- to low-spin state via pressure and heat. There were several changes, not least those in the magnetic properties, as well as the strength and length of the Fe-ligand bonds. This made it of interest as a data storage medium.

A recipe for binding and catalysis by pectate lyase sounds like an excerpt from a cookbook, but **Arefeh Seyedarabi**'s talk was more about killing vegetables than cooking them. He discussed an important reaction that a bacterium uses to invade plant tissues via a secondary infection, and the requirements for this to happen including the presence of Ca and the cleavage of C-O bonds.

The coffee and tea where just around the corner (not a hike away, as at the main meeting) and gave us a nice break to absorb the information that we had been given. The lectures soon started again with **Andres Goeta** giving a keynote on *Getting Hot Results from cold Data*. This was initially an overview of what techniques you can use and the benefits you get from low or variable temperature studies, moving into the history of the devices up to the present day with several interesting examples.

David Berry's talk on *Pharmaceutical Co-crystals - Screening via hot stage melts* gave us an insight into how difficult good co-crystals can be to get when screening a lot of different samples. He first had to define a co-crystal, then showed us a 3-component phase diagram that he had produced. It seemed initially that there were only tables of negative results, but after he went on to use the hot stage Kofler technique to screen, there were many more co-

crystals being formed. This was a good example of how finding the right conditions to grow crystals can be vital.

Liana Vella-Zarb used her shiny MAC to talk about *Automated comparison of computational structures and experimental diffraction data* with lots of flashy animations and a few smurfs for good measure. Poor data is something that most of us are good at collecting, so it is always good to hear about techniques that help you process it. Structure determination from powder spectra can be hampered where the data consist of broad lines or where there are insufficient peaks. Liana first produces a theoretical structure and uses this as a starting point in processing the experimental pattern. If there are several possibilities, the similarity to the data can be determined using PolySNAP to whittle it down. With several successes so far, this technique looks promising for the future.
Markus Fries' *Crystallographic insights into the mechanism and specificity of pectin methylesterase* involved some really squiggly wiggly proteins! Pectin methyl esterase (PME) desterifies the methyl galacturonate esters in the polysaccharide pectin, thus catalyzing the invasion of plant tissues. He looked at seven complexes between pectin and PME, which give insight into the action of this novel esterase at the molecular level.

Some people just like to show off; for **Shu Yan Zhang** a tiny crystal is too small, so why not put a jet engine in the beam instead! *Engineering applications of X-ray Diffraction* was an interesting talk, showing another field in which crystallography is used (energy dispersive diffraction). Measuring the residual stress on aircraft components is important, as you don't want a crack in the engine when you're a thousand feet up. We were presented with some of the techniques that can be used at large synchrotron and neutron facilities as well as new developments in a lab-based high X-ray diffractometer for bulk residual strain evaluation (HEXameter). A nice talk to end the session but even better pictures!

The now traditional (and slightly ominous) 1-minute poster pitches were this year accompanied by quacking ducks, horns, and to finish people off a bell, not to forgetting the occasional national anthem! The poster session itself gave everyone a chance to show off their work, whether they were talking or not. After many conversations with a glass of wine, we decided that the pub was an excellent place to carry on the "scientific" talking. The evening entertainment was greatly improved by the fact that the young crystallographers had provided everyone with a foam stress ball.
From the standard of talk the day before, the expectations were high for the second day and we were not disappointed. The keynote was delivered by **Andrea Hadfield**: *Chasing lactate dehydrogenase in circles: making crystal movies.* Normally the problem with studying protein or other natural products in the solid state is that we only get to see the end result, with perhaps an intermediate, and therefore don't get to see the full cycle. Andrea described work she had done following the dehydrogenation of lactate by slowing down the reaction by a combination of cooling and pH inhibiters designed to fast capture the intermediates. The reaction has to be in-situ, so all the reactants involved need to be present. Luckily in this case, there were large solvent channels in the crystal that allowed for this. The reaction goes through lots of transition states and by freezing several of these she was able to make an animation representing the continuous loop involved. The animation showed just how much movement was required in such processes allowing greater understanding in the future.

Gemma Little's talk *A high pressure study of Gallosilicate Natrolite* examined the superhydrated zeolite structure of natrolite, using a high pressure cell on a soggy (with water) crystal. The experiments were carried out at ISIS on the powder neutron instrument PEARL with a diamond anvil cell. Rietveld refinements of the data gave the structure.

New synchrotron sources provide exciting opportunities to expand the possibilities in crystallography although stronger beams with higher flux also present new problem. **Robert Davies**' talk *Radioprotectant screening for cryocrystallography* discussed the attempts that are being made to protect protein crystals from the intense radiation that can quite literally burn a hole in your crystal. The only way to protect your crystal in the past was to cool, and although this is beneficial, further protection is also required. By adding free radical scavengers to soak up any electron radicals that are formed by the beam, further damage can be prevented. This was clearly shown in the test he performed and the next stage is to attempt it with a real crystal.

It is not common for a superhero to present a talk at the young crystallographers but this year Concrete boy (alter ego **Stephen Cairns**) came to tell us about his *Synthesis and structural studies of ettringite group of minerals*. Delayed ettringite formation in concrete is a problem in construction where it forms cracks and reduces the stability of the building. The structure of ettringite contains a high quantity of water molecules. The current structure was determined using X-ray diffraction, which is not able to locate the hydrogen positions so Stephen has been carrying out neutron experiments at both ISIS and ILL on natural samples. He is also using his powers to try and synthesise ettringite in the lab. Hopefully his work will provide useful answers to help Malaysian truckers get across falling down bridges!

Alexander Pohl asked *Why couldn't Bragg solve the structure of nickel cyanide?* and apparently it isn't because he wasn't smart enough. The fact is that he didn't have the equipment; he needed a synchrotron and then maybe a neutron source. Problem solved!
More cool animations were in store for us in **Gareth Lloyd**'s talk *Molecular Motion within Crystals*. Predicting how and when changes will happen in a crystal is a complex problem. By doing dynamic calculations on the structure, he was able to show the small amount of movement required for a solvent to move from one cavity to the next. These produced nice videos, where they distorted (danced around) to allow the molecules to move past. Looking at the thermal displacement parameters, he came up with amusing baby talk abbreviations, as well as a lot more interesting science.

The very successful meeting was drawn to a close with us (bio-terrorists, potato killers, superheroes and crystal squeezers as well as the rest) all ready to see what the BCA itself had to offer.

Martin Adam
University of Glasgow

Dinner in Canterbury

BCA FOUNDER MEMBERS AT CANTERBURY:
When the BCA was founded in 1982, opportunity was given to become a "Founding Member" for a donation of £100 and then get ten years without further subscription. Some of us hesitated a bit too long and missed the chance, but fortunately 52 people did take up the offer to give this helping start to the fledgling organisation. Five of these ware at the 25th Anniversary meeting, and looking in very good shape! Pictured here at the dinner are: **Terry Willis**, **Hilary Muirhead**, **Kate Crennell**, **Judith Howard** and **Mike Hart**.

ANDREA HADFIELD, new chairman of the Biological Structures Group thanks **Richard Pauptit** for his time in that role - or is she picking up the pieces?

YOUNG CRYSTALLOGRAPHERS
in pop-group mode

Crystal Structure Refinement: A Crystallographer's Guide to SHELXL

P. MÜLLER, R. HERBST-IRMER, A.L. SPEK, T.R. SCHNEIDER AND M.R. SAWAYA (EDITED BY P. MÜLLER).

GEORGE SHELDRICK'S programs have dominated small molecule crystallography for almost 30 years, and though I am not aware of the exact proportion of published crystal structures for which SHELXL has been used for refinement, I would be surprised if the figure were much less than 90%. The program is now being used increasingly by protein crystallographers, particularly for refinement against high-resolution data sets.

This book is intended as complement to the SHELXL manual, and while there is inevitably material which is common to both, the book gives the reader access to more introductory material (for example on restraints and rigid bodies), step-by-step worked examples, and advice on problems like hydrogen atom placement, twinning and disorder. It is an invaluable source of practical advice for new users of SHELXL: one of my students has successfully taught himself to use the program from this book, and has been able to tackle some tricky disorder problems as a result.

The first two chapters describe the structure of the SHELX suite, some basic concepts such as the difference between restraints and constraints and definitions of *R*-factors etc. Chapters 3 and 4 cover the treatment of hydrogen atoms and atom-type assignment. The examples chosen to illustrate the latter are interesting, based on samples of somewhat murky provenance, where atom-assignment is not at all obvious from the supposed chemistry. Chapter 5 describes disorder. This is the best practical account of disorder modelling that I have seen, though I would have mentioned the van der Sluis-Spek SQUEEZE procedure on the grounds of its life-enhancing quality. After a short chapter on pseudosymmetry, the subject of twinning is covered in Chapter 7, again with some first-rate examples. The final chapters cover artefacts, validation and macromolecular refinement.

It is worth emphasising that this book is about crystal structure refinement with SHELXL. It does not cover crystal structure solution or interpretation, though it does contain chapters on validation, while the chapter on artefacts highlights some possible pit-falls in interpretation of results. Neither does the book contain much material on the theory of structure refinement, and there is no discussion of non-linear least squares, normal matrices, alternative weighting strategies or derivation of standard uncertainties. It presents a thoroughly SHELX world view in which, for example, F^2 refinement is right and *F*-refinement wrong. This is just as the authors intended it, but readers who wish to learn about the theory of refinement would need to go elsewhere, for instance the books edited by Giacovazzo or Clegg in the same IUCr series.

There are a number of typographical errors and some phrasing will sound unconventional to native English speakers. Overall, though, the style of the writing is a very accessible, with a constant emphasis on practicalities. The illustrations are excellent. The drive to accessibility occasionally leads to over-simplifications; in one case for example, the phase of a structure factor is described as being hidden in the atomic coordinates.

This is a welcome addition to the IUCr series of crystallography text books; other books in the same series include Coppens' book on *X-ray Charge Densities and Chemical Bonding, Fundamentals of Crystallography* by Giacovazzo et al., and the 'Durham School Book' (*Crystal Structure Analysis: Principles and Practice*) by Clegg *et al.* This book can be recommended unreservedly to anyone who wishes to use SHELXL for refinement.

Simon Parsons
University of Edinburgh

Oxford University Press, 2006.
Price: **£49.95** (hardback)
ISBN 0-19-857067, 232 pages

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, Macclesfield. To offer a talk please contact a session organiser

2nd to 3rd July 2007
Small Angle Scattering Special Interest Group, ILL, Grenoble

See below for details:

7th November 2007
Pharmaceutical Special Interest Group, AstraZeneca, Macclesfield, Cheshire

MORNING SESSION: General pharmaceutical applications.

ORGANISERS: Anne Kavanagh & **Roy Copley**

AFTERNOON SESSION: Will include structure solution from powder data - microstructural applications and Rietveld quantification. Talks on these topics are particularly invited but more general talks are welcomed.

ORGANISERS: Anne Kavanagh & **Roy Copley**

8th November 2007
Autumn Meeting, AstraZeneca, Macclesfield, 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

Small Angle Scattering Special Interest Group

2 - 3 July 2007 ILL, Grenoble
CALL FOR PAPERS

FEES: Full £180, Concessions and Speakers £90. Please consider offering a talk at this meeting by contacting an organiser.

ORGANISERS: Richard Morris, Dave Taylor and **Jeremy Cockcroft.** The programme will start at 9am on the Monday morning with a tour of the ILL facilities and will finish for a 12:30 lunch on Tuesday to allow delegates to travel home that day. Delegate numbers are limited and the meeting fees will include Sunday and Monday nights B&B accommodation in the facility Guest House, Dinner at a restaurant on Monday, lunches on Monday and Tuesday.

REGISTRATION IS NOW OPEN: Please note that, because we are offering an all-in fee, we will only use a paper based registration process for this meeting. This will ensure that payment (to cover the venue costs) is received with the booking. The limited places will be allocated on a first come basis, any unsuccessful applications and cheques will be returned. Successful application fees cannot be refunded under any circumstances.

BURSARIES: A limited number of sponsored bursaries are available for this meeting. The bursary will cover the meeting fee but NOT travel. Bursars will be expected to give a short oral contribution on their work at the meeting. To apply for a bursary please complete a registration form and write "Bursary application" across the top of the form.

SPEAKERS INCLUDE: Peter Laity (Cambridge), **Vladimir Kogan** (PANalytical), **Andrew Harrison** (ILL), **Peter Laggner** (Hecus), **Charles Dewhurst** (ILL) and **Alberto Saiani** (Manchester).

TRAVEL: See the ILL transport page under:
www.ill.fr/pages/menu_g/howtocome.htm

DRAFT PROGRAMME:

Monday 2nd July 2007
9:00 Tour of the ILL facilities
10:30 Coffee
11:00 Contributed talks
12:30 Lunch
14:00 Contributed talks
15:30 Tea
16:00 Contributed talks
17:30 Adjourn
Evening: Dinner in town (included in the cost)

Tuesday 3rd July 2007
9:00 Contributed talks
10:30 Coffee
11:00 Contributed talks.
12:30 Closing Remarks & lunch.

More details will be posted on the website: www.crystallography.org.uk/ig as soon as they become available.

CCG News

New Committee:

Following the elections at the AGM in Canterbury, the new CCG Committee is:

Chair: **Richard Cooper**
Deputy chair: **Andrew Bond**
Secretary/Treasurer: **Alex Griffin**
YC representative: **Susanne Huth**
Student representative: **Stephen Cairns**
Representative on BCA Coouncil: **Jonathan Charmant**

Ordinary members:
Hazel Sparkes
Amber Thompson
Steve Moggach
Harriott Nowell
Ross Harrington

MORE PRIZES

In addition to the prize awarded to **Andrew Bond**, a copy of *International Tables for Crystallography Volume A: Space-group symmetry* was donated by IUCr and awarded to **Pete Wood** (Edinburgh) for poster PP02: A study of the compression of small molecule crystal structures using Hirshfeld surfaces.

The judges also gave three honourable mentions to the following posters:
CP08: **Peter Galek** - Predicting structure directing interactions from molecular properties: a knowledge based model of H-bonding propensity in organic crystals.
CP25: **Anna Collins** - Crystal structure and packing in a series of chalcone derivatives.
IP10: **Lynne Thomas** - Non-conventional scattering studies of materials using a laboratory image plate diffractometer.

CCG AUTUMN MEETING

This year's Autumn meeting will be held on Wednesday 14th November 2007 at Diamond Light Source. The meeting theme will be "Chemical Crystallography at Diamond". Confirmed speakers include **Dave Allan**, **Paul Raithby** and **Bill Clegg**. The meeting is sponsored by Bruker AXS. Details and registration will be available at http://crystallography.org.uk/ccg shortly.

Chirality, Polarity and All That

THE three crystallographic sums of the Puzzle Corner in Issue No. 99 were designed to draw attention to aspects of the symmetry of crystal structures of practical use to the structure analyst. Moreover, they reflect my interest in the determination of absolute structure and absolute configuration, and chirality and achirality in crystals. As these topics are only sparsely treated in *International Tables for Crystallography*, it is not a routine task to solve this puzzle. Moreover, the proper way to deal with question (b), although it may be done in a more ad-hoc way, and the only way to answer question (c) is by way of the Euclidean normalizers of the space groups. These are little known to structure analysts, but nevertheless contain much useful information. There is a presentation in Chapter 15 of I*nternational Tables for Crystallography Volume A*. In essence the Euclidean normalizer of a space group encapsulates the symmetry of the space group itself e.g. the symmetry of a proper pictorial representation of the symmetry elements of a space group.

Turning to the puzzle itself, the first sum in each question refers to a count of space-group types into certain classes and the second sum (in parentheses) refers to the count of the corresponding geometric crystal classes. For (c) there is no corresponding classification in terms of complete geometric crystal class so there is no subsidiary sum in parentheses.

(a) 92 + 65 + 73 = 230 (11 + 11+ 10 = 32); Here the underlying concept is that of 'absolute structure' and its determination by the study of intensity differences between Friedel opposites *hkl* and $\overline{hkl}$.

(a) Classifies the space-group types depending on whether the crystal structure is centrosymmetric or non-centrosymmetric and on whether the crystal structure is chiral or achiral. Working in this way there are three classes of structures:

CA - centrosymmetric achiral crystal structures, for which 92 space-group types are possible. All space-group types in the corresponding 11 geometric crystal classes are present. Structures in this class are invariant under inversion through a point, an operation that physicists call parity. Absolute structure is undefined (meaningless) for a CA structure.

NC - non-centrosymmetric chiral crystal structures for which 65 space-group types are possible. All space-group types in the corresponding 11 geometric crystal classes are present. For structures in this class inversion through a point generates the enantiomorphic structure which can not be brought into congruence with the initial structure by rotation and translation. Historically, as Frank Allen and Dieter Schwarzenbach informed me, these 65 space-group types were correctly determined by Sohncke some twenty years before the derivations by Fedorov and Schoenflies of the 230 space groups. Sohncke did not believe that rotoinversions (rotoreflections, isometries of the second kind) were symmetry operations, presumably because you can not apply them to a rigid body. Absolute-structure determination of an NC crystal specifies which enantiomorph is present.

NA - non-centrosymmetric achiral crystal structures for which 73 space-group types are possible corresponding to complete sets of 10 geometric crystal classes. It is confusing to many people, but true, that for structures in this class, inversion through a point generates a structure which is not identical to the initial structure (since it is non-centrosymmetric), but is also not an enantiomorph since the structure is achiral. In fact, for structures in this class, inversion through a point is always equivalent to a rotation. You can invert the structure by rotating it and the inverted structure is just a rotated version of the initial structure, i.e. a structure in a different orientation. Without a shadow of doubt, it is where dealing with the NA class of structures that authors of scientific papers and authors of crystallographic software make the most enormous bloomers. For NA crystals, absolute-structure determination defines a rotation of the specimen.

By definition there are no centrosymmetric chiral crystal structures.

(b) 68 + 162 = 230 (10 + 22 = 32); there are 68 space-group types in 10 complete geometric crystal classes where an origin for the crystal structure can not be fixed by relation to a symmetry element in either 1, 2 or 3 directions. For the other 162 space groups in 22 complete geometric crystal classes (some centrosymmetric and some non-centrosymmetric), the origin can always be fixed on a symmetry element. Of the above 68 space-group types, twenty in 5 geometric crystal classes are those of chiral crystal structures (NC) and the remaining forty-eight in 5 geometric crystal classes are those of achiral crystal structures (NA). Crystals in any of the above 68 space-group types may display first rank polar tensorial properties such as pyroelectricity, whereas it is symmetry-forbidden for crystals with any of the other 162 space-group types.

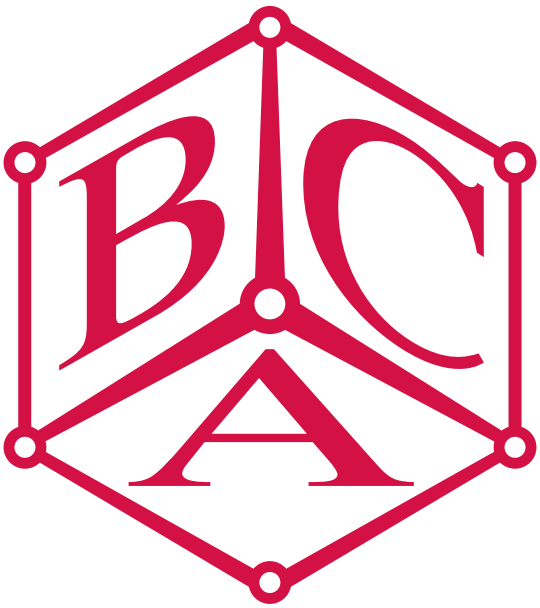
If the crystal structure is in space group *P*1, one may position the origin freely in three directions; if the geometric crystal class is *m* the origin may float parallel to the mirror plane in two directions; in the classes 2, *mm*2, 4, 4*mm*, 3,

3*m*, 6 and 6*mm*, it is along the principal symmetry axis that the position of the origin may be freely chosen. One may find this information in Tables 15.2.1.2-4 of *International Tables for Crystallography Vol. A* under the heading 'Basis vectors'. The basis vectors which are premultiplied by an epsilon (ϵ) are the directions for which the origin can not be fixed with respect to a symmetry element. In this way, one finds the number of directions and the directions themselves.

Crystal-structure refinement in any of these 68 space-group types has particular problems. Firstly, the origin has to be fixed in some way, and many modern refinement programs use an optimized method developed by Flack and Schwarzenbach (1988). Older, less satisfactory procedures fixed the appropriate coordinates of the heaviest atom. Secondly, with incorrect measurement and data handling procedures, there is a risk of incurring bias in the atomic coordinates along the directions for which the origin can not be fixed by a symmetry element. The effect, known as a 'polar dispersion error', was discovered by Ueki, Templeton and Zalkin (1966) and quantified by Cruickshank and McDonald (1967). In structure solution there is an effect known under the name of partial-polar ambiguity where one sees one part of the structure correctly and the other part as inverted through a heavy atom. I think, however, this effect is not limited to the above 68 space-group types but is general to any non-centrosymmetric space group.

(c) 207 + 2x11 + 1 = 230; The sum concerns a classification of the space-group types by the geometric crystal class of the Euclidean normalizer of the space group. One finds the symbol for the Euclidean normalizer, presented in a way related to those of space groups, under the heading 'Symbol' in the tables mentioned above. The geometric class of the Euclidean normalizer is not given directly but may be deduced in the same way that one deduces the geometric crystal class from a space-group symbol. So, for 207 space-group types, the geometric crystal class of the Euclidean normalizer is identical to that of the holohedry of the space group, i.e. the crystal class of the lattice translations, which is the criterion giving rise to the classification in terms of the 7 crystal systems. These are the normal or boring space-group types. For 22 space-group types, arranged in 11 pairs, the geometric crystal class of the Euclidean normalizer only contains rotations and no rotoinversions, the class thus being a subgroup of the holohedry. These 22 are the only truly chiral space-group types as they occur as enantiomorphic pairs. All other space-group types are achiral, as they do not occur in enantiomorphic pairs. And, last but by no means least, there is one other space-group type for which the geometric crystal class of the Euclidean normalizer is centrosymmetric but not a holohedry. This is space group No. 205 $Pa\bar{3}$. The symbol of its Euclidean normalizer is $Ia\bar{3}$, which means the normalizer is in $m\bar{3}$, an index 2 subgroup of the holohedry $m\bar{3}m$. Some of the funny behaviour of $Pa\bar{3}$ can be seen in the space group absences *0kl* : $k=2n$. Note that this condition applies for $k=2n$ and not for $l=2n$ as one might naively imagine for a cubic crystal. For fun, ask yourself the question 'Is it thus possible to distinguish between *b* and *c* in this plane?'. Another ramification occurs in twinning by merohedry. For all the other 229 space groups, non-space-group-absent reflections in one twin domain overlap non-space-group-absent reflections in another domain, and space-group-absent reflections in one twin domain overlap space-group-absent reflections in another domain. Only in space group $Pa\bar{3}$ do non-space-group-absent reflections in one twin domain overlap space-group-absent reflections in another domain. So, you can directly estimate the twin fractions by studying the space-group-absent reflections in the *0kl* planes. As a further bit of fun, ponder the question as to why what some structure analysts call 'obverse-reverse twinning' in rhombohedral crystals might have been included here and why it has not been.

Howard Flack



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.

3-10 June 2007
Sixth European Workshop in Drug Design, Certosa di Pontignano, Siena (Italy)
Information from: ewdd@unisi.it

4-8 June 2007
Fundamentals of X-ray Powder Diffraction Pennsylvania
www.icdd.com/education/xrd.htm

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

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

11-13 June 2007
New and emerging sources of intense beams of particles and short-wavelength radiation, Lund, Sweden
www.maxlab.lu.se/emergingsources/index.html

11-15 June 2007
Advanced Methods in X-ray Powder Diffraction Pennsylvania, USA
www.icdd.com/education/xrd.htm

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

13-16 June 2007
16th Croatian-Slovenian Crystallographic Meeting, Petrcane, Croatia
www.hazu.hr/kristalografi

15-17 June 2007
Canadian Light Source 10th Annual Users' Meeting Saskatoon, Saskatchewan, Canada
www.lightsource.ca/uac/meeting2007/

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/

18-22 June 2007
EMBO'07 Exploiting Anomalous Scattering in Macromolecular Structure Determination ESRF-EMBL, Grenoble, France
www.esrf.fr/events/conferences/embo2007

19-23 June 2007
Crystallization: Focus on Membrane Proteins Brookhaven National Laboratory, USA
www.nsls.bnl.gov/newsroom/events/workshops/2007/crys/

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

22-24 June 2007
Scattering on Liquid-Liquid Interfaces, Snekkersten, Denmark
http://sinq.web.psi.ch/sinq/instr/amor/ws/liquid-ws.html

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/

28-29 June 2007
Modern Drug Target Crystallography and Structure Based Drug Discovery La Jolla, CA, USA
www.ruppweb.org/workshops/Molsoft_workshop_2007.htm

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

1-6 July 2007
ICMAT 2007 - Synchrotron Radiation for Making and Measuring Materials Symposium. Suntec City, Singapore
http://mrs.org.sg/conference/icmat2007/symposia/sym-n/

1-7 July 2007
Gordon Research Conference on Electron Distribution And Chemical Bonding: Dynamics And Densities, South Hadley, MA, USA
www.grc.org/programs.aspx?year=2007&program=elecdist

2-3 July 2007
Small Angle Scattering SIG, ILL, Grenoble, France
www.crystallography.org.uk/ig/

6 July, 2007
Third Nucleic Acids Forum, Reading
www.rsc.org/NucleicAcids

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/

18-21 July 2007
Current Trends in Microcalorimetry Boston, USA
www.microcal.com/index.php?id=402

21-25 July 2007
3rd ISCB Student Council Symposium (SCS3), Vienna, Austria
www.iscb.org/submissions/index.php?id=14

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

5-11 August 2007
Zurich Crystallography School 2007 - Bring Your Own Crystals, Zurich, Switzerland
www.oci.uzh.ch/diversa/xtal_school

8-17 August 2007
The Zurich Crystallography School 2007 An intensive summer school for small-molecule crystallography. Organic Chemistry Institute, University of Zurich
www.oci.uzh.ch/diversa/xtal_school

10-12 August 2007
3rd BioXAS Study Weekend - Satellite Meeting of BSR2007. Saint Aubin, France
www.synchrotron-soleil.fr/workshops/2007/Third-BioXAS-SWE/

12-17 August 2007
9th EMU School: Nanoscopic Approaches in Earth and Planetary Sciences. Munich, Germany
www.9th-emu-school.de/

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/

18-25 August 2007
9th PSI Summer School: Correlated Electron Materials. Zuoz / Engadin, Switzerland
http://sls.web.psi.ch/view.php/science/events/Conferences/2007/Zuoz2007/Scope.html

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>

26-30 August 2007
Medical Applications of Synchrotron Radiation Saskatoon, Saskatchewan, Canada
www.lightsource.ca/masr2007/

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

2-7 September 2007
MSSC2007 - Ab initio Modelling in Solid State Chemistry. Torino, Italy
www.iucr.ac.uk/cww-top/mssc2007.pdf

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

4-14 September 2007
10th Oxford School on Neutron Scattering Oxford
www.oxfordneutronschool.org

5-7 September 2007
CCP4-sponsored protein structure workshop, Carlisle
www.chem.gla.ac.uk/protein/gala

5-8 September 2007
Structural Biology of Disease Mechanisms Murnau, Germany
www.murnauconference.de/

10 September 2007
8th Swiss Light Source Users MeetingVilligen-PSI, Switzerland
http://sls.web.psi.ch/view.php/science/events/Conferences/index.html

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

12-13 September 2007
Annual Meeting of Swiss Crystallographic Society (SGK/SSCr), Villigen, Switzerland
http://diffraction.web.psi.ch/sgk-sscr-2007.htm

13-18 September 2007
XIV International Conference on Small-Angle Scattering (SAS-2009), Oxford
www.isis.rl.ac.uk/largescale/loq/SAS2009/SAS2009.htm

16-21 September 2007
ElCryst2007 - New Instruments & Methods for Electron Crystallography. Aachen, Germany
www.elcryst2007.de/

17-21 September 2007
Symposium on New Opportunities and Challenges in Material Research using Synchrotron and Free Electron Laser Sources Warsaw, Poland
www.e-mrs.org/meetings/fall2007/I.html

24-26 September 2007
Surface Modification Technologies (SMT 21), Paris, France
www.c2s-organisation.com/smt21=20

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

7-13 October 2007
Hercules Specialised Course (HSC5) on Synchrotron Radiation and Neutrons for Cultural Heritage Studies, ESRF, Grenoble, France
www.esrf.fr/NewsAndEvents/Conferences/HSC/HSC5/

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

29-31 October 2007
Short course on amphiboles Rome, Italy
www_crystal.unipv.it/amphiboles/home.htm

7 November 2007
Pharmaceutical SIG, BCA IG, AstraZeneca, Alderley Park, Cheshire
www.crystallography.org.uk/ig/

8 November 2007
Autumn Meeting, BCA IG AstraZeneca, Alderley Park, Cheshire
www.crystallography.org.uk/ig/

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

21-23 May 2008
Surfaces and Interfaces in Soft Matter and Biology: the impact and future of neutron reflectivity, ILL, Grenoble, France
www.ill.fr/Events/rktsymposium/

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

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

7-11 July 2008
10th EMU School High-resolution electron microscopy of minerals. Nancy, France
www.lcm3b.uhp-nancy.fr/emu10/

21-26 July 2008
XRM2008 9th International Conference on X-ray Microscopy. ETH Zurich, Switzerland
http://xrm2008.web.psi.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