

# Crystallography News

British Crystallographic Association

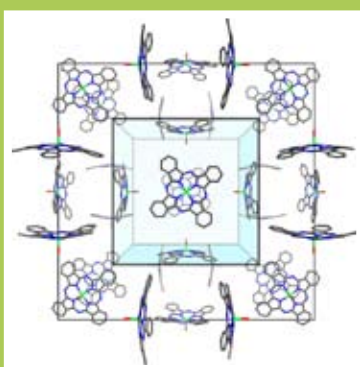


Issue No. 105 June 2008

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## BCA Spring Meeting 2008 - York p9-25



Secretary's Report p6

Protein Structure Workshop p7

Exhibitors p16

Repairing the Bank's Sub-prime Assets p28

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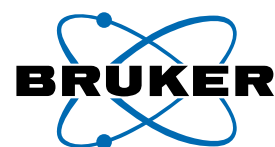
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think forward

Crystallography





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# Contents

From the President .....	2
Council Members .....	3
From the Editor .....	4
Puzzle Corner and Corporate Members .....	5
Secretary's Report .....	6
Announcing the 15th CCP4 .....	6
Protein Structure Workshop	
Financial Statement .....	7
BCA 2008 Meeting .....	9-25
Two new York accounts .....	9
Main Speakers .....	11
The Young Crystallographers .....	13
Exhibitors .....	16
Symposia .....	18
Atoms to Patterns Exhibition Opens .....	26
Repairing the Bank's Sub-prime Assets .....	28
News from the Groups .....	29
Kyoto IUCr Crystallographic Computing School .....	29
Meetings of Interest .....	30

### *This month's cover:*

Awards to Tony Crowther and the Goulds; Young Crystallographers at the dinner; an interested spectator in the centre



# From the President



**IT** is my great pleasure that I start this column by welcoming **Carl Schwalbe** as the new editor of **Crystallography News**. The **BCA Council** is most grateful to him for taking on this important role within the organisation and we wish him every success.

Let me again express the thanks of the BCA to the outgoing editor, **Bob Gould**, for his sterling work over the last 6 years. His efforts have been very much appreciated and we wish him a relaxing retirement.

I have just returned from the very successful Spring Meeting at York where there was an outstanding scientific programme covering all aspects of crystallography from powder diffraction on Mars to elucidating the structures of viruses! The four plenary speakers set a very high standard and this was followed by all the other contributors. **John** and **Ivana Evans**, and the programme committee, are to be thanked for their outstanding contribution to the whole meeting. With due respect to previous organisers of Spring Meetings, I do not think that there has ever been such a carefully planned and well organised Meeting and John and Ivana must take the credit for this.

As in previous visits of the BCA Spring Meeting to York the venue and the facilities were excellent and the catering was of a particularly high standard. The support of the University of York Conference Office is gratefully acknowledged. Also, as always, our thanks go Northern Networking Events for their support and for dealing with all the administration associated with the conference. Finally, our thanks go to all our sponsors and exhibitors without whose support it would not be possible to hold the Meeting in its current form.

Thinking ahead, next year's Spring Meeting will be held at

Loughborough University starting on Monday 20th April with the Young Crystallographers sessions and running until Thursday, 23rd April, 2009. **Simon Parsons** has very kindly agreed to act as the programme chair. The programme committee has already had its first meeting and the theme of "Dynamic Crystallography" has been chosen for the Meeting.

At the York Meeting **Sheila Gould** retired from her post as BCA treasurer at the end of her three-year term. We are most grateful to her for all her hard work and for keeping the BCA finances on an even keel through the turbulent world financial situation.

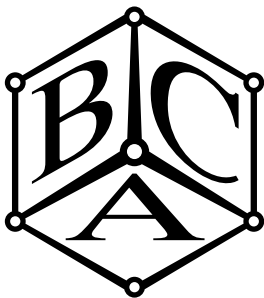
So **Bob** and **Sheila Gould** have both retired from their BCA posts after many years of supporting the BCA in an immeasurable number of ways. We thank them both most sincerely and wish them well for the future. We hope to see them at many more BCA Meetings.

Also, at York, **Chick Wilson** resigned as Education Co-ordinator because of the pressure of other commitments. Chick has been on Council for the past 11 years including a term as President. His overwhelming enthusiasm and drive will be sadly missed and we thank him for his many and varied contributions to the BCA.

I am very pleased to be able to report that Harry Powell has been elected as the new BCA treasurer. We welcome him to Council and wish him well in his new post. I am also pleased to announce that **Mike Probert** has been co-opted to Council as the new Education Coordinator and he will be working closely with me to promote educational aspects of the BCA. I am very much looking forward to working with him.

Finally, our thoughts now turn to the IUCr XXI Congress at Osaka running from 23rd to 31st August. There will be a strong BCA representation at the Meeting and I look forward to seeing many of you there.

**Paul Raithby**



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Full committee details on the BCA website [www.crystallography.org.uk](http://www.crystallography.org.uk)  
Spring Meeting Registration and Subscriptions: [www.crystallography-meetings.org.uk](http://www.crystallography-meetings.org.uk)

# From the Editor



**THIS** is my first issue as Editor in succession to **Bob Gould**. No doubt you can easily notice that the apprentice has taken over from the master! **Bob's** blend of deep knowledge of crystallography, academic wit and the ability to cajole contributions from a wide variety of crystallographers is

irreplaceable. Fortunately, many influences remain the same, starting with the aforementioned contributors, foremost among whom is our ever-eloquent President. Much administrative work is done by Northern Networking. Their calm efficiency makes them almost invisible between BCA meetings, but at the meetings we can appreciate their fine personal qualities. The identity of the printers, **William Anderson and Sons Ltd.**, is only revealed in a few modest lines on the masthead page. To begin to appreciate their role, imagine getting your local rag to print "P<sub>2,2,2,1</sub>". Now suppose that a verbose Editor writes an unusually long column, an equipment supplier wants an extra page to introduce a beautiful new piece of kit, yet a meeting timetable has to remain in the centrefold. This type of problem, worthy of inclusion in one of Bob's Puzzle Corners, is solved in every issue.

For those of you who don't know me very well, here is a bit of background. I grew up in Ohio. Unsurprisingly since Ohio is just across Lake Erie from Ontario, some people think my accent is Canadian. I did my PhD research at Harvard with "Colonel" **William Lipscomb**. Along with many colleagues, I determined the structures of boron hydrides, those unusual cages where each boron atom seems to make unreasonably many bonds. We admired the Colonel's genius as he made sense of the bonding and won the Nobel Prize in Chemistry. For my postdoctoral research I worked with **Wolfram Saenger** and **Fritz Cramer** at the Max Planck Institute for Experimental Medicine in Göttingen, Germany. There I developed my lifelong interest in pharmaceutical crystallography. In 1972 I looked for an academic position back in the U.S.A. but found little because of a round of budget-cutting. I decided to "park" in England for a few years until things got better and therefore took up a lectureship at Aston University. I have been at Aston ever since, receiving a Personal Chair in 2007 and going part-time during the current academic year. One thing that made me decide to stay here permanently is the cordial collaboration I developed with synthetic chemists at Aston, most notably

**Malcolm Stevens**, whose anti-cancer drug temozolomide is approaching "blockbuster" status. Another important factor is the friendship and cooperation I have always received from British crystallographers, with none of the nasty competition that occurs in some other disciplines and cultures.

The cover of this issue prominently features the Young Crystallographers, now a fully fledged Group within the BCA. Their presence at the BCA meeting at York in April added sparkle and enthusiasm, and the record of this meeting in this issue is mainly based upon their personal accounts. The cover also features **Tony Crowther**, who was the BCA Prize lecturer, and **Bob** and **Sheila Gould** as they received an award to for their sterling (literally, in Sheila's case) service to the BCA. The overall theme of the meeting was "Structure, Property and Function". From a poster by **Madeleine Helliwell**, in a box on the cover is a robust phthalocyanine framework into which various metal ions can be placed to tune the catalytic properties. One of the keynote lectures, "Putting the Fun in Functional Molecules" by **Paul Attfield** "did exactly what it said on the tin" and summed up the ethos of the meeting. Many of the photographs from York in this issue were contributed by **Dave Taylor, Duncan Sneddon, Bob Gould** and **Andrea Fallas**, whose skill is much appreciated.

The emphasis on the Young Crystallographers is balanced by some Old Crystallographers in the Puzzle Corner, reflecting my interest in the history of crystallography. There is a picture contributed by **Mike Glazer**, where the task is to identify the crystallographers, and I have made a list of famous past and present crystallographers who have to be matched to their (sometimes part-time) job titles.

Finally I want to draw your attention to the photographs on pages 16-17 which I took of the exhibition stands at the BCA meeting. This is not because of any artistic merit in my photography. Indeed, I don't think I answered the following questions particularly well. "Should I zoom or pan to take in the extensive PANalytical display? At the far end of a row of stands, could I avoid leaving Oxford Cryosystems out in the cold? Could I insert the lake as a background for the Waters display?" Nevertheless, these pictures illustrate the new hardware and software which enable us to achieve exciting new things. Even if you are the theoretical kind of crystallographer who doesn't need equipment, consider that without our exhibitors' contribution the registration fee would have been painfully higher and there would have been nothing but water to drink!

**Carl Schwalbe**



# Puzzle Corner

**PART 1.** Name the crystallographers in the picture



**PART 2.** The names of 11 distinguished crystallographers are given in alphabetical order, along with the job titles (full- or part-time) for 10 of them. Match the title to the crystallographer and name one crystallographic achievement of each.

**William H. Bragg**

*Chancellor, Bristol University*

**Auguste Bravais**

*Clarinetist, Minneapolis Symphony Orchestra*

**Georges Friedel**

*Dean of Science, Lille University*

**Robert O. Gould**

*Director, Ecole Nationale des Mines, St. Etienne*

**Herbert A. Hauptman**

*Professor of Mathematics and Experimental Physics, Adelaide Univ.*

**Dorothy M. Hodgkin**

*Professor of Mineralogy, University of Cambridge*

**William N. Lipscomb**

*Professor of Physics, Ecole Polytechnique, Paris*

**William Hallows Miller**

*Researcher, U.S. Naval Research Laboratory*

**Louis Pasteur**

*Senior Member, Institute for Cancer Research, Philadelphia*

**Arthur L. Patterson**

*Vicar Apostolic of the North*

**Niels Stensen**

*For the answer to the previous Puzzle Corner please see p.28*



## 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 March 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:

**David Massey | BCA Administrative Office**

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Oxford Diffraction  
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# BCA Secretary's report 2008

**IN April 2007 I took over as BCA secretary from Christine Cardin. I would like to thank her for her assistance in helping me in my new role.**

As secretary, I record the minutes of the council meetings and with helpful prompting by **Bob Gould** add articles on BCA business to Crystallography News.

This year **Sheila Gould** finished her role as treasurer and we all owe her a great deal of thanks. We are delighted to welcome **Harry Powell** as our new treasurer. Bob Gould is now standing down as editor of Crystallography News and we all thank him for the wonderful editorship he has provided and all his hard work on producing such a high quality magazine and wish Carl Schwalbe all the best in his new role as Editor.

The website is also undergoing changes and we have on-line registration again this year after its successful inauguration for the Kent Spring Meeting last year. It is much more convenient and I have used it myself. We have online payments for interest group meetings too since cheques are becoming progressively obsolete. The PCG now have a wiki for their webpage to enable more rapid updating.

The Council has discussed email usage, following the lead of industrialists who need to be careful about email lists getting into the wrong hands. They use compiled email lists or BCC so as not to disclose addresses to others. Once an email is sent you have no control over it. Please let Northern Networking through the BCA Website and group secretaries know your up to date email address. On a related matter the IUCr's world wide directory of crystallographers which is accessible via the IUCr website needs to be kept up to date to be useful, so please add your entry if you are a practising crystallographer and update it if you are already in it.

The Interest Groups have been very active and the Young Crystallographers have formally become an Interest Group. The Biological Group held their summer school in St Andrews and winter meeting on the Structural Investigation of Gene Regulation in London; the Physical Group winter meeting was on New Techniques and Instrumentation for structure solution of magnetic structures and the Durham Rietveld School was held earlier this month. The Industrial Group had a meeting on small angle scattering in Grenoble taking advantage of the good rates during the summer downtime and in November held a pharmaceutical special interest group meeting back to back with their autumn meeting in Macclesfield. The CCG had their autumn meeting at Diamond in November on Chemical Crystallography at Diamond. The Young Crystallographers have another satellite meeting at this spring meeting and continue to explore ways they can work within the BCA and are actively

involved in development of the BCA website.

This year we have the IUCr congress in Osaka and there will be a UK delegation of BCA members. The council is also considering a bid to host the European Crystallographic Association meeting in 2013, probably in Edinburgh.

**Georgina Rosair**

April 2008

## Announcing the 15th CCP4 Protein Structure Workshop

**FROM 3rd-5th September 2008 this annual meeting will allow crystallographers and interested structural biologists from Northern UK laboratories to present their latest research and hold a morning workshop on a special topic of interest, all in a relatively informal atmosphere. This meeting has often been known simply as "Galashiels" but will again return to last year's successful venue, Carlisle, at St. Martin's College. This year the workshop will "boldly go to the final frontier" - MEMBRANE PROTEINS - as its specialist topic.**

Registrants are requested to provide a talk title (perhaps but not necessarily related to the special topic) as the meeting will continue to provide an invaluable opportunity for younger group members (PhD students and postdocs) to present their work to a friendly external audience and pick up useful tips. Registrant costs will be subsidised by CCP4 and other external sponsors\*.

\*Interested commercial sponsors please contact the organisers for registrant and exhibition costs.

Organising committee:

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A web page with additional information and registration details is available at  
<http://www.chem.gla.ac.uk/protein/gala>

# Financial Statement

## The British Crystallographic Association

### Summary Financial Statements for year ended 31 December 2007

**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:

	2007	2006
Grants and sponsorship	11,013	425
Donations	6,831	1,905
Annual Conference(5)	99,195	90,951
Meetings of groups	36,369	3,783
Crystallography News	22,944	17,773
Membership Subscriptions	24,714	19,702
Net Income from trading	16	13
Investment income	4,100	6,027
Interest received	4,899	2,341
IUCr Bursary	-	23,780
<b>TOTAL INCOME</b>	<b>210,081</b>	<b>166,700</b>

#### EXPENSES:

	2007	2006
Direct Charitable expenditure(2)	172,259	119,957
Management & administration(3)	28,884	27,827
<b>TOTAL EXPENDITURE</b>	<b>201,143</b>	<b>147,784</b>

#### NET INCOME:

	2007	2006
	8,938	18,916
Unrealised gains (losses) on investment assets	(4,149)	4,896
<b>NET MOVEMENT IN FUNDS</b>	<b>4,789</b>	<b>23,812</b>

Balances brought forward at 1 January	217,766	193,954
Balances carried forward at 31 December	222,555	217,766

#### ASSETS:

	2007	2006
<b>Fixed assets</b>		
Tangible assets	5	5
Investments	70,592	93,145
Total	70,597	93,150
<b>Current assets</b>		
Stock	493	493
Debtors	16,928	2,850
Cash at Bank	143,503	138,891
Total	160,924	142,234

**LIABILITIES:** amounts falling due within one year (7,436) (16,386)

**LIABILITIES:** amounts falling due after more than one year (1,530) (1,232)

**NET ASSETS** 222,555 217,766

#### INCOME FUNDS:

	2007	2006
Restricted funds (4)	93,071	85,413
Unrestricted funds (4)	129,484	132,353
<b>Total</b>	<b>222,555</b>	<b>217,766</b>

## 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

	2007	2006
Subscription to International bodies	6,569	4,032
Annual conference (5)	96,526	87,860
Meetings of groups	8,591	5,281
Crystallography News + Newsletters	24,301	18,367
Course fees and accommodation	27,000	1,615
Grants and sponsorship	5,440	1,202
Awards & bursaries	882	-
Arnold Beevers Bursary Fund	2,950	1,600
<b>Total</b>	<b>172,259</b>	<b>119,957</b>

### 3. GOVERNANCE

	2007	2006
Administration fee	20,781	22,066
Accounting fee	3,936	3,819
Insurance	392	378
Bank and security charges	155	134
Special Interest Group Administration	1,958	108
Council Members' expenses	1,662	1,295
Depreciation-tangible fixed assets	-	27
<b>Total</b>	<b>28,884</b>	<b>27,827</b>

The full BCA accounts for 2007 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 2007

4. STATEMENT OF FUNDS	Brought Forward	Incoming Resources	Resources Expended	Gains (Losses)	Carried Forward
<b>UNRESTRICTED FUNDS</b>					
General Fund	<u>132,353</u>	<u>155,179</u>	<u>(153,899)</u>	<u>(4,149)</u>	<u>129,484</u>
<b>RESTRICTED FUNDS</b>					
IUCr bursary fund	23,781	3,063	-	-	26,844
Arnold Beevers bursary fund	16,398	3,149	(2,950)	-	16,597
Dorothy Hodgkin prize fund	8,538	99	(585)	-	8,052
Chemical group teaching school	7,045	33,095	(28,290)	-	11,850
Chemical group fund	5,055	2,504	(5,900)	-	1,659
Industrial group fund	6,784	8,936	(5,698)	-	10,022
Biological Structures group fund	<u>17,812</u>	<u>4,056</u>	<u>(3,821)</u>	-	<u>18,047</u>
<b>Subtotal</b>	<b><u>85,413</u></b>	<b><u>54,902</u></b>	<b><u>(47,244)</u></b>	<b>-</b>	<b><u>93,071</u></b>
<b>Total of Funds</b>	<b><u>217,766</u></b>	<b><u>210,081</u></b>	<b><u>(201,143)</u></b>	<b><u>(4,149)</u></b>	<b><u>222,555</u></b>

5. Spring Meeting 2007 University of Kent at Canterbury	
<b>INCOME</b>	
Sponsorship	7,050
Registration	71,895
Exhibition	21,769
Bursaries	1,750
<b>Total</b>	<b>102,464</b>
<b>EXPENDITURE</b>	
Accommodation & Meals	26,590
Facilities	12,800
Catering	16,428
Social Event	5,701
BCA Speakers Expenses	8,090
Refunds	2,825
Abstract Book	5,078
NNE Fee	15,187
Administration	5,485
Printing & Stationery	2,355
<b>Total</b>	<b>100,539</b>
<b>TOTAL INCOME</b>	<b>102,464</b>
<b>TOTAL EXPENDITURE</b>	<b>100,539</b>
<b>MEETING SURPLUS</b>	<b>1,925</b>

All the transactions for the 2007 Spring Meeting were made through the BCA account, and consequently these detailed meeting accounts are reported as part of the BCA financial report

### Treasurer's Report 2007

This was a busy year for the BCA and its constituent groups. Overall we had a surplus of £4,789 during the year ended 31 December 2007, and the Association has no material guarantees or commitments which could affect its future solvency. The general fund had a deficit of £2,869 after a decrease of £4,149 in the value of the investments, but the reserve funds operated by the Groups and the School had a overall surplus of £7,658. The income from our investments brought in £8,999 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. In the current climate we are holding more of our reserve as interest-generating cash. Our investment portfolio was valued at £70,592, and this also provides 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.

The Young Crystallographers symposium before the Spring Meeting in Canterbury was well attended and appreciated, and sponsors were generous in their support too. 30 bursaries were awarded to the Spring Meeting, ten of which were commercially sponsored. We also 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 not been required by the organisers of the meeting in Osaka, Japan this year, so the monies are accumulating in the reserve fund, and will be offered to the meeting in Madrid 2011 in due course.

The Chemical Group biennial Crystallography School was held at Durham University in March, and the organisers are to be congratulated on running, as ever, a very successful event with 78 participants and 10 tutors.

Crystallography News has broken even this year on a turnover of £22,944. The BCA owes a debt of gratitude, as ever, to

its advertisers and sponsors who generously support our activities. The surplus from the Spring Meeting, though small, is always welcome, and the sponsorship enables the costs to be kept affordable to many.

Subscriptions to international bodies were £6,569, 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 expanding the interactive conference website to include payment of membership and group meeting fees, are £20,781. This facility seems to be much appreciated and it does make life easier for the Treasurer too! The expertise and hard work of Northern Networking Events Ltd is very much appreciated.

Membership income is up by £5,012 this year as the increase in subscription rates came through. There were 16 Corporate Members. Also as a result of the increase in membership subscription and some donations, the amount received from the Inland Revenue in Gift Aid was also up this year to £1,558. These monies were allocated to the Arnold Beevers Bursary Fund, and this Fund was also boosted by a transfer of £829 bank interest income from the BSG, for which the BCA is very grateful. Gift Aid will be affected by the decrease in standard rate income tax this year.

This is my last report as Treasurer, and I would like to thank everyone, in particular Chick Wilson, Paul Raithby, members of Council, Gill and the team at Northern Networking Events, and our accountant Bob Young for all their help throughout the year, and the whole of my tenure of this office.

Sheila Gould

Hon Treasurer

The full BCA accounts for 2007 are available as an e-mail attached file from the BCA administrative office.

# BCA 2008 Meeting



**THE** following description of the recent BCA meeting at York has been compiled from reports by bursary recipients. Two accounts are reproduced in full, and for each session I have combined parts of other reports by a procedure akin to sintering a powder. I hope that most report writers will be able to recognize at least a couple of their own sentences. Your contributions are appreciated!

Some general points are worth noting at the outset. A recurring theme was the recipients' heartfelt gratitude to the Arnold Beevers Bursary Fund. In many cases the grant made the difference between attending the meeting and not being able to attend. Donors to the Fund can be well pleased with the good they have done. **Graham Stinton** pointed out that the Young Crystallographer speakers at the meeting represented a relatively small number of institutions: all the submitted oral abstracts were from just six. Writing as a structural biologist, **Andrea Fallas** found the sessions to be friendly and fun but was disappointed by the small turnout of young biological crystallographers. The lesson is clear: if you are from outside the "Big 6" institutions and/or you are a biological crystallographer and you missed the York meeting, do come next year! Several people commented that the highlight of the Young Crystallographers' day was undoubtedly the "flash presentation" session, where budding crystallographers battled for a bottle of bubbly to present their poster in exactly one minute. **Patrick Dall'Aglio** and **May Marsh** mentioned that the poster session was very enjoyable and they particularly liked the "match your ticket" game, which gave a good opportunity to interact with scientists from other disciplines. As a non-biologist **John Findlay** praised the 15-minute chairman's introduction to the "*Ligand Binding and Drug Design I*" session given by **Rod Hubbard**, stating "I found it very interesting and frantically scribbled down as many notes as I could. The presentation not only helped me to understand (and enjoy) the rest of the session but I left feeling that I really learned something." This additional means to encourage crystallographers to venture outside their own "comfort zone" might well be adopted more widely. This section begins with two accounts reproduced in full that convey the spirit of the meeting.

**Carl Schwalbe**

## The Goose-Challenger's Story

**AFTER** last year's trip to the South (a place of fear and suspicion for an adopted Yorkshire-man) the decision to hold this year's Spring meeting in York was well received. We were especially glad that we arrived fresh and ready on Monday morning, as it was soon obvious that the local geese would attack sandwiches at any overt sign of weakness; thankfully it later became clear that they would retain a casually threatening demeanour but avoid outright violence for the duration of the meeting.

The Young Crystallographers' sessions kicked things off in the usual style with a great selection of fine talks, pretty posters and excellent science, the difference this year being the first ever YCG AGM; we have arrived! (A big thank you to all who have made it possible to say that).

**Tony Crowther** opened the main meeting, honouring the career of **Michael Rossmann** by displaying his contribution to the solution of macromolecular structures. Highlighted were the structure of haemoglobin and a number of viruses along with their cellular attachment architectures, scary looking things indeed. After lunch the parallel sessions started. I attended Structures from Pharmaceutical Powders. **Alastair Florence** discussed the application of structural solution from powder diffraction to a range of carbamazepine analogues, spotting common packing and H-bonding motifs along the way and importantly associating them to the chemical changes. **Vincent Favre-Nicolin** followed, discussing the problems and processes of getting from lab powder data to a structure and displaying the power of his excellent free software, Fox (available at <http://objcryst.sourceforge.net/Fox>). **Matthew Johnson** (GSK) concluded the session offering a perspective on the various applications of PXRD in the pharmaceutical industry, one interesting example of this being the quantitative detection of a polymorph impurity down to 1.5% via Rietveld analysis.

After some caffeine and a biscuit **Gérard Coquerel** (Jekyll and Hydrate) proved that a hydrate can be much more of a Jekyll than a Hyde when used as a means of racemate resolution in modafinil. In this system R/S resolution was only possible in the presence of water, with knowledge of the ternary phase space. This knowledge, Gérard proved, he and his group have in spades. **Alan Kennedy**'s first port of call displayed the potential perils of spellcheckers, as *Mony a Meickel Mays a Muckel* (many small things make a large thing) transformed into *Mock Turtles*. He followed this by giving experimentalists something to feel ashamed of as he showed

the lack of large scale systematic studies within organic salts. He then went on to explain his experimental methodology of using a 'simplified' molecule as a means of building up a databank to allow structure-property prediction, showing there are feasible alternatives to writing code. **Royston Copley** then finished the session displaying the hydration of Carvediol, a racemic molecule that clearly didn't want to behave, requiring SSNMR data and the crystal structure of the R enantiomer to understand the disorder present in the racemate. Also shown in this talk was the interesting hydration/dehydration behaviour of the single enantiomer, displaying the power of optical microscopy when combined with a secondary technique and a generous helping of logical thought.

The Applied Crystallography Showcase allowed **Ian Oswald** to give his YCG prize-winning talk again on energetic materials under pressure, specifically focussing on the explosives RDX and HMX. In this talk he outlined the new phases he had discovered using the Paris-Edinburgh cell (not small enough to fit in the palm of your hand!) and confirmed the previously reported phase transitions. In an unscheduled appearance **Judith Shackleton** then followed describing the techniques she had used to map a toroid and its correct manufacture (TEDDI, RIBEC, and resistivity) concluding that the scale correlation between techniques and the lattice parameters had implications for manufacturing. She concluded by showing a video of her first take-off as the pilot of a small plane, a novel ending to a very interesting talk. The next Judith was **Judit Debreczeni** (AZ) discussing the application of protein structure determination to the drug development process, first explaining the possible industrial applications before giving specific examples. Of interest was the protein associated with leptin signalling (PTPLB), knowing the structure of which aided the development of a number of potential active compounds for diabetes and obesity. **Mark Farnworth** (Pilkington Glass) showed how they used X-rays not only to determine if the growth of coatings was correct in orientation but also as a means of determining how much glass was in their glass. **Suzanne Harte** (Pharmorphix) then described the various techniques they apply in conjunction with XRD to screen for pharmaceutical salts and the challenges associated with screening for new pharmaceutical phases. **David Rendle** concluded the session giving a showcase of how XRD is applied to forensic science for various purposes, from identification of substances to intelligence gathering. I found it fascinating to see how such techniques can trace a batch of illicit drug from local supplier back to its country of origin. All in all a well planned and interesting session.

As ever this was a really well organised, well attended meeting that was full of good science. The conference dinner, although interrupted for a few more prizes, was as raucous and fun as usual, and led directly to the lack of reporting on the final day; on which there were some very fine talks (**Peter Müller's** Plenary and the Design of Functional Materials session were both great). Thankfully getting home was as simple as arriving, leaving the geese to their next unwitting victims.

**Dave Berry**  
University of Bradford

## The Hopeful Travellers' Account

**THE Spring BCA meeting was held at the stunning location of the University of York this year and overall a great success. We attended the Young Crystallographers meeting, but missed part of the first plenary as we tried to arrive on time by train (what a surprise!!!).** The well organised event hosted a number of 15 minute presentations from a wide variety of science. The Young Crystallographers aim to give an opportunity for PhD students and PostDocs to gain experience of talking in front of a relaxed and unpressured scientific audience. The presentations were of high quality and we gained many inspirational ideas including techniques of slurries in capillaries for powder diffraction and a number of alternative programs e.g. FOX and Olex2. Some talks unrelated to our own work were fascinating, and good background explanation made it very easy to follow. It was also a good possibility to try our own presenting skills (poor suffering audience!). The one minute poster presenting was chaotic and funny as usual, as well as the evening program (good of them to open the bar).

The main BCA meeting started for us after lunch on the 8th April with a variety of sessions from different subject areas. One session of particular interest was on Functional Molecular Materials, especially talks by **Jeremy Rawson** and **Guillermo Mínguez**, because these were relevant to our subject areas.

The second talk in the session 'Sulfur-Nitrogen Radicals: Systematic Design of Spin-Transition Materials' was given by **Jeremy Rawson** from Cambridge. He discussed the packing of  $7\pi-\pi$  thiazyl (S/N) radicals and their possibility of forming a stable crystalline phase or dimer. This depends on the packing, and they can switch between the monomer and dimer structure with light. He wants to try some work under pressure as well. It was a really good talk, especially as he is not a crystallographer but introduced a lot of new ideas which needed a crystallographic analysis. His talk definitely left the audience with a lot to think about.

One of the stand-out talks for us at the York spring BCA meeting was by **Guillermo Mínguez** from the University of Sheffield, titled 'Non-Porous Materials Can Also Take Up Gases'. His talk focused on the reversible uptake of HCl gas by a non-porous crystalline framework, through a sequence of bond cleavages, with a change in coordination geometry from distorted tetrahedral to square planar. It was interesting to see that a lot of the work had been followed by X-ray powder diffraction, with good solutions being found using the DASH software, as there were no crystals of suitable size for single crystal analysis. The project was thorough and many different analytical techniques were used backing up his ideas of the suggested reaction process. All in all, an excellent talk.

Another useful aspect of the meeting was the DASH

workshop. It was extremely helpful to have hands-on experience with knowledgeable instructors available for any queries.

The BCA conference dinner was enjoyed by all with free wine and beer from Bruker and PANalytical. The main presentation ceremony was guided excellently with much enjoyment from seeing worthy prize winners.

**Steffi Schiffers, Anna Stevenson and Mark Warren.**  
University of Bath

## The Main Speakers at York

### BSG PLENARY: A Tale of Two Careers

**THE** BSG plenary lecture which opened the main meeting was an excellent talk given by **Tony Crowther**, subtitled "From molecular replacement to the structure of viruses". The lecture honoured **Michael Rossmann**, who has made major contributions to the field of macromolecular crystallography. Tony started with Michael's early career and his work with Max Perutz on haemoglobin leading to the concept of molecular replacement. Both men worked in this field, developing some of the theoretical machinery including rotation functions. While they applied different methods (Crowther using electron microscopy, Rossmann X-ray crystallography) both studied proteins and viruses. Crowther finished with details of his recent work relating the structure and activity of the Hepatitis B virus.



### PCG PLENARY: Charge Order in Oxides - Putting the Fun into Functional Materials

**PAUL ATTFIELD** from the University of Edinburgh started off day two of the conference. A bit of extra fun arose from the

argument between Paul's laptop and the projection system early on in the lecture! He started by outlining what charge ordering (CO) is - the ordering of different charge states of an atom or a molecule in the crystal.

This effect can bring about metallic to insulator transitions as the CO sets in. While many CO materials are inorganic, organic charge ordering has been seen. He gave a number of reasons why CO is an important phenomenon. It is typically associated with superconductivity and colossal

magnetoresistance. It can be quite difficult to quantify CO using crystallographic techniques for a number of reasons including the potential for micro twinning in single crystals and the lowering of symmetry that a CO transition can induce. The small distortions give rise to very small superstructure peaks. He went on to give a number of examples, with work confirming the presence of CO in magnetite using powder diffraction and X-ray resonance studies. A model for the underlining theory was also presented.

### IG PLENARY: X-Ray Diffraction on Mars?



**THE** third plenary lecture of the meeting led us into the AGM and perhaps more importantly the conference dinner! It was given by **Rob Delhez** of the Delft University of Technology, and its eye-catching title was bound to attract plenty of people.

The first part of his talk outlined why one might be interested in researching space and in particular Mars. Apart from being our closest neighbour Mars also shares an early history comparable to Earth. While a lot of research has focused on Mars, there remain many questions which X-ray diffraction (XRD) could answer. The rest of the talk detailed the technical and scientific challenges that would face a potential diffractometer on Mars. He introduced us to the NASA and ESA XRD instruments, CheMin and Mars-XRD due to fly to Mars in the next few years as part of mobile scientific laboratories. Both feature X-ray fluorescence (XRF) as well as XRD. XRF and XRD together offer a highly complementary picture of a mineral's composition. The ability to combine different techniques into a single field-adapted piece of equipment is a useful application, and will no doubt be used by geologists and mineralogists in terrestrial field work in years to come. The build requirements for the two instruments differ greatly with the Mars-XRD being much smaller than its US counterpart and having very tight requirements. Rob is involved in the development of the European instrument. The lecture was very interesting and gave a nice insight into some really exciting frontiers in crystallography.

## CCG TEACHING PLENARY: Dead End Highway 13 - the Carriage of no Return

**BRIGHT** and early in the morning after the conference dinner **Peter Müller** from MIT took us on a drive through some of the trickier areas of structure refinement. He started by passing on the regards of the American Crystallographic Association's standing committee on education. He then outlined what makes a good structure and the different types of errors that can hinder a refinement. Apart from systematic errors there are, in Peter's view, avoidable errors and really avoidable errors! The latter can take the form of mistyped lattice vectors, for instance. Peter focused on the former and gave a number of examples where avoidable errors could occur. These included assignment of atom types and dealing with (or failing to deal with) disorder in a system. He suggested a number of ways to check and deal with both problems. In particular the use of restraints in refining disorder was strongly suggested due to the high correlation of data for the disordered atoms. Such restraints can come from many

sources and people shouldn't be afraid to use them as additional data for the refinement. Despite running short of time and not being able to cover everything - there are plenty of avoidable errors - those crystallographers managing to get up in time heard some good advice on dealing with difficult refinements.

**Anthony M. Reilly**, University of Edinburgh  
**Sarah Lister**, University of Durham



## Prize Lectures

**TWO** excellent lectures were given by the CCG and PCG prize-winners (**Kirsty Anderson** and **Laurent Chapon** respectively). In particular, Kirsty's lecture on crystal structures with  $Z' > 1$  attracted general interest well beyond the boundaries of chemistry. She noted that around 8.8% of structures in the Cambridge Structural Database have a  $Z'$  greater than one, and that values of  $Z'$  range from 1/96 to 32 with even numbers more common than odd. In addition to database work looking for potential explanations as to why some compounds form high  $Z'$  structures, she has been conducting a number of experimental studies to try to obtain verification of her theories. During her talk she also discussed the limitations of the current definition of  $Z'$  and the need for further clarification to deal with the presence of amongst other things solvent molecules.

Next we heard from Laurent, the PCG prize winner, who is associated with the new generation GEM neutron diffractometer recently constructed at the ISIS pulsed neutron source. He talked about "Neutron Magnetic Scattering Study in Multi-Ferroics  $\text{RMn}_2\text{O}_5$ ". The audience remained engaged in his lecture even after the pictures of Nicole Kidman had gone. An informative overview of the propagation of magnetic moments in space was presented whilst at the same time serving up more in-depth information on Laurent's extensive work on neutron magnetic scattering of multiferroics for those left wanting more.

**Laura Budd**, University of Edinburgh  
**David Free**, University of Durham  
**David Millar**, University of Edinburgh  
**Hazel Sparkes**, University of Durham



*Laurent Chapon receiving the PCG award at the lecture session*



*Other prizewinners at the conference dinner*





Other prizewinners at the conference dinner



Other prizewinners at the conference dinner

## The Young Crystallographers

**ONCE** again the Young Crystallographers' meeting, divided into four sessions, preceded the main BCA meeting by a day. The presentations demonstrated convincingly that a lot of enthusiasm and clear explanation of good science can be packed into a 15 minute talk.

The first session was chaired by **Susanne Huth. Ehmke Pohl** of Durham University opened it with his enlightening plenary lecture *Why is macromolecular crystallization so difficult and why do we still obtain suitable crystals?* He discussed some of the theory behind crystallization and summarized some of the current strategies in use to obtain crystals of macromolecules suitable for X-ray crystallography.

**Gordon Cunningham** gave the first student talk of the session with his talk entitled *Application of high-throughput cluster analysis to multiple data types - differential scanning calorimetry and infrared data*. Gordon told us of methods that allow DSC, IR, PXRD and Raman datasets to be compared with each other using a variety of cluster analysis methods.

**Alexandra Bowyer** gave a talk on *The 3D structure of L-Threonine dehydrogenase (TDH) from Thermococcus kodakaraensis, an enzyme involved in amino acid metabolism*. The enzyme THD is one of two major pathways by which degradation of the amino acid L-threonine occurs. So far she has been able to determine a structure from X-ray diffraction, but has not been able to establish thus far whether the enzyme requires a second catalytic  $Zn^{2+}$  ion at the active site, which could possibly bind at the site to stabilise long loops of the tertiary structure that have poor electron density in the crystal structure.

**Helen Maynard** gave us an overview of *High pressure*

*crystallography* in which she pointed out that pressure is in fact the biggest physical variable that we can play with, and has applications in all aspects of science. She also discussed her future plans for investigating a potential new high pressure phase of methane, whose high-pressure behaviour is important in models of the outer planets such as Neptune, where it comprises ~10-15% of the planet's mass.

In his talk *a molecular dynamics approach to equilibrium structures in crystals*, **Anthony Reilly** discussed a new method using molecular dynamics simulations that allows time-averaged experimental structures to be corrected to equilibrium positions. Differences between simulated equilibrium and time-averaged structures are used as corrections for experimental structures. Potential uses include the ability to determine new forms for the Debye-Waller factor to model systems with curvilinear motion.

Next, **Marc Schmidtman** gave his talk on *H-transfer and polymorphism in  $IN_2$ -OA*. Marc discussed the four different polymorphic forms of molecular complexes of isonicotinamide with oxalic acid,  $IN_2$ -OA, which demonstrate some unusual hydrogen bonding schemes and a tendency towards the appearance of polymorphism.

The final event scheduled for this session was an introduction by **Richard Gildea** to *Olex-2: the new molecular tool*, which was intended to whet the appetite for the Olex-2 workshop on the final afternoon of the BCA meeting. This new open source molecular graphics program offers solution, refinement and manipulation of small molecule crystal structures. It was surprising and impressive that we got not only a PowerPoint presentation about this program, we saw it working in real time too!

This opening session set a very high standard for the meeting, which was reinforced in the subsequent sessions.

After a break for tea and coffee, the meeting resumed under the chairmanship of **Duncan Sneddon** with a keynote from **David Allan** on *Beamline I19: A Facility for Small Molecule*

*Single-Crystal Diffraction at Diamond*. He informed us of some of the reasons we may want to use synchrotron radiation to study single crystals, which include the high flux, tunability and low divergences of the X-ray beam. A series of photos illustrated the progress that is being made with the construction of the new beamline. The talk left members of the audience thinking of experiments to perform once the beamline is completed.

Next in the programme was a study by **Leo Chavas** on *Structural studies of vesicle trafficking*.

**Stefanie Schiffrers** then gave a talk on *Solid state reactions with photocrystallography* where she described her research into kinetic studies of [2+2] photoreactions under light and pressure. The combination of spectroscopic and crystallographic techniques allows the study of light-induced metastable and transient species, enabling the study of the structure of materials as they change.

**Shaun Evans'** talk on *Structures and transitions in light lanthanides at high pressure* discussed how a range of different close-packed crystal structures of trivalent lanthanide elements can be accessed by the application of pressure.

In the last talk of the day, **Graham Stinton** discussed *The structure of molecular nitrogen at high pressure using X-ray diffraction and maximum entropy maps*. He explained how maximum entropy mapping (MEM) uses electron density, rather than discrete atoms, to model a structure, which can be particularly useful for modelling highly-disordered systems, or where data is incomplete.

Finishing the day's sessions after the group's AGM were the entertaining poster flash presentations, with poster contributors invited to plug their poster for up to one minute (but not a second longer!). The poster session followed giving other members of the YCG the opportunity to present their research. This was accompanied by a buffet dinner and a fair quantity of free wine!

Next morning the final session of the meeting was well attended despite the previous evening's festivities. **David Beveridge** of HARMAN technology Ltd. began this session with his intriguingly titled keynote, *Crystals, Grots and X-rays*, in which he told us of the enjoyment and challenge involved in identifying unknown compounds using a variety of techniques, including X-ray powder diffraction.

**Mark Warren** gave his talk on *Time-resolved photo-crystallographic investigation of metastable species*, during which he discussed some examples of linkage isomerism involving nickel nitro complexes. Irradiation of a sample at low temperature causes the NO<sub>2</sub> ligand to undergo linkage isomerism, resulting in a change in coordination mode from the N-bound to the O-bound isomer. The use

of synchrotron radiation is essential for allowing short data collections and the use of smaller crystals, which ensures that the whole crystal is photoexcited.

Next, **Riccardo Montis** presented his research on A simple salt with a complex structure; *4-aminopyridine hydrochloride with Z' = 30!* A structure of 4-aminopyridine hydrochloride has been determined which contains 240 molecules in the unit cell, with Z' = 30, which would appear to be the second highest value for Z' found to date.

In her talk entitled *Magnetic coupling in model cubic V, Ni and Cu structures comprised of interlinking HF<sub>2</sub><sup>-</sup>, HCl<sub>2</sub><sup>-</sup> and HFCl<sup>-</sup> ligands*, **Lorreta Lawton** discussed her research into the dependence of magnetic coupling strength on exact exchange content, hydrogen bond length and proton position using the CRYSTAL06 computational code. This code was used because it allows for mixed hybrid-exchange calculations which combine both the Hartree Fock and density functional theory approximations to yield more accurate coupling constants.

**Iain Oswald** gave an explosive (!) lecture on *High pressure structural studies of energetic materials*. We learnt the importance of crystal morphology in the explosives industry, where for example the detonation velocity is proportional to the density of the polymorph, and also the shock sensitivity of a particular polymorph is of vital importance. Iain discussed his research into high pressure polymorphs of the military explosive RDX

**Susanne Huth** followed with her talk on *Crystal chemistry of functionalised organic molecules - a structural systematics approach*, in which she told us of her work studying crystal packing patterns together with the application of solid state energy calculations. Through the use of libraries of closely related compounds she has been able to carry out a systematic analysis of non-covalent interactions exhibited in 1,8-substituted anthraquinones.

**Andrew O'Neill** brought the final session to a close with his talk entitled *Nucleation studies of substituted aromatic compounds*. Andrew has been performing in-situ X ray scattering studies of the initial crystal nuclei formed at the earliest stages of the nucleation process, in an attempt to increase understanding of this process.

The range of topics covered in the YCG satellite meeting reflected the vast array of interests held by members of the group. This kind of interdisciplinary forum allows for the open discussion and exchange of ideas that is vital to keeping the UK at the forefront of crystallographic research for generations to come.

**Richard Gildea**, University of Durham  
**Helena Shepherd**, University of Durham  
**Andras Kallay**, University of Glasgow



Session 1



Session 2



Session 3

# Exhibitors BCA 2008 Spring



Alpha



Oxford Cryosystems



MARresearch



Hiltonbrooks



Incoatec



Oxford Diffraction



Oxford University Press



PANalytical



Xenocs

# g Meeting, York



Rigaku



STOE Thermal



Taylor & Francis



Waters



ICDD



CrystalMaker



Douglas Instruments



Molecular Dimensions



Bruker

## Applied Crystallography Showcase

**THE** winner of the 'Industrial Group Young Crystallographers Prize', **Iain Oswald** from the University of Edinburgh, gave the first presentation on *High Pressure Studies of Energetic Materials*. He used the Paris-Edinburgh cell to study effects of extreme conditions on a military explosive, 1,3,5-trinitrohexahydro-1,3,5-triazine, also referred to as RDX. His work has successfully determined the structure of  $\gamma$ -RDX at high pressure. He concluded that using high-pressure techniques can provide detailed information about structure and behaviour of energetic materials under high-pressure conditions. Furthermore, it didn't destroy the Paris-Edinburgh cell!

**Judith Shackleton** from the University of Manchester gave the second talk titled *Direct Correlation between Ferrite Microstructures and Electrical Resistivity*. Judith helpfully explained what ferrites are and the importance of what they are used for. She gave an overview of how these ferrites were prepared and the results of the analysis done using Tomographic Energy Dispersive X-ray Imaging (TEDDI). This technique has a stage which allows scanning in 3D. The result showed that lattice parameters were larger at the inner and outer surface of the sample, as was to be expected because of the loss of Zn. Her research also considered Remote Electron Beam Induced Current (RIBEC). This method measured the electrical properties; however it showed no contrast compared to the method above, so resistivity measurement was used instead. This method showed some variations which were consistent with TEDDI.

The next talk was by an industrial member, **Judit Debreczeni** who works at AstraZeneca, Alderley Park. Judit spoke about protein structures in drug discovery. She gave an insight into protein crystallography in the pharmaceutical industry by discussing the stages and steps required and the timescale used in industry and the high-throughput methods used in screening. She referred to a classical example, p38 MAP kinase, and discussed how pyrazolamines are inhibitors of this rheumatoid arthritis target. Modelling was unsuccessful but a new binding pocket was identified. Additionally she talked about targeting ptp1b, where high-throughput screening failed to deliver any leads but NMR screening was used. The studies revealed a secondary binding site which can be targeted.

The next talk was from **Mark Farnworth** from Pilkington. Mark spoke about glass and methods they use to analyse and measure glassy phases in refractory material. X-ray diffraction becomes important in the analysis of thin microcrystalline coatings.

**Suzanne Harte** of Pharmorphix presented a talk about the work carried out at this specialist company in Cambridge. The company carries out solid form research for its clients who have active compounds. Pharmorphix provide services for clients throughout the different stages of drug discovery and development, which can be from salt selection through to patent protection strategies. The techniques this company offers to fully understand solid-state properties of a drug range from spectroscopy to microscopy, thermal analysis to HPLC and stability studies to XRD.

**David Rendle**, who discussed the *Applications of XRD within Forensic Science*, gave the final talk of this session. This was most interesting as he presented how anything and everything can be considered as forensic evidence and then, if it is wholly or partially crystalline, be analysed using XRD. He outlined how XRD is valuable to forensic scientists as it is non-destructive and versatile in the analysis of organics, inorganics, and metals. It also allows forensics teams to distinguish between polymorphs and racemic from optically active forms.

**Hafsa Javed**,  
University of Bradford



**Back row** - Chris Staddon (Chair), David Rendle, Mark Farnworth, Iain Oswald

**Front row** - Judith Shackleton, Suzanne Harte, Judit Debreczeni

## Big is Beautiful

**THIS** session, chaired by **Judith Shackleton**, marked a good contrast to some of the usual topics found at a crystallography conference. The general topic of this session was how neutrons and X-rays are used with large-scale samples-- no nanomachines in this session! **Supriyo Ganguly** from the Open University gave the first talk entitled *Analysis of weld residual stress in prototype engineering components and structures using pulsed neutrons*. In essence this talk was about the quality of welds and how to make sure that the techniques used to weld materials together can produce a strong bond that shouldn't fail. This can of course be somewhat inconvenient if a weld should fail on say an aircraft. On the upside this could distract you from worrying about your luggage in Heathrow! The talk showed that neutron TOF diffraction could be used to better understand the process of welding materials together along with examining the residual stress within these materials created during these processes.

The second talk was given by **George Bibby** from Rolls Royce who was using X-ray backscattering to look at residual stress in turbine blades. This process was aimed at replacing fatigue testing and is used among other methods to ensure that changes in manufacturing practice will not have a detrimental effect on the component in question. The instrument was an interesting piece of equipment, where the source and detectors move leaving the bed static, which is a simpler solution than moving a large sample. The talk also emphasised the need for careful measurements and the controlling of errors and this can lead to surprisingly accurate results.

The final talk was from **Michael Drakopoulos** from JEEP at Diamond who gave a presentation on the features of a beam line that is being built to a quite unique specification. It is capable of handling large samples within an external building along with providing a unique capability to carry out a wide range of experiments on large objects as well as being able to study processes on site. This beam line should prove to be interesting when it comes online in October 2009.

**Duncan Sneddon**,  
University of Glasgow



George Bibby, Michael Drakopoulos, Judith Shackleton (Chair), Supriyo Ganguly

## Calculating Properties from Structure



Chick Wilson, Jamshed Anwar, John Mitchell, Simon Coles  
(Michael Probert not available)

**THIS** final parallel session of the meeting was chaired by **Simon Coles** who put together a really good set of speakers. Opening the session was **Jamshed Anwar** from the University of Bradford. His talk focused on understanding polymorphic behaviour and phase transition using molecular simulation. He started by highlighting the importance of such processes to industry with the story of a drug formulation changing polymorph and losing solubility. While crystallography can tell us about structure, we cannot learn about the thermodynamics and mechanism. Molecular dynamics can potentially give us this information. Some work on a martensitic-type phase transformation in DL-norleucine was presented. This synthetic amino acid forms bilayers through hydrogen bonding. These bilayers shift relative to each other when the transformation comes. This can proceed via molecule-by-molecule shifting or via whole bilayers moving. With the aid of some well-crafted movies he showed that the concerted motion of bilayers is not only possible but a significant contribution to the overall transformation.

The second half-hour talk was given by **John Mitchell** from the University of Cambridge. John started his talk by outlining the various ways computation techniques can impact in chemistry: from theoretical chemistry all the way to informatics. He then gave a number of interesting examples of informatics in action. These included predicting solubility of compounds using the Random Forest technique! Each tree in the forest applies a subset of a number of different criteria for solubility and gives a decision on solubility or insolubility. A more robust approach involving thermodynamic integration and lattice-energy calculations was also detailed. The use of a spam filter to discern between biologically active and inactive compounds was another really interesting example of informatics.

The third speaker was **Chick Wilson** from the University of Glasgow. He gave a shorter fifteen minute talk on the input of theoretical chemistry into his research. The talk was jam-packed full of many, varied examples, most of which Chick didn't have time to go through! The computational method of choice was plane-wave density functional theory and the focus was on using theory to further the understanding of various systems. Some highlights were the studies of proton transfer and energetics of polymorphism where theory and experiment match closely in predicting which polymorph is favoured.

The last talk of the session was given by **Mike Probert** from the University of Durham. Concentrating on one particular aspect of his abstract, he chose to focus on determining charge density maps rather than on their application. He discussed the important requirements for achieving meaningful results in multipole refinements. Data reduction is a key aspect of this and with many different programs and methods for integrating the data it's easy to see why problems might arise. Calibration of the diffractometers is also an issue which must be addressed.

**Anthony M. Reilly,**  
University of Edinburgh

## Jekyll and Hydrate

**CHAired** by **Anne Kavanagh**, the session consisted of talks by three speakers. The catchy title probably helped to guarantee this session a good attendance even at its late afternoon time with the poster session still to come.

The first speaker was **G rard Coquerel** of the University of Rouen with the presentation *The Different Roles of Water Molecules in Chiral Discrimination in the Solid State*. The talk gave an insight into the fact that the simple water molecule can have very important effects in discriminating the chirality of a crystallised molecule, as very often it is important to the molecular recognition of the molecules and not just there to fill gaps. He showed this visually through diagrams of molecules held together by bridging water molecules and through the use of ternary phase diagrams

Next up was **Alan Kennedy** from the University of Strathclyde with the Glaswegian title of *Mony a Meickel Maks a Muckel* that he assures us means "many small things make a big thing". This was linked to his presentation through the idea of investigating many very similar molecular systems to build up a database of knowledge that then can be used to predict the outcome of a crystallisation experiment. He envisages that if we can predict the outcome of the crystallisation, we shall be able to predict the properties of the materials from their starting materials. Alan showed this through preparing numerous salts of substituted benzoates that differed in the group 2 metal counter-ion as well as the identity and the position of the substituent. He ranked them in order of their solubility, which is a key factor in the pharmaceutical drug design.

Last up was **Royston Copley** from GlaxoSmithKline, with the presentation *The Complex Solid-State Structure of Carvedilol Phosphate: A Case Study of a Pharmaceutical Hydrate*. Royston has been working with the active pharmaceutical ingredient carvedilol phosphate that is used in heart medicine as a beta-blocker. He told the story of the complex nature of the hydrate, which initially proved difficult to crystallise. He showed that it took many techniques, including X-ray diffraction and solid-state NMR, to work out the nature of the disorder found near the chiral centre and concluded by saying that one

of the most interesting techniques was video microscopy of the diffractometer used to show how the water was entering the dehydrated crystals.

**Craig Martin,**  
University of Glasgow



*G rard Coquerel, Roy Copley, Anne Kavanagh (Chair), Alan Kennedy*

## Ligand Binding and Drug Design

**THIS** symposium chaired by **Rod Hubbard** attracted so many contributions that it extended over two sessions. Rod was an active chairman, starting the session with a very helpful fifteen minute crash course in drug discovery methods and the procedures involved in getting a new drug from the lab to release. This was specifically aimed at those in the audience who were not up to speed with the background to the talks that were to follow.

Next, **Tom Davies** presented *Fragments, Structures and Drug Discovery*. He talked about fragment based drug discovery and its advantages over the more common high-throughput screening methods as well as explaining drug potency factors and illustrating how X-ray diffraction can be advantageously applied as a biophysical screening technique. He stressed the concept of ligand efficiency, whereby a small fragment with a moderate binding constant is more amenable to development than a much larger molecule that binds somewhat more strongly. He also introduced *Pyramid* as a tool for bringing together biophysical techniques (such as XRD) to assist in fragment based drug discovery.

To end the first session **Nicolas Foloppe** gave his talk: *Exploiting Crystal Structure for Ligand Discovery and Design*. The focus was on the drug discovery methods employed at Vernalis. This includes a reverse fragment based approach where inhibitors are deconstructed and used to increase the



quantity of drug candidates generated and also improve the overall quality of those candidates. He provided a good insight into part of Vernalis' drug design process. Examples from company experience were interesting in their own right and clarified how these methods are used.

After a break the lecture series resumed with *The Structure of a Chondroitin Sulphate A Binding Domain in Placental Malaria* by **Matthew Higgins**. It is well known that malaria is a deadly parasitic disease, causing around 500 million cases and 2 million deaths per year. What may be less appreciated is that malaria poses a particular threat in pregnancy because the parasites bind to the surface of the placenta and restrict blood flow to the foetus. Matthew reported the crystal structure of the domain of one of the parasite's adhesive proteins that binds to chondroitin sulphate A. This study gives insight into the molecular basis of this interaction and should provide guidance for antimalarial drug discovery.

Another frightening disease was addressed by **Chris Phillips** in *HIV-1 Reverse Transcriptase Structure-Based Drug Design*. About 40 million people are currently living with HIV. The disease can be held in check with combination treatment that includes a non-nucleoside reverse transcriptase inhibitor (NNRTI). Because of the danger of viral resistance, continued drug design in this area is important. Over 50 crystal structures of different NNRTI enzyme complexes have been determined, leading to conclusions about structure-activity relationships against wild type and mutant enzymes.

**Stephen Curry** concluded the stimulating and wide-ranging session with *Crystallographic Analysis of Metabolite and Drug Binding to Human Serum Albumin, a Pharmaceutical Trouble-Maker*. Whereas the previous speakers examined targets that were to be hit hard with drugs, human serum albumin (HSA) is a highly abundant target that should usually be missed. Due to its abundance and high binding capacity, HSA often captures a large fraction of administered drug doses, thus reducing their effective concentration. Only occasionally HSA binding is useful to smooth out the peaks and troughs of concentration. Stephen showed that specific molecular recognition and nonspecific matching of polarity are both important influences on drug- HSA binding.

**John Findlay**, University of Glasgow  
**Carl Schwalbe**



Matt Higgins, Rod Hubbard (chair), Tom Davies, Nicolas Foloeppe, Stephen Curry, Chris Phillips

## PDF Workshop, and Local Structure and Disorder in Crystalline Materials

**AN** excellent introduction to local structure was given in both the PDF (pair distribution function) workshop and the subsequent talks in the main conference. The PDF workshop, run by **Matt Tucker** from ISIS and **Thomas Proffen** from the Los Alamos National Laboratory helped by **Andrew Goodwin** from Cambridge, highlighted the information which can be obtained through diffuse scattering, present in all powder X-ray diffraction data. The long-range/average information normally gained from a powder XRD pattern through Rietveld refinement can be greatly complemented by the study of the diffuse scattering. Whilst two compounds may have a similar average structure, their local structure may be extremely different. Through total scattering experiments, the PDF profile may be obtained, which can be used across a range of powders from amorphous materials to disordered crystalline systems. Of particular interest was the ability of the PDF method to see dynamic disorder in crystalline systems

The first parallel session of the meeting dealt with understanding the imperfections in crystals. Chaired by **Matt Tucker**, the session started with a talk by **Thomas Proffen**. He introduced the topic of diffuse scattering – the underlying intensity in a diffraction pattern that arises from deviations from the perfect structure. Such deviations can be a result of vibrations or defects. He outlined the procedure for converting a powder neutron diffraction pattern into a PDF that reveals each interatomic distance in the system. As a result the short, medium and long range order of the system can be probed. Thomas outlined some of the requirements of getting a good PDF, which include a large Q range and good counting at high Q, the result being that neutron reactor sources aren't that suitable for the method. On the high resolution neutron powder diffractometer NPDF at Los Alamos, PDF's extending out to 20 nm can be determined. Thomas finished with some test cases including gold nanoparticles. Some of these are so small they can be totally characterised with the method.

The next speaker was **Sharon Ashbrook** from the University of St. Andrews. She is looking at disorder in solids using magic-angle-spinning NMR. The technique was introduced in the talk. It is quite powerful and can tell us a lot about the NMR active nuclei in the sample including different coordination environments and disorder. The MAS NMR technique was combined with theoretical NMR spectra determined using the NMR-CASTEP code. Sharon then gave some examples of her work including studies of a class of compounds called pyrochlores, which have a potential use in storage of radioactive materials. Using the NMR active nucleus  $^{89}\text{Y}$  the sites typically occupied by actinides can be studied. Here the data from

defects simulated in NMR-CASTEP were of particular use in validating aspects of the model. Disorder of  $^{45}\text{Sc}$  in perovskites was also discussed. It was impressive, then and later during the conference, to observe the growing interest among the crystallographic community for solid state NMR as a complementary method. Indeed, the technique was not only mentioned by an NMR expert like Sharon, but also by a significant number of speakers during the whole conference.

**Simon Hibble** from the University of Reading then gave a shorter talk returning to the theme of pair distribution functions. He discussed work on some transition metal cyanides such as MCN or  $\text{M}(\text{CN})_2$ . While the compounds might seem simple, the PDF technique was applied to understanding the negative thermal expansion in both types of compound. The PDF clearly show that this originates from buckling of the structure in one and two dimensions. He also showed the complementary nature of PDF with EXAFS. Both techniques determine the Ni–C and Ni–N distances (in  $\text{Ni}(\text{CN})_2$ ) to be the same.

The final speaker of the session was **Alex Hannon** from the ISIS facility. He also talked about PDF's, this time focussing on the interpretation of thermal motion. He started by outlining the origins of the peak within PDF analysis – resolution, thermal motion and disorder. In principle, Rietveld refinement should give us a handle on thermal motion. However, using thermal parameters from a Rietveld refinement to refine PDF's can often lead to a poor fit. Alex explained that this is due to the different way in which thermal motion is detailed in the two methods. PDF's give distances that take into account correlated motions of atoms – while Rietveld doesn't. Bond lengths from powder diffraction will often be shorter than PDF bonds as result. Three polymorphs of  $\text{GeO}_2$  were used to illustrate this point in a talk that highlighted some important aspects of crystallography.

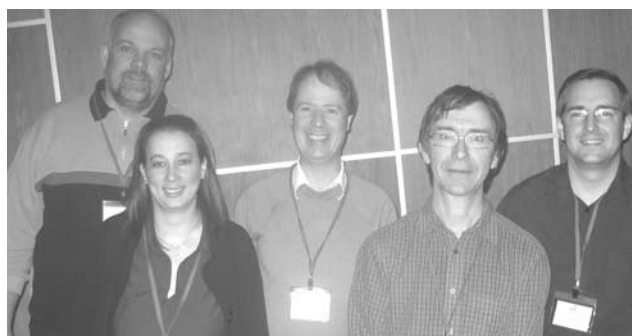
The session made a stimulating start to the parallel sessions of the meeting with some very good talks highlighting two powerful methods for studying disorder in a variety of materials.

**Anthony M. Reilly**, University of Edinburgh

**Julia Payne**, University of Durham

**Anne Soleilhavoup**, University of Durham

**Sarah Lister**, University of Durham



*Thomas Proffen, Sharon Ashbrook, Alex Hannon, Simon Hibble, Matt Tucker*

## Neutrons in Biology

**THIS** session chaired by **Garry McIntyre** (Institut Laue Langevin, ILL) provided a fascinating insight into the use of neutron scattering techniques in biology. Garry initially gave a brief introduction to the topic discussing how there are currently around 20 solved structures of proteins by neutron diffraction. He also gave a list of facilities currently available including LANL at Los Alamos, New Mexico, ISIS in the UK, ILL in France and the proposed facility MANDI at the new SNS (Spallation Neutron Source), USA.

The first speaker was **Matthew Blakeley** (ILL), who spoke about neutron protein crystallography at the ILL. Matthew explained why neutrons are useful as they can 'see' hydrogen atoms much more effectively than X-rays due to the large scattering length for hydrogen (and deuterium) which is comparable to that of carbon. Hydrogen atoms are of great importance in the determination of enzymatic mechanisms and as such neutron scattering provides a definitive method to access these details even at diffraction resolutions such as  $2\text{\AA}$ . The new neutron Laue diffractometer LADI-III is dedicated to high resolution ( $1.5\text{\AA}$ – $2.5\text{\AA}$ ) protein crystallography and has been operational since March 2007. LADI-III is a 'quasi Laue' diffractometer working in the range of  $2$ – $3\text{\AA}$  wavelength with a 5–25%  $\delta\lambda/\lambda$  bandpass. This somewhat restricted wavelength band avoids the increased background signal that would result from using the wider band of the full white beam but nevertheless represents a more efficient use of the emitted neutrons than a monochromatic beam. LADI-III also features a cylindrical detector which allows the instrument to cover a large area of reciprocal space, including full back scattering and thereby longer wavelengths which scatter more strongly than shorter wavelengths. Matthew's presentation highlighted the significant gains in performance over the previous instrument, LADI-I; the improvements in detector design and the readout system allowed a 2–3 fold gain in detection efficiency. It was explained that this has permitted data collection at higher resolution using both shorter exposure times and smaller crystals. These improvements were illustrated through various examples of recent projects including an anti-freeze protein crystal of  $0.13\text{ mm}^3$  which is significantly smaller than the typical sizes previously required for this instrument, and yet a resolution of  $2\text{\AA}$  has been achieved. The example of cytochrome c oxidase illustrated how freeze-trapping intermediates has allowed protonation states of key histidine residues to be determined.

The second speaker, **Lee Brammer** (University of Sheffield) described the proposed instrument LMX (Large Molecule Crystal Diffraction) at Target Station 2 at ISIS, UK. There is currently the shared SXD (Single Crystal Diffractometer) at ISIS working in the wavelength range of  $0.2$ – $1.0\text{\AA}$  with 11 area detectors. The proposed new instrument LMX will be dedicated to the study of larger unit cells (up to  $\sim 30,000\text{\AA}^3$ ) at high resolution (of the order  $1$ – $1.2\text{\AA}$ ) or very large unit cell

volumes at lower resolutions (e.g. proteins with 240,000 Å<sup>3</sup> unit cell volume at 2 Å resolution or 10<sup>6</sup> Å<sup>3</sup> unit cell volume at 2.5 Å resolution). The new instrument will incorporate a sample chamber capable of cryocooling to 5K with moderate pressure, detectors with 2 $\pi$  coverage and Time of Flight (TOF) Laue diffraction. Its brilliance improves on the already successful Protein Crystallography Station 'PCS' at Los Alamos. The TOF measurement technique allows the data to be measured in effect in 3D, i.e. position and time, and the full white beam to be used rather than 'quasi Laue'. This instrument will be based at Target Station 2, the new cold neutron source at ISIS which generated its first neutrons in December 2007, offering higher flux and a 10Hz pulse rate. LMX is proposed for phase 2 of the upgrade program which will take place between 2009 and 2012. Lee explained that the science areas of interest for this instrument will be the study of large scale chemical systems and biological macromolecules. This will permit data collection on high molecular weight biological structures including multi-molecular complexes and molecular machines as well as pharmaceutical applications of ligand-protein interactions.

Moving from instrumentation to sample preparation, the third speaker **Susana Teixeira** (Keele University) discussed the Deuteration Laboratory at the Grenoble Partnership for Structural Biology. The Deuteration Laboratory was set up in 2003 as a collaboration between the ILL and the Grenoble EMBL outstation. It moved into the Partnership for Structural Biology in 2006 and has a thriving user programme accessible through a peer review process. Susana explained that because deuterium produces a stronger signal than hydrogen when using neutron scattering while reducing incoherent background scattering, deuterium labelling of samples is a powerful tool. It improves the sensitivity of crystallography experiments and lowers the background noise. Visibility is enhanced, and smaller crystals can therefore be used. Biological samples can be fully deuterated via expression in deuterated medium, normally using *E. coli* (although other expression systems are also available). Selective labelling of amino acids or nucleotides can also be carried out to highlight specific parts of a system.

This was followed by **John Helliwell** (University of Manchester), who detailed the main methods available for the determination of protonation states in proteins. Biology rests on chemical reactions, which in turn involve hydrogen atoms or protons; however determination of their positions is challenging for protein crystallography. John first described the use of bond length analysis in Asp and Glu residues using high resolution X-ray data (better than 1.3Å). The protonation state of a residue is determined by comparison of carboxyl group bond distances with expected C=O and C-OH bond lengths, taking into account the associated errors determined from a full matrix refinement inversion. John also discussed the use of neutron diffraction and perdeuterated proteins in order to determine the protonation states of histidine residues where a hydrogen (as deuterium) atom can be located at

a resolution as low as 3Å. The Cruikshank DPI (diffraction-component precision index) parameter was also discussed and its use for estimating the average standard error and hence diffraction resolution required in order to positively infer protonation from X-ray data using bond lengths. Finally John briefly discussed the use of pKa prediction tools for the determination of protonation states of ionisable groups and the scrutiny of such programs using structures with known protonation states determined from neutron data.

The final speaker of the session was **Stephen Prince** (University of Manchester), who provided an insight into crystallography of membrane proteins with contrast matching at low resolution by using the ILL diffractometer DB21. He discussed the use of contrast matching in order to render specific parts of the molecule of interest (the protein, DNA, RNA or detergent for example) invisible by using a buffer containing the appropriate percentage of D<sub>2</sub>O. Referring to work on the peripheral light harvesting complex of the purple bacterium *Rhodospseudomonas acidophila*, Stephen illustrated how map fitting combinations of contrast matching neutron data to about 13Å resolution collected on DB21 and X-ray data collected to 2.0Å have allowed the determination of the volume of the crystal occupied by detergent and the detergent location within the crystal lattice.

The question time was reserved until after all the speakers. Questions ranged over topics such as the approximation of initially ignoring the hydrogen atoms on the ionisable side chains and on the timetable for the new instruments (including those in Japan, the UK and the USA). Reference was made to the poster session which included an assessment of the risk of structural changes due to protein deuteration, namely that significant differences were seen in a recent CSD survey but that the differences were small and indeed below the usual level of bond distance and angle determination of protein crystallography. Cases however of resonance structures that would be affected by the heavier, i.e. deuterium, isotope would form a point of risk; clearly a combined X-ray and neutron structural analysis would be the most powerful in such circumstances. There were also benefits in all studies of a combined X-ray and neutron approach to maximise diffraction data-to-parameter ratios, and software was now available in PHENIX and nCNS to undertake such joint protein model refinements.

**Stuart Fisher**, Institut Laue Langevin, France and School of Chemistry, University of Manchester

**Shona Gillespie**, EPSAM, Keele University



Matthew Blakeley, Garry McIntyre, Lee Brammer, Stephen Prince, Susana Teixeira, John Helliwell

## Structures From Pharmaceutical Powders

**CHAired** by **Kenneth Shankland**, this session featured three speakers who covered the range from technical advances to industrial uses with lots of interesting results in between.

The first speaker was **Alastair Florence** from the University of Strathclyde who, under the title *Challenges and Opportunities for Structure Determination from Laboratory Data in Physical Form Discovery*, gave an enthusiastic presentation on some of his findings as part of the CPOSS (Control & Prediction of the Organic Solid State) project. Alastair began by introducing the experimental approach to structure determination using powder data (SDPD) and the difficulties and benefits which it brings. He moved on to talking about carbamazepine (CBZ) and the search for a catemeric form of carbamazepine which has been predicted but never produced despite the numerous investigations which have been carried out on CBZ. He then discussed the search for polymorphs in three analogues of CBZ which differ by small chemical changes such as swapping C for N or changing a double bond to a single bond: 10,11-dihydroxycarbamazepine (DHC), Cyheptamide (CYH) and Cytenamide (CYT). DHC only forms catemers. Since the only difference between DHC and CBZ is the absence of a double bond, this may offer further support for the existence of a catemeric form of carbamazepine. Importantly, CYH has both a catemeric polymorph and a dimeric polymorph, and the two structures show common features. Alastair finished off with a few tips for successful structure solution from powder diffraction. This talk was of great interest as it highlights links between computational studies and lab work through to identifying and solving new forms via XRPD using several structure determination programs.

The second speaker was **Vincent Favre-Nicolin** from the Institut Nanosciences and Cryogenie and Universite Joseph Fourier (Grenoble) whose talk was entitled *Solving Structures Using Fox and Flexible Modelling*. Vincent is involved in the development of programs suitable for structure determination from powder diffraction (SDPD). After a brief history of SDPD he discussed direct space methods and some of the advantages which have led to an increase in their popularity, including the advantage of making use of a *priori* structural knowledge. Moving on to the Fox program, we heard how it has been developed to deal with more flexible molecules with numerous degrees of freedom. This is of course a highly important development, and it is very important that structure determinations can be carried out quickly. To ensure this a GRID network has been set up using the computing power of over 400000 computers, enabling up to 56 free torsion angles to be used in SDPD. Interestingly, he showed how having too many restraints for a structure solution can sometimes be unhelpful. He also demonstrated that using high resolution

data, though essential for Rietveld refinement, can greatly slow down structure solution from powder diffraction data. Despite the obvious advantage of significantly reducing the number of parameters, the use of Z-matrices does have a few drawbacks; however we also heard methods of overcoming these problems, in particular the use of flexible restraints. Vincent showed some of the program's functionality using cimetidine as a test case. He rounded out his talk with a discussion on how to resolve problems which may be faced such as a wrong model, preferred orientation issues or the program running too slowly. All of the material discussed was illustrated with a wide range of examples including a polymer.

The final speaker was **Matthew Johnson** from GSK who spoke about *A Pharmaceutical Industry Perspective of SDPD*. Matthew first took us through the drug development process (discovery to development to manufacture to market) highlighting the stages of the process where the solid state form is of importance. He also went through a list of required information about the solid form and whether powder diffraction can provide this information or if a single crystal is required. The final part of his talk revolved around indexing which is a key technique in the early stages of drug development. It allows for salt and polymorph screening and can be used to identify extraneous peaks in diffraction patterns which may suggest the presence of polymorphs or impurities. Matthew also discussed how data collected from other analytical techniques along the development process, such as solid state NMR, TGA and DSC, can be incorporated into model building for structure solution. Such factors such as potential H-bonding, solvation state, molecular connectivity and Z' value can all be of huge benefit when trying to solve structures from powders. This was an interesting insight into the differences in scale between university and industrial powder diffraction through the sheer amount of data that is produced by big companies on a daily basis. This talk brought a thoroughly enjoyable session to a close.

**Laura Budd**, University of Edinburgh  
**Gordon Cunningham**, University of Glasgow  
**Guillermo Mínguez**, University of Sheffield  
**Andrew O'Neill**, University of Glasgow



Matthew Johnson, Alastair Florence, Vincent Favre-Nicolin, Kenneth Shankland (chair)

## Small Is Smart

**WITH** the promise of topics bearing the trendy prefix nano-, this session, chaired by **David Beveridge**, was sure to attract interest. The information provided by X-ray powder diffraction can be of great value in developing the industrial potential of these novel materials. However, a technical challenge arises from the broadening of reflections as the crystallite size decreases.

**Steve Norval** (Intertek MSG) in *Powder Diffraction of Nanomaterials* surveyed the established and emerging uses of nanopowders, nanocolloids, nano-oxides and nano-metals. He discussed techniques applicable to such materials for phase identification, quantification, study of microstructure, in situ monitoring, etc., and predicted an important future for powder diffraction.

**Chris Staddon** (University of Nottingham) was the spokesman for a cross-E.U. collaboration also involving the Charles University in Prague on *X-Ray In-Plane Scattering of GaN Nano-Rods*. Gallium nitride based semiconductors are gaining in technological importance, but the numerous defects frequently present limit their usefulness. However, GaN nano-rods are generally defect free. While it is relatively straightforward to determine the correlation length of the nano-rods along their growth axis, it is difficult to determine the mean in-plane lateral dimensions. Previous X-ray studies have required synchrotron radiation. However, Chris

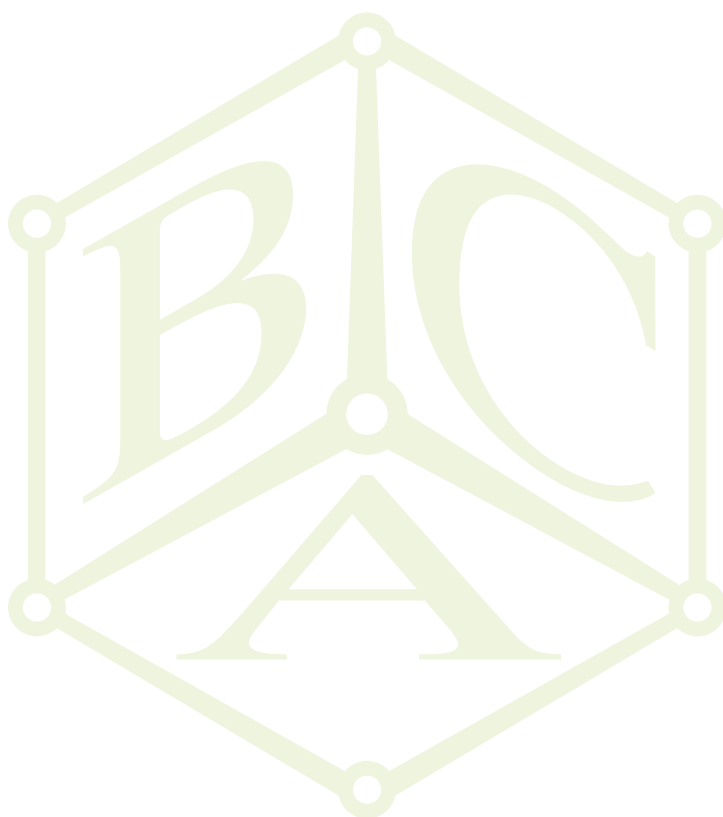
reported success in using home laboratory equipment. The technique relies on comparison of simulations and experimental data.

**Chris Gilmore** (University of Glasgow) described *Solving Crystal Structures of Zeolites Using Powder Diffraction and Electron Crystallography*. Zeolite structures frequently are difficult to solve because of poor crystallinity and small crystallite size. Powder patterns are plagued by peak broadening, and electron diffraction studies also suffer from problems. Chris reported new techniques for solving structures *ab initio* from both electron diffraction and powder data, using density building functions and density histogram matching methods along with entropy maximization and likelihood analysis.

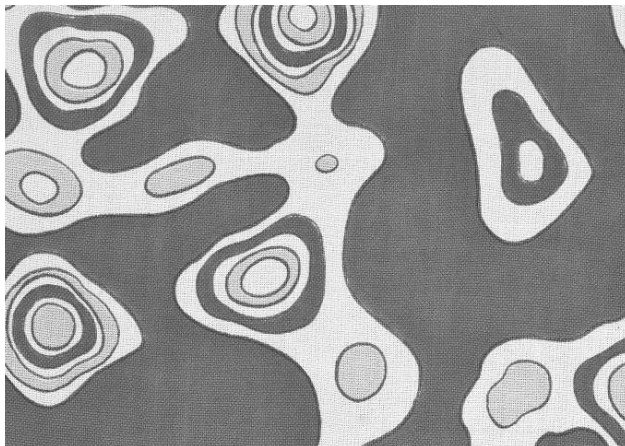
### Carl Schwalbe



David Beveridge (chair), Steve Norval, Chris Gilmore, Chris Staddon



# From Atoms to Patterns



*Afwillite, studied by Helen Megaw V&A Images/Victoria and Albert Museum, London*

## From Atoms to Patterns Exhibition Opens

**AS** described in the last issue of *Crystallography News*, this exhibition at the Wellcome Collection of crystal structure designs from the 1951 Festival of Britain will run until 10 August. The online version [www.wellcomecollection.org](http://www.wellcomecollection.org) provides a variety of interesting information. The show was officially opened on 23 April with a short speech by the BCA's own **Mike Glazer**. Fulfilling the Curator's intention to expose the beauty of crystal structures to a wide audience, the approximately 200 invited guests included members of the press, museum people and design artists.

In the abridged extracts reproduced below from the book by **Lesley Jackson**, the Curator, it becomes evident that **Helen Megaw**, the originator of the idea, was perceived to be taking a professional risk by venturing out of academia and associating with trade and commerce. Many of the crystallographers who supplied her with images remained anonymous. However, their pride was evident in their choice of textiles, such as **Alice Bragg's** beryl lace and **Gisela Perutz's** methaemoglobin print dress. Thus there are excellent precedents encouraging you to wear your BCA tie with pride!

"On 20 February 1946 Dr. **Helen Megaw** came up with an intriguing proposition: 'I should like to ask designers of wallpapers and fabrics to look at the patterns made available by X-ray crystallography. I am constantly being impressed by the beauty of the designs which crop up... without any attempt of the worker to secure anything more than clarity and accuracy... I think the combination of really

attractive pattern with the assurance of scientific accuracy would win a lot of attention.'<sup>1</sup>

"In May 1949 Professor **Kathleen Lonsdale** from University College, London used some of Megaw's slides of crystal structures to illustrate a lecture about crystallography to the Society of Industrial Artists. **Mark Hartland Thomas**, Chief Industrial Officer from the Council of Industrial Design, was in the audience. He immediately realised the potential of this material and wrote to Megaw offering to place her patterns with manufacturers. Shortly afterwards he came up with the idea of a special design project linked to the forthcoming Festival of Britain in 1951. The Festival was intended as a platform for British ingenuity and creativity in science, technology and the arts, so a project combining all three seemed ideal, he believed: 'My idea is to make a small group consisting of a manufacturer of each of the following, namely: dress textiles, furnishing textiles, carpets, pottery, linoleum and wallpaper, with a view showing goods in these categories decorated with crystallographic patterns.'<sup>2</sup>

"Although from different professional spheres, **Mark Hartland Thomas** and **Helen Megaw** made a highly effective team; he respected her expertise as a scientist and ensured that her high-minded aspirations for the project remained sacrosanct; she trusted in his ability to find sympathetic manufacturers and, literally, to deliver the goods. In the end, 28 firms participated in the Festival Pattern Group, producing a total of 80 designs. Crystal structure furnishings provided the main décor in the Regatta Restaurant on the South Bank and were also displayed in the Dome of Discovery. They also featured prominently in the Exhibition of Science at the Science Museum, as well as forming a part of the Land Travelling Exhibition.

"As Adviser on Crystal Structure Diagrams, **Helen Megaw** selected all the scientific material used by the Festival Pattern Group and liaised directly with other crystallographers. This explains why, in addition to her own contributions, so much of the material was supplied by her colleagues at the Cavendish Laboratory (Bragg, Taylor, Perutz, Kendrew and a research student called June Broomhead), partly because they were doing such interesting work, but also because they were on the spot. Other diagrams were sourced from crystallographers Megaw already knew well, or well enough to approach, mostly at other universities (her old friend **Dorothy Hodgkin** at Oxford, Professor **Gordon Cox** and Dr. **G.W. Brindley** at Leeds, Professor **John Monteath Robertson** at Glasgow), but also in industry (Charles **William Bunn** and **Myra Bailey** at ICI). With hindsight Megaw's choice of crystallographers reveals amazing astuteness and



*Souvenir Book of Crystal Designs, Published by HM Stationery Office for the Council of Industrial Design, 1951*

prescience, including three scientists who would go on to win the Nobel Prize: **Max Perutz** and **John Kendrew** in 1962, **Dorothy Hodgkin** in 1964. All three were working in the field of proteins,

the newest and most difficult and elusive area of crystallographic research.

“All the crystallographers were sworn to secrecy, and in fact, apart from Megaw, whose role was openly acknowledged in subsequent publicity, their names were deliberately withheld at the time. The reason for this appears to have been concern (presumably on Megaw’s part) to protect their scientific reputations, in particular the perceived need to separate their serious academic research from the appealing, but obviously more light-hearted, interpretations of their diagrams by the Festival Pattern Group.

“The response from crystallographers was overwhelmingly positive. Megaw reported a few days after the Festival opened that she was ‘besieged by inquiries from colleagues and acquaintances to know what is... being made, where it can be had, and at what price.’<sup>13</sup> **Lawrence Bragg** wrote to **Hartland Thomas** to say how thrilled he was with the results: ‘When in 1922 I worked out the first crystal of any complexity that had been analysed, aragonite, I remember well how excited my wife was with the pattern I showed her as a motif for a piece of embroidery. Ever since then, especially when I was in Manchester, I have been urging industrial friends to use these patterns as a source of inspiration, and I was delighted when Miss Megaw... told me some two years ago that she had aroused your interest. The patterns she showed me yesterday are the practical realization of what we have long wished to see.’<sup>14</sup>

“Bragg’s pride is underlined by the fact that at the International Congress of Crystallography in Stockholm (27 June - 3 July 1951) his wife, Lady **Alice Bragg**, wore a spectacular evening dress made of Beryl lace, one of her husband’s crystal structures. **Max Perutz** (himself the son of a textile manufacturer) was evidently approving as well. His wife, **Gisela Perutz**, wore a printed rayon dress featuring his diagram horse methaemoglobin at the conference, while **Helen Megaw** sported a blouse made of crepe silk based on one of her structures of atwillite. ‘A lot of the men from Cambridge have been wearing the ties,’ she reported to **Hartland Thomas**; ‘also someone had sent a tie with a Patterson diagram of insulin to Dr Patterson, the American inventor of that type of diagram, and he is wearing it with pleasure.’<sup>15</sup>

“After all their hard work in bringing the project to fruition, it must have been gratifying to the two chief protagonists, **Mark Hartland Thomas** and **Helen Megaw**, to receive such enthusiastic feedback. **Hartland Thomas** observed at the time: ‘Though the chief idea of the Festival Pattern Group was to get leading manufacturers together on a design project and though we were careful to stress that the crystal structure diagrams could not be a ready-made short cut to good design, I always felt that there was more to it than that - if only to add an emotional apprehension to the intellectual study of scientific patterns. / I had not quite realised that the crystallographers’ delight in their patterns expressed an interest in their form that had an importance in scientific understanding.’<sup>16</sup>

- <sup>1</sup> Letter from Helen Megaw to J.R.M. Brumwell, 20/2/1946 (V&A Archive of Art Design 1977/3/12).
- <sup>2</sup> Letter from Mark Hartland Thomas to Helen Megaw, 20/6/1949 (AAD 1977/3/33).
- <sup>3</sup> Letter from Helen Megaw to W. Haigh, Dobroyd, 12/5/1951 (AAD 1977/3/208).
- <sup>4</sup> Letter from Sir Lawrence Bragg to MHT, 11/5/1951 (Design Council Archives, University of Brighton 5384-4).
- <sup>5</sup> Letter from Helen Megaw to Mark Hartland Thomas, 4/7/1951 (DCA 5384-4).
- <sup>6</sup> Letter from Mark Hartland Thomas to J.R.M. Brumwell, 19/7/1951 (DCA 5384-4).

**Lesley Jackson is the Curator of *From Atoms to Patterns - Crystal Structure Designs from the 1951 Festival of Britain* at the Wellcome Collection, 183 Euston Road, London, 24 April - 10 August 2008.**

This article is an edited version of a longer essay called ‘The Story of the Festival Pattern Group’ in the accompanying book: ***From Atoms to Patterns - Crystal Structure Designs from the 1951 Festival of Britain*** by Lesley Jackson, published by Richard Dennis Publications (ISBN 978 0 9553741 1 1). The book includes illustrations of all the designs produced by the Festival Pattern Group and ***An A-Z of Crystal Structures*** documenting the scientific sources of all the designs. Copies, priced at £20, can be ordered from: [books@richarddennispublications.com](mailto:books@richarddennispublications.com)



Wellcome Library, London

# The Bank's Sub-prime Assets

## Repairing the Bank's Sub-prime Assets

**IN** mid-April as I write this, hardly a news broadcast goes by without a gloomy report about the crisis in sub-prime mortgages and its effect on the banks. We crystallographers have a bank, too, the Protein Data Bank; and it too has some sub-prime assets. In most cases the problem is no worse than some peeling paint and a few squeaky floorboards, but in one recent case [for a discussion of its significance see G. Miller (2006) *Science*, 314, 1856-1857] whole houses were built back to front!

As a small-molecule crystallographer I have the benefit of validation by CheckCIF. My usual first reaction to the comments that come back is to feel insulted; but after calming down and making the recommended changes, I produce a much improved paper. Macromolecular crystallography provides more scope for creativity, and therefore also for making mistakes. An important microsposium at the 2007 European Crystallographic Meeting in Marrakech dealt with the topic of structure validation and quality control. This session covered the range from getting the sequence right and eliminating some sources of error in data collection to determining the protonation state and applying the most suitable refinement

restraints. These technical advances should improve the reliability of future macromolecular structure determinations. Of course they can do nothing about dodgy structures already in the bank. Fortunately, the existing structures are the subject of the worldwide Protein Data Bank remediation project. For what I suspect is a small fraction of the salary that a forensic accountant would charge for sifting through a bank's financial assets, these researchers have gone through the archive [K. Henrick et al. (2008) *Nucleic Acids Research*, 36, D426-D433]. The remediation group did not have the temerity to tinker with the coordinates since it would have been all too easy to replace obvious errors with subtle bias, but the changes they have made are important. A Chemical Component Dictionary has been defined and applied to atom names, atom types, residue names and residue assignments for all monomer units and small-molecule ligands. Inconsistencies between the chemical and coordinate sequences have been resolved. The capability of representing viruses has been enhanced. Citations, especially the infuriating "To be published", have been brought up to date. Typographical errors and parsing errors have been corrected as much as possible. The improvements should be of benefit to all of us who examine and compare macromolecules with the aim of discerning structural regularities or designing ligands.

**Carl Schwalbe**

## Puzzle Corner... ...MARCH ANSWER

**THE** unencrypted text occurs in the March 2008 issue on page 26 in column 1 and consists of the paragraph:

*Everyday products decorated with patterns based on crystal structures are the subject of this innovative show, which brings together an eclectic array of textiles, wallpapers, fashion, furniture, laminates, carpets and tableware. Drawings of atomic structures will sit alongside the designs they inspired reflecting the unique collaboration between Britain's leading post-war scientists and manufacturers.*

There were several correct answers with good comments. We liked Jim Trotter's: "I cheated a little, by simply looking quickly through the whole issue for a paragraph of about the right length, starting with an 8-letter word, in which the first and third letters were the same - and quickly found it on page 26. Worse, I have to admit, I did not even type out the answer, but just read it in on my scanner, with an OCR program!

But this month's winners are Simon and Ricky Hibble, whose letter follows:

Rather than using brute force methods we used a mixture of inspiration and "collaboration" to solve this problem on our Easter holiday. We discussed various strategies including brute force matching of word lengths, use of letter frequencies and started working on the two and three letter words. I convinced my son (Ricky, 12 that day) that we might try more elegant and inspired methods such as guessing what one of the longer words could be. We were disappointed not to find "diffraction" or "crystallography" but our "collaboration" rapidly led to discovering this word encrypted as "gpddrzpvruiapi" and a rapid solution.

Puzzles are clearly an excellent way of attracting younger readers. Ricky has just started studying symmetry at school and the carpet patterns provide a talking point.

**Simon and Ricky Hibble**

University of Reading  
and Magdalen College School



# News from the Groups

## News from the Groups



### CCG AUTUMN MEETING 2008:

*"New Methods in Chemical Crystallography"*

Sponsored by **Oxford Diffraction**

Wednesday 12 November 11.00 - 17.00,  
Newcastle University

This meeting will feature a range of speakers presenting current research in X-ray crystallographic techniques. The topics include: application of charge-flipping solution methods to modulated crystal structure data; parametric diffraction studies; combining X-ray structural data and computational chemistry; and modelling diffuse X-ray

scattering from disordered materials. Confirmed speakers include:

**Dr Trixie Wagner** (Novartis Pharma AG, Switzerland)

*"Advancing into higher dimensions - a practical approach to modulated structures"*

**Dr Lynne Thomas** (University of Glasgow)

*"Bragg scattering and beyond... Getting more from diffraction patterns"*

**Dr Natalie Fey** (University of Bristol) *"Building knowledge bases from structural data"*

## 2008 Kyoto IUCr Crystallographic Computing School - Sharing our knowledge

### KYOTO CRYSTALLOGRAPHIC Computing School

Kansai Seminar House, Kyoto, Japan

Monday 18th - Saturday 23rd August 2008

(just prior to the Osaka IUCr 2008 congress)

[www.iucr.org/iucr-top/comm/ccom/kyoto2008/](http://www.iucr.org/iucr-top/comm/ccom/kyoto2008/)

Organisers: **Prof Anthony Spek** (Utrecht), Prof. **Min Yao** (Sapporo), Dr **Ralf Grosse-Kunstleve** (Berkeley), Dr **Harry Powell** (Cambridge), Prof. **Atsushi Nakagawa** (Osaka),

**Lachlan Cranswick** (Chalk River)

Speakers have been drawn from across the crystallographic computing community, covering both powder and single crystal methods, from minerals through small molecules to proteins and macromolecular assemblies. They include **Ralf Grosse-Kunstleve** (LBNL, Berkeley), **Rob Hoof** (Bruker AXS, Delft), **Garib Murshudov** (YSBL, York), **Gábor Oszlányi** (Hungarian Academy of Sciences, Budapest), **Tom Terwilliger** (LANL, Los Alamos), **Brian Toby** (APS, Argonne) and **David Watkin** (Chemical Crystallography, Oxford), among others.

### INTRODUCTION:

During the first conference on crystallographic computing held at the Pennsylvania State College, USA in 1950, **Ray Pepinsky** noted that solving the major computing problems would 'require many minds. Our aim here is to share what we know - to cross-pollinate our minds.'

### SCHOOL AIMS:

To have the crystallographic computing experts of the present, help train and inspire a generation of experts for the future. This will be achieved by the use of an excellent (and full) program of lectures and tutorials. Speakers are listed at: <http://www.iucr.org/iucr-top/comm/ccom/kyoto2008/speakers.html>

### THE VENUE

The 2008 Crystallographic Computing School will be held at the Kansai Seminar House in Kyoto. Kyoto is the cultural center of Japan with its long history. The modern city treasures its heritage with its 1600 Buddhist temples, 400 Shinto shrines, and its exquisite gardens. Kyoto is also a center of Japanese tradition.

The Kansai Seminar House was originally derived from a movement initiated in Germany by the Christian Churches soon after World War II. The influence reached Japan in the 1960's and the Kansai Seminar House was founded in Shugakuin, Kyoto in 1967. Contributions came from the Christian Academy Movement of Germany, churches affiliated with NCC-USA, and Japan.

<http://www.iucr.org/iucr-top/comm/ccom/kyoto2008/venue.html>

### COSTS (AND ACCOMODATION)

We hope, pending completion of sponsorship contributions, that we may be able to keep the entire costs for participants (including accommodation and meals) below the equivalent of 500 Euros.

<http://www.iucr.org/iucr-top/comm/ccom/kyoto2008/registration.html>

**Existing sponsors are listed on the webpage and currently include:**

IUCr2008 Osaka and International Union of Crystallography (IUCr)

<http://www.iucr2008.jp/>

Bruker AXS <http://www.bruker-axs.de/>

Cambridge Crystallographic Data Centre: <http://www.ccdc.cam.ac.uk/>

CCP4 <http://www.ccp4.ac.uk/>

Hampton Research: <http://www.hamptonresearch.com/>

Infocom <http://www.infocom.co.jp/bio/>

Oxford Diffraction <http://www.oxford-diffraction.com/>

Phenix <http://www.phenix-online.org/>

Rigaku: <http://www.rigaku.com/>

SJI Japan Ltd <http://www.sji.co.jp/>

# Meetings of interest

**FURTHER** information may be obtained from the meetings website. 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](mailto:cockcroft@img.cryst.bbk.ac.uk) or to the Editor. The help of Dr Simon Parsons and the IUCr listing is gratefully acknowledged.

## June 2008

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- 5th European Charge Density Meeting (ECDM5) - Gravedona, Italy, 6-11 June 2008.
- IWPCPS-10 - 10th International Workshop on Physical Characterization of Pharmaceutical Solids. Bamberg, Germany. 8-13 June 2008.
- ISSRNS 2008 - 9th International School and Symposium on Synchrotron Radiation in Natural Science. Ameliowka, Poland. 15-20 June 2008.
- SNBL Workshop - Simultaneous Raman-X-ray diffraction/absorption studies. ESRF, Grenoble, France. 18-19 June 2008 .
- International Summer School - Structure Determination from Powder Diffraction Data. Paul Scherrer Institut, Villigen, Switzerland. 18-22 June 2008.
- Protein Crystallography Europe Amsterdam, Netherlands. 19-20 June 2008.
- 17th Slovenian-Croatian Crystallographic Meeting Ptuj, Slovenia. 19-22 June 2008.
- Protein Crystallography Europe Amsterdam, Netherlands. 19-20 June 2008.
- 21st International Conference on X-ray and Inner-Shell Processes Paris, France. 22-27 June 2008.
- The Zurich School of Crystallography 2008 University of Zurich, Switzerland, 22 June - 5 July 2008.
- 2nd Midnight Sun Meeting on Drug Transport & Delivery Tromsø, Norway. 25-27 June 2008.
- Colloque de l'Association Française de Cristallographie - Rennes, France, 7-10 July 2008.
- Gordon Research Conference: Diffraction Methods in Structural Biology , Lewiston ME USA. 13-18 July 2008.
- XRM2008 9th International Conference on X-ray Microscopy. ETH Zurich, Switzerland. 21-26 July 2008.
- SRMS-6 - 6th International Conference on Synchrotron Radiation in Materials Science. Campinas, Brazil. 20-23 July 2008.
- 5th LANSCE Neutron School - Magnetism in bulk and Nanostructured Materials. Los Alamos National Laboratory, Los Alamos, New Mexico, USA. 23 July-1 August 2008.

## August 2008

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- Summer School on Applications of Synchrotron Radiation Techniques in Earth and Environmental Science Oxford, UK. 12th-15th August 2008.
- 7th PSI Summer School "Probing the Nanometer Scale with Neutrons, Photons and Muons" Zuz, Switzerland. 16-22 August 2008.
- Kyoto Crystallographic Computing School Kyoto, Japan. 18-23 August 2008.
- 21st Congress of the International Union of Crystallography 2008. Osaka, Japan. 23-31 August 2008.
- ECTP2008:18th European Conference on Thermophysical Properties. Pau, France. 31 August - 4 September 2008.

## July 2008

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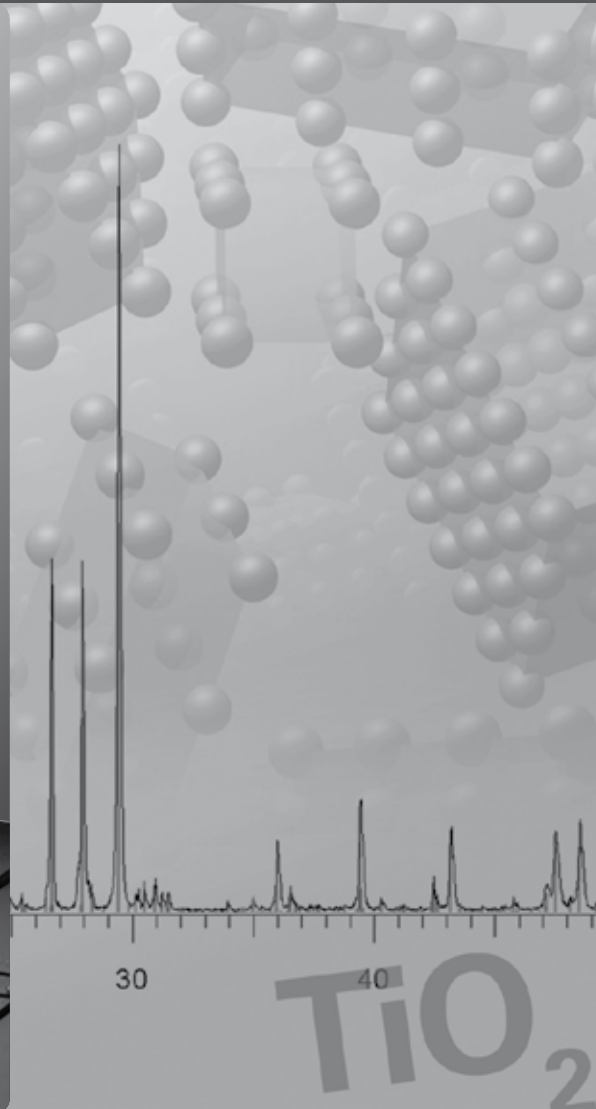
- Surface X-ray and Neutron Scattering, SXNS10 Paris, France. 2-5 July 2008.
- ICQ10 - 10th International Conference on Quasicrystals. Zurich, Switzerland. 6-11 July 2008.

## September 2008

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- 7th International Workshop on Polarised Neutrons in Condensed Matter Investigations - Tokai, Japan, 1-5 September 2008.
- 12th JCMS Laboratory Course - Neutron Scattering Jülich/Garching, Germany. 1-12 September 2008.





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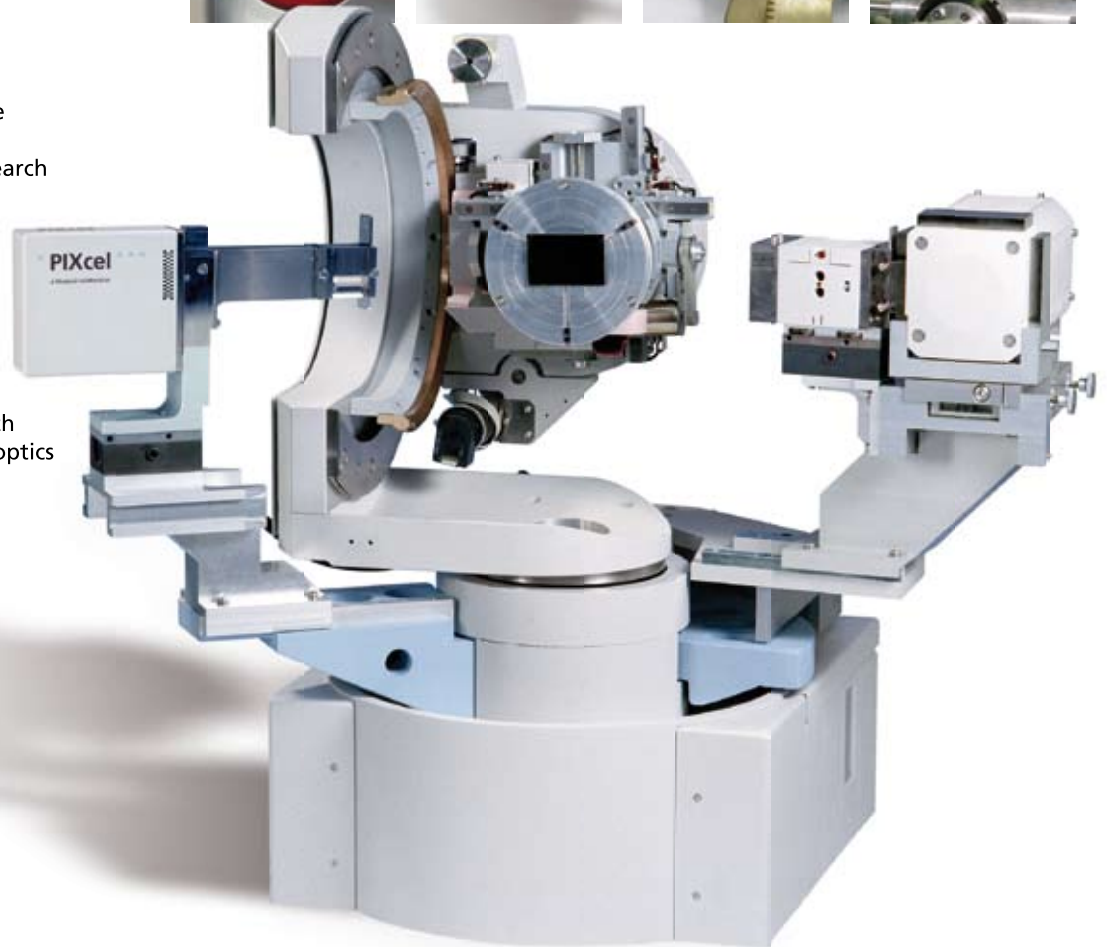


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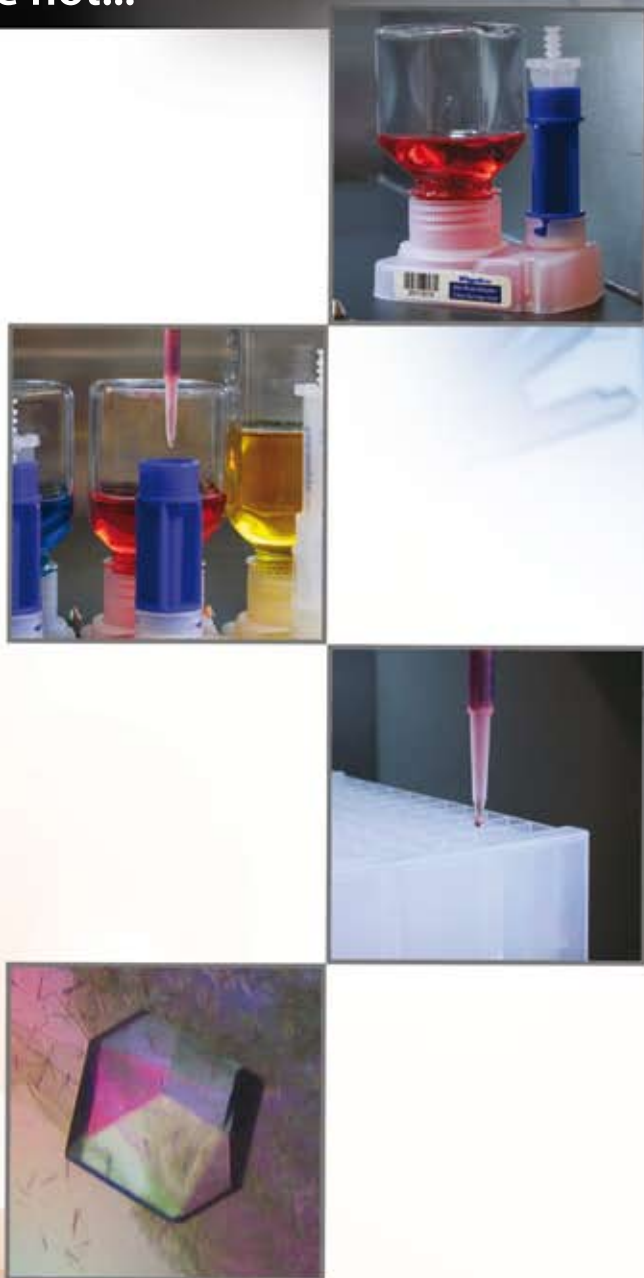
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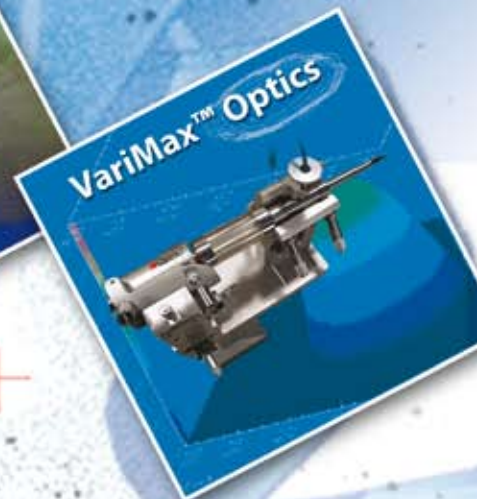
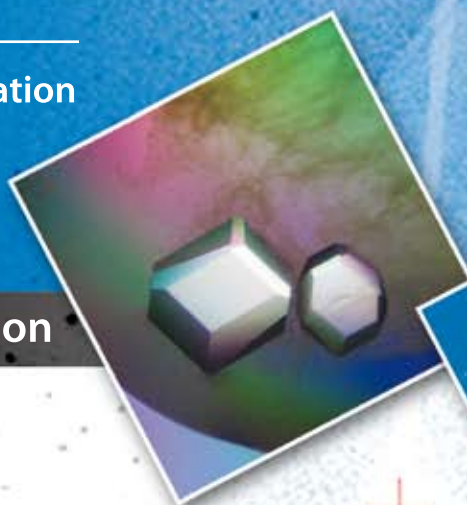


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