Crystallography News

British Crystallographic Association

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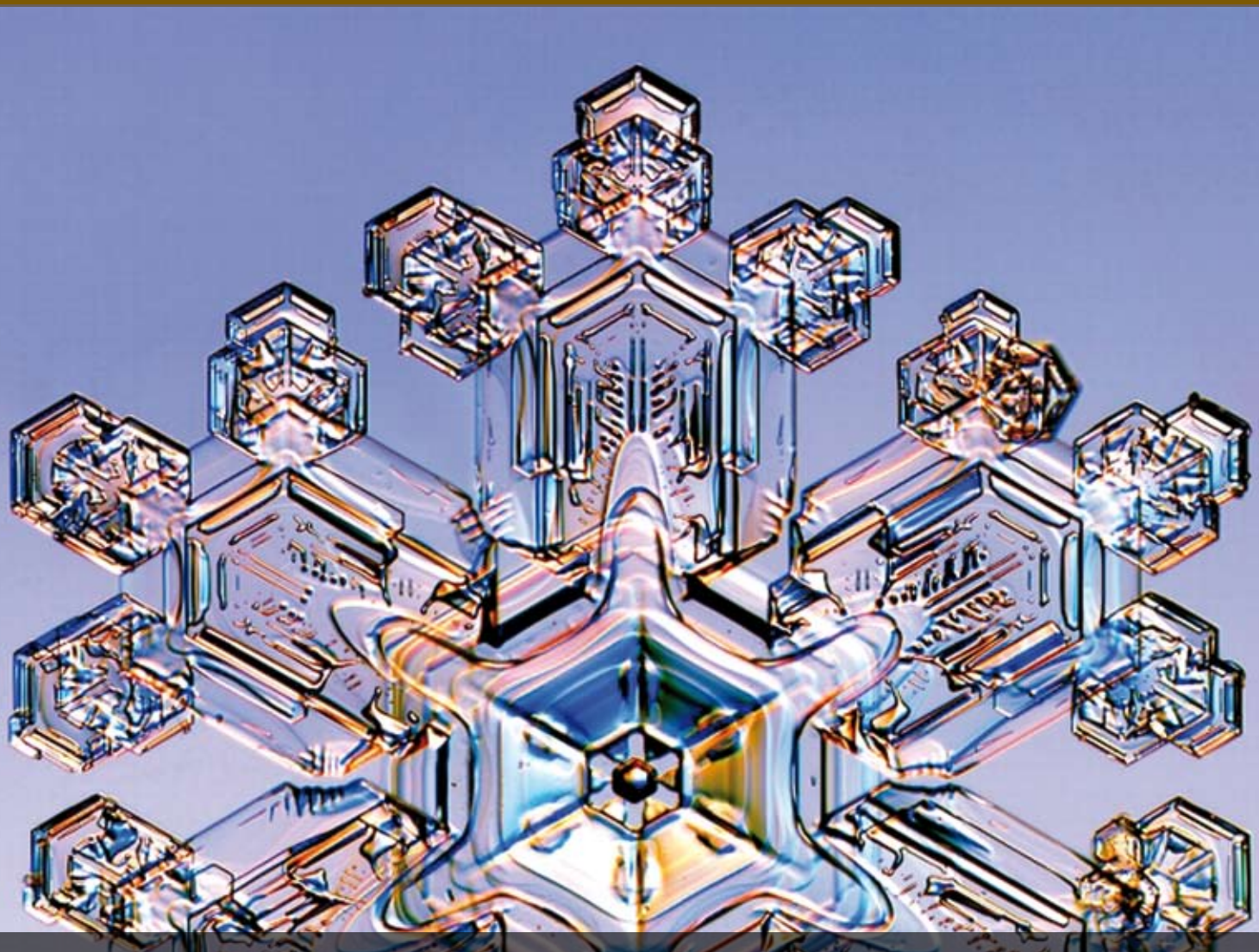

Loughborough 2009 p7-14

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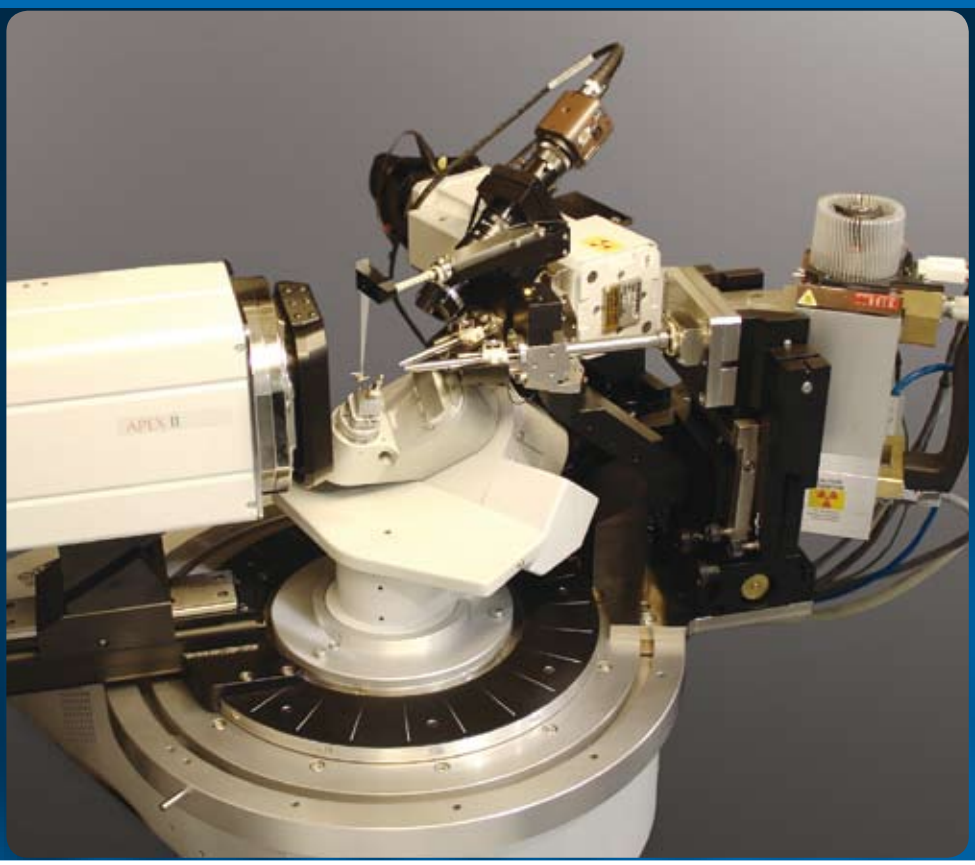

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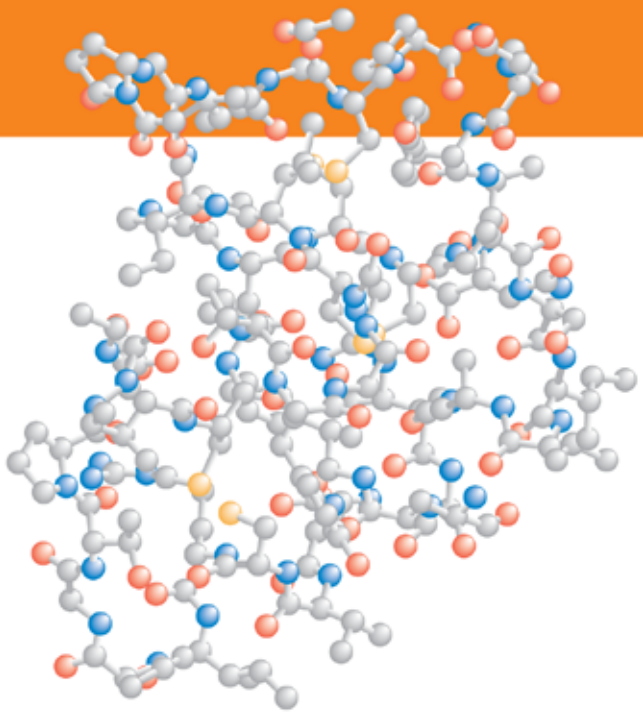

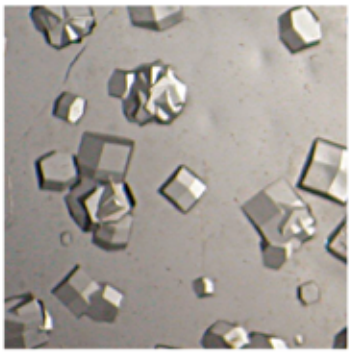

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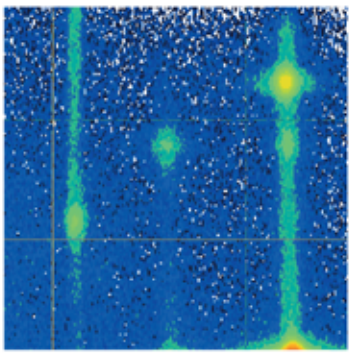

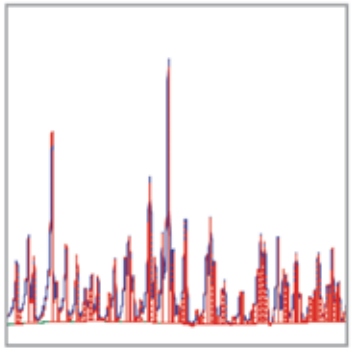

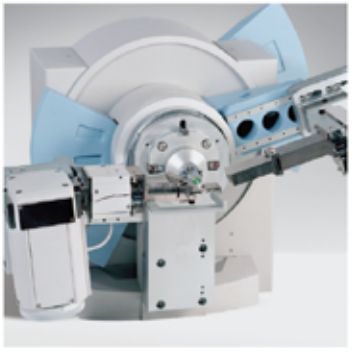

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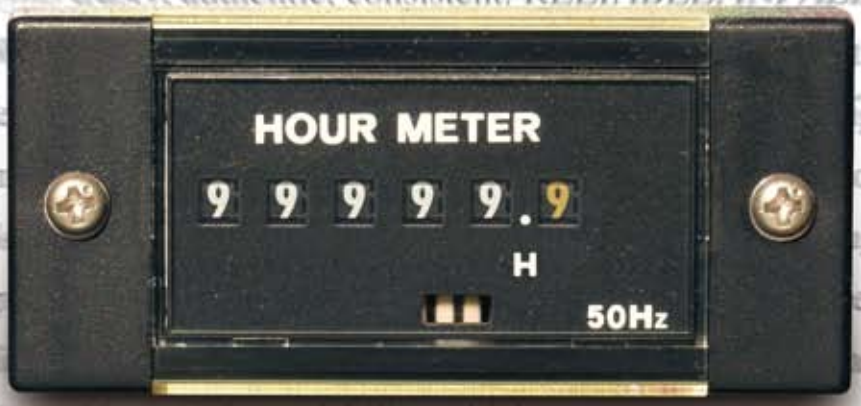

reliability \re-li-abil-i-ty\noun

—Synonyms trusty, authentic, consistent, RELIABLE, INFALLIB

TRUSTY

can be de

consisten

a reliabl

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Contents

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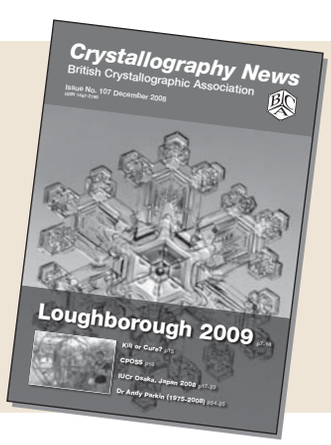
BCA explorers discover a buckyball in Kyoto; a snow crystal photographed by Prof. Kenneth Libbrecht.



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From the President

BY the time this column appears in *Crystallography News* the Christmas vacation will almost be upon us so let me wish all our readers a very Happy Christmas and a peaceful and prosperous 2009. It has been another busy year for the BCA. I think that all would agree that the Spring Meeting at York was a great success with a very wide ranging and enjoyable scientific programme. The other "big meeting" of the year was the IUCr Congress, held in Osaka, Japan, during the last two weeks of August. The BCA was very well represented there with many contributors to the scientific sessions. I led the UK delegation of **Sandy Blake**, **Georgina Rosair**, **Harry Powell** and **Chick Wilson** at the General Assembly where it was confirmed that Madrid would host the next IUCr Congress, in 2011, and that Montreal would be the hosts in 2014. The UK delegation also gave **Chris Gilmore**, who was standing for IUCr President, our full support. Unfortunately, he was not successful in the election but **Sine Larsen** (Denmark) was a very worthy winner and we send her our warmest congratulations. Chris continues as an Ordinary member of the Executive Committee. In addition nine UK representatives were elected to the various IUCr Commissions so that UK representation remains strong in the International Union.

There were also several meetings of the European Crystallographic Association during the Osaka Congress. During these meetings we received support for the UK to submit a bid to host the ECA meeting in 2013 and **Sandy Blake** has kindly agreed to chair a working group to plan the bid which will be put forward at the Istanbul ECA-25 Meeting next August. During the Osaka Meeting came the very sad news of the passing of **Andy Parkin** after a short illness. Andy was one of the founder members of the Young Crystallographers and, in his short career, made many contributions to the BCA at all levels. His gentle sense of humour and his tireless encouragement of others will be greatly missed. Our thoughts are with his wife and relatives at this very sad time. An obituary for Andy highlighting his many contributions to crystallography can be found later in this issue of *Crystallography News*.

Looking to the future, as you will also see in this issue, the programme for the Spring Meeting at Loughborough, to be held between Tuesday 21st and Thursday 23rd April, 2009, is almost complete. I would like to thank **Simon Parsons** and the Programme Committee for their sterling efforts. As usual the Young Crystallographers will run a satellite meeting starting on Monday, 20th, and there will also be a special symposium in honour of **Frank Allen** commencing at lunchtime on the Thursday. It is also a great pleasure to welcome back the XRF community this year so that there really will be something to excite everyone.

I have to report that **Jeremy Karl Cockcroft** has recently retired as our webmaster after many years of sterling service. I am sure that you would wish to join me in thanking **Jeremy Karl** for all the hard work that he has put in. A working group of **Sandy Blake**, **Simon Coles**, **Richard Cooper** and **Mike Probert** has taken over the running and development of the website for the time being and we hope to bring nominations for a new webmaster to the AGM, at the Spring Meeting. Also, at the AGM, we have to elect a new President and three Ordinary members. The Secretary is looking forward to receiving your nominations for all these important posts in the near future.

Paul Raithby

BCA Council 2008

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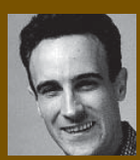

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Full committee details on the BCA website **www.crystallography.org.uk**

Spring Meeting Registration and Subscriptions: **www.crystallography-meetings.org.uk**

From the Editor

ICE. In the form of snowflakes, how it delighted us when we were children! It may be more of a chore for us now, but clearing a fall of snow from the driveway and footpaths still engenders a warm glow of accomplishment and provides the perfect excuse to enjoy a big mug of hot chocolate. Where we definitely don't want ice is on the surface of the sample or within the mother liquor in a low-temperature diffraction experiment. Cryo-cooling has improved the accuracy of small-molecule crystallography and brought about a revolution in macromolecular crystallography, but it must be applied knowledgeably. This issue features an article by Elspeth Garman on cryo-cooling and radioprotection.

It also ties in well with a CCP4 Study Weekend that Elspeth is running in January 2009, on "Experimental Phasing and Radiation Damage". Other specialist meetings (and their organisers) announced in this issue are Control and Prediction of the Organic Solid State- State of the Art and Challenges (**Sally Price**) in March and Aperiodic 09 organised for the Aperiodic Commission of the IUCr (**Ronan McGrath**) in September. A good selection of group meetings illuminates the dull months of November and December. The Pharmaceutical Special Interest Group of the Industrial Group held its autumn meeting in Loughborough on 5th November, followed by the Physical Crystallography Group at their traditional venue, Cosener's House in Abingdon, on "Neutron Diffraction and Complementary Techniques". A week later it was the turn of the Chemical Crystallography Group in Newcastle on "New Methods". The irresistible attraction that Geordieland holds for crystallographers is confirmed by the Biological Structures Group winter meeting, 16th December at the University of Newcastle, on "Protein : Nucleic Acid Interactions". These specialist meetings and group meetings may not attract as much attention as the big annual BCA meeting or the spectacular Congress of the IUCr, but they provide a valuable complementary experience: a chance for experts in one field to discuss it intensively in an informal atmosphere.

The cover of this issue shows the discovery of a fullerene on a side trip to Kyoto by intrepid BCA explorers **Georgina Rosair**, **Paul Raithby**, **Christine Cardin** and **Yu Gan**. Inside we have several reports on the IUCr Congress held this summer in Osaka, Japan. With seven different microsymposia running simultaneously and up to three coincident keynote lectures each reporter's perspective was bound to be different. It may even seem that some of us attended entirely different meetings! A certain amount of microsymposium-hopping was possible. Most speakers apparently took their cue from the outstanding punctuality of Japanese railways and kept to their allotted time, even without bullying from the distinguished scientists chairing their sessions. We have the recipients of Arnold Beevers bursaries to thank for most of the reports. From the excitement evident in their accounts it is clear that their experiences in Osaka both enhanced their technical knowledge and fired their enthusiasm.

The donors to the bursary fund and people who admired Arnold Beevers should be very happy with the results of such generosity. Many of these bursary recipients will originally have acquired their skills in crystallography at one of the Intensive Schools in Durham. The next occurrence of this School in 2009 is announced in this issue. Please remember, too, that the deadline for submission of abstracts for the 2009 European Crystallographic Meeting will be March 15.

I conclude with a personal tribute to **Andy Parkin** in addition to the obituaries appearing in this issue. As an (over) enthusiastic adopter of dSNAP I tried to apply it in various appropriate and inappropriate situations. Thanks to Andy's perceptive and tactful advice I could concentrate my efforts and obtain useful results.

Carl Schwalbe

Puzzle Corner

SOLVING this puzzle should be feasible even after excessive consumption of mince pies. Fill the blanks with appropriate responses to the clues. Then look askance at what you have done to find a message from the Editor.

— — — — — — —
Author of space group notation

— — — — — — —
Author of space group notation

— — — — — —
Policeman or penny that may become a target

— — — — —
Greek axis in Dutch diffractometer

— — — — — — —
Type of cell containing the protein studied by Kendrew

— — — — — — —
Beam used in diffraction experiments

— — — — — —
Scientist who shared the Nobel Prize with Kendrew

— — — — — —
Type of crystalline sample that can be used for identification and, sometimes, structure determination

— — — — — — —
Element used in red phosphors on cathode ray tubes

— — — — — — — — —
Scientist who postulated wave-particle duality

— - — — —
Beam used in diffraction experiments

— — — — — — —
Iron (II)

I have not yet received an answer for the word search in the September Puzzle Corner. As a means of stimulating the intellect after excessive consumption of holiday goodies, it will be left open for answers until the next issue.

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.
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From the Treasurer

FOLLOWING a decision by Council, the BCA is moving its bank accounts from HSBC to the Charities Aid Foundation Bank, CAF Bank. The principal motivation for this change is that CAF Bank treats its customers as charities, whereas HSBC (in common with all major UK banks) offers business banking terms, even to those customers who do have charitable status. CAF Bank is the only suitable bank for the BCA that has links from the Charity Commission's website.

The move will have a number of advantages for the BCA, among which are:

- The increase in interest revenue will allow BCA to offer several more student bursaries every year.
- Interest rates closer to those available to personal customers at other banks. Business bank accounts are run by banks according to commercial terms, and rarely give significant interest rates; businesses are expected to invest to gain a return by other means.
- Transfers during working hours between current and savings accounts are performed on the same day, so that the current account balance does not need to be kept artificially high for long periods in expectation of having bills to pay.
- Working with a bank intended for charities should mean that there will be no confusion about the BCA's status as regards its bankers.

For those members whose only financial dealings with the BCA is payment of the annual subscription and the Spring Meeting registration, this move will make almost no difference.

Payments will still be made to the British Crystallographic Association. If payment is by cheque or credit card, there will be no difference noticeable to the member.

Subscriptions Currently Being Paid by Standing Order

Payment by standing order has been a source of problems for many years for the BCA. At the last count, there were just over 300 standing orders being paid with respect to the annual subscription; of these, over 140 were incorrect. Most of these incorrect payments were for membership rates that had been current some time in the past, but others were duplicates (i.e. several members appear to be paying twice), and some could not be traced to a payee. Moving to a new bank allows the BCA to ensure that all members are paying the correct subscription and are doing it once only!

If you wish to pay your annual subscription by standing order and also wish to remain a member of the BCA for 2010, you will need to complete a new standing order form and return it to our administrative office; this is because the banking system does not allow standing orders payable to one bank to be transferred to another.

Subscription Payments by Direct Debit

We are taking the opportunity of the move to offer the option of paying by direct debit. This will allow the BCA to collect the correct subscription fee from all members who choose this method of payment, and to update the fee in accordance with resolutions passed by the membership at the AGM. The BCA will offer a 10% reduction in membership fee for those who choose to pay their subscription by direct debit for 2010, in order to encourage take-up of this option.

A number of members have mentioned that they feel uncomfortable with making payments by direct debits. In order to address this concern, I am happy to emphasize that the current payment options will continue, and there will be no penalty for any member who decides to pay by standing order, cheque or credit card.

Loughborough 2009

BCA 2009 Spring Meeting 21st-23rd April 2009 University of Loughborough

http://www.crystallography-meetings.org.uk/

THE BCA Spring meeting in 2009, which has the theme Dynamic Crystallography, will run from 11:30 on Tuesday 21st April to 13:30 on Thursday 23rd April. The meeting will also incorporate parallel sessions on X-ray Fluorescence.

Prior to the main meeting, the Young Crystallographers session will commence on Monday 20th April. After the main meeting, there will be a Symposium for Dr Frank Allen to mark his retirement as Executive Director of the Cambridge Crystallographic Data Centre. This will commence at 14.00 pm on Thursday 23rd April and conclude at 13.30 pm on Friday 24th April 2009.

All scientific lectures including the Young Crystallographers will take place within the James France Building on the Loughborough University Campus.

We will have our traditional Commercial Exhibition, located in the James France Building Exhibition Area. Due to the popularity of the Young Crystallographers session at the Spring Meeting in York, the Commercial Exhibition will be open from 19.00 on Monday 20th April and will close after the morning coffee on Thursday 23rd April. As well as being open during all refreshment breaks, delegates will have the opportunity to visit all stands during the poster and exhibition buffet dinner on Tuesday 21st April.

Registration and refreshment breaks during the main scientific programme will take place within the Exhibition centre. The Young Crystallographers session on Monday 20th April will take place within the Exhibition Centre lecture theatre and the evening buffet will be held in the exhibition hall.

For more information on the exhibition and sponsorship opportunities, or for any other enquiries about registration or accommodation, please contact David Massey at the BCA Administrative Office, **01355 244966** or email **bca@glasconf.demon.co.uk**

Registration

Early Registration Costs (before 16th March 2009)

Full Registration	**£210.00**
Student/Unemployed/Retired	**£105.00**
Non-Member Surcharge	**£35.00**
One-Day Registration (no concessions)	**£105.00**

Late Registration Costs (after 16th March 2009)

Full Registration	**£260.00**
Student/Unemployed/Retired	**£105.00**
Non-Member Surcharge	**£35.00**
One-Day Registration (no concessions)	**£130.00**

Accommodation

There are two types of accommodation available at the University of Loughborough.

Standard B&B	**£35.00** per night
En-suite B&B	**£51.00** per night

All accommodation is situated in the village area within the University campus. Standard accommodation is within the Faraday Building and en-suite accommodation is located also within the Faraday Building along with the Cayley and Royce Buildings. Breakfast and dinner will be served within the Elvyn Richards Dining Hall.

Check-in time is from 15.00 and keys must be returned on departure no later than 09.30.

Catering

Morning and afternoon refreshments from Tuesday 21st April - Thursday 23rd April will be served in the Exhibition Centre. Refreshments and lunch for the Young Crystallographers will be served within the Elvyn Richards Dining Hall.

Breakfast and dinner (including the Conference Dinner on Wednesday 22nd April) will be served in the Elvyn Richards Dining Hall.

The Young Crystallographers Buffet Dinner on Monday 20th April and Poster and Exhibition Buffet Dinner on Tuesday 8th April will be served within the Exhibition Centre.

All lunches and evening meals must be booked in advance and will be ticketed.

Packed Lunch	**£6.50**
Dinner on campus (Monday 16th April)	**£15.00**
Conference Dinner	**£35.00/£20.00** *for concessions*

Please be aware that if packed lunches and evening meals

are not selected on the registration form and paid for prior to attending the meeting it is the individual's responsibility to make alternative arrangements.

Social Events

On Tuesday 21st April, the poster and exhibition reception will be held in the early evening. A buffet meal with wine will be served within the Exhibition Centre. Delegates will have the opportunity to meet with the exhibitors and poster presenters in a relaxed and informal setting. There will not be an additional charge for attending this evening reception, but sponsorship is welcome.

The Conference dinner will be held on Wednesday 22nd April in the Elvyn Richards Dining Hall at a cost of **£35.00/£20.00** for concessions.

Car Parking

Those wishing to park within the University Campus must request a car parking permit on the registration form. Permits along with joining instructions will be sent along with registration confirmations. Parking is free, but must be pre-ordered.

Email Facilities

Computer access will be available within the library at the University of Loughborough. Wireless is also available in certain designated areas on campus. Email logins are free. Please visit the registration desk for access.

Abstract Submission

Poster Abstract Deadline - **2nd February 2009**
Please submit abstracts for posters using the Word template available from
http://www.crystallography-meetings.org.uk/abstracts.htm

Please ensure that all abstracts are submitted using the template available from **http://www.crystallography-meetings.org.uk/abstracts.htm**. Please do not use old versions of the template from previous years.

BCA Bursaries

A limited number of bursaries are available from the Arnold Beevers Bursary Fund to cover the cost of registration, two nights' standard accommodation, lunches from Tuesday 21st - Thursday 23rd April, evening buffet on Tuesday 21st and the Conference Dinner on Wednesday 22nd April. The bursary will not cover travel expenses and recipients will be expected to present a poster and produce a report on part of the meeting.

Council is again seeking commercial sponsors of Spring Meeting Bursaries at £250.00 per student and it is hoped that some Named Bursaries will be awarded at this meeting.

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

The closing date for all applications is Monday **2nd February 2009**. Only on-line applications via the conference website: **http://www.crystallography-meetings.org.uk** will be accepted.

Insight into Loughborough

Loughborough is at the heart of England in the northern most part of the county of Leicestershire. Being centrally placed, it is well served by road, rail and air links. Main line road and rail networks link Loughborough directly with the rest of the country and the town itself is served by excellent bus services. Loughborough University is less than two miles away from Junction 23 of the M1 motorway. London is one-and-a-half hours away by train, Birmingham one hour and Manchester and Leeds around two hours. There are regular scheduled flights from UK, European and international destinations to East Midlands Airport, only 8 miles away. Loughborough is an ancient market town, and local attractions include a bell foundry museum, the Great Central Steam Railway and a number of country parks.

Travel Information

Loughborough lies at the heart of the UK motorway system, 1 mile from Junction 23 on the M1 and only 8 miles from East Midlands Airport, giving ready access to most parts of the UK and Europe via daily scheduled flights.

Security barriers are in operation at each entrance to the campus. Visitors are asked to report to one of the gatehouses where staff will issue a pass and direct you to your destination.

BY ROAD:

From M1 (Junction 23) or the A6, follow the signs to the University.

FOR 'SAT-NAV' USERS:

To help ensure your satellite navigation system gets you to Loughborough University correctly, use the postcode LE11 3TZ when setting your destination.

(Important: If coming into Loughborough using any other postcode, please follow signposts to 'University' to ensure you are directed to the main entrance.)

CAR PARKING

University and public car parks are marked on the campus map. Parking on campus is restricted. Those wishing to park within the University Campus must request a car parking permit on the registration form. Permits along with joining instructions will be sent along with registration confirmations. Parking is free, but must be pre-ordered.

Disabled visitors are requested to telephone our Security Office on the number below before visiting so that suitable parking can be arranged.

For more information contact the Security Office on **01509 222 141**.

BY RAIL:
90 minutes from London St Pancras. Approximately 10 minutes by taxi or bus from Loughborough train station.
www.midlandmainline.com
http://www.kinchbus.co.uk/timetables/sprint.aspx

BY AIR:
8 miles from East Midlands Airport and convenient for Birmingham Airport (M42).
www.eastmidlandsairport.com
www.bhx.co.uk

TRAVELLING BY COACH OR BUS:
Coach and bus services to and from other parts of Leicestershire and the UK operate from the centre of Loughborough.

Travel by National Express or regional bus services to Loughborough then connect with local Kinch bus town services to the Loughborough University campus.

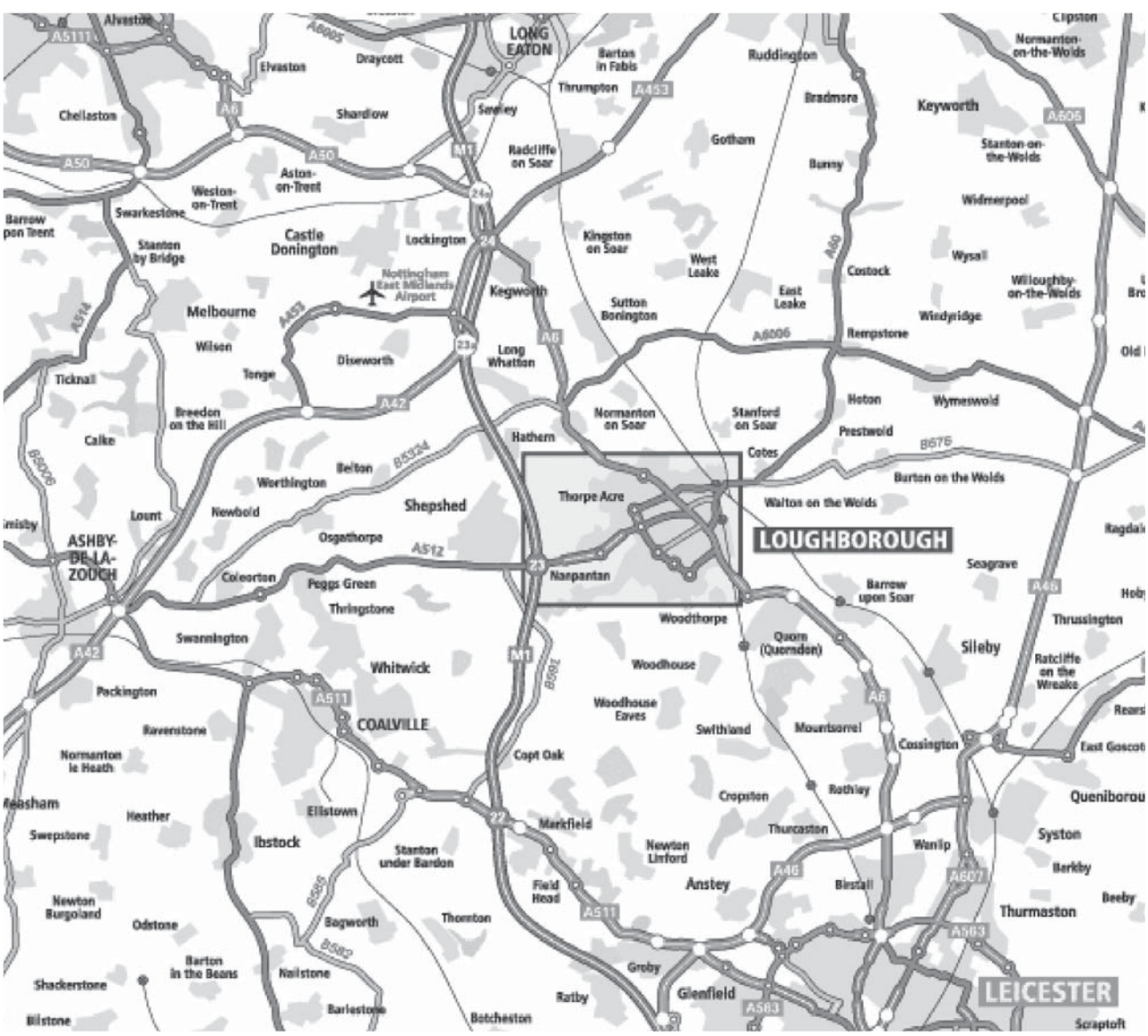
For enquiries about all these services call Traveline on **0871 200 22 33.**

OTHER USEFUL PLANNING SERVICES
National Express - **www.nationalexpress.com**
Trent and Barton Buses - **www.trentbuses.co.uk**
Traveline East Midlands - **www.travelineeastmidlands.org.uk**

University Shuttle Bus Service
Kinchbus Number 7 commences from Loughborough Railway station and brings you straight to campus.

Alighting points on the campus include:
Students' Union
Pilkington Library
Wolfson School
Holywell Park

In term time this service runs every 10 minutes Monday to Saturday daytime until 5.45 pm. A Monday to Friday evening service operates every 30 minutes until 8.40 pm during term times only. Sunday service runs from 11 am until 7.20 pm.



Timetable, AGM Loughborou

	Day 0 Monday 20th April	Day 1 TUESDAY 21st April				Day 2 WEDNESD		
9:00		Lecture Theatre 1				Lecture The		
9:15		Young Crystallographers 4				Plenary IG (X		
9:30								
9:45						Coffee 9.45		
10:00								
10:15						Parallel sessions		
10:30		Registration/exhibition 10.30-11.30			Lecture Theatre 4	Lecture Theatre 1	Lecture Theatre 2	
10:45						Reactivity in Crystals-1 (CCG)	Reactions in Macromolecular Crystals (BSG)	
11:00					XRF General (XRF)			
11:15								
11:30		Lecture Theatre 1						
11:45		Lonsdale Lecture 11.30-12.30					BSG AGM 11.45-12.30	
12:00								
12:15								
12:30		Lunch/exhibition/registration 12.30-13.30				CCG AGM 12.30-1.15	Lunch/AGM	
12:45								
13:00	Lecture Theatre 1							
13:15	Young Crystallographers 1							
13:30		Sessions 13.30-15.00				Sessions 13.3		
13:45		Lecture Theatre 1	Lecture Theatre 2	Lecture Theatre 3	Lecture Theatre 4	Lecture Theatre 1	Lecture Theatre 2	
14:00		Computational Crystallography (CCG/PCG)	New Synchronation Instrumenation (BSG/CCG)	Multiferroics (PSG)	XRF General (XRF)	Reactivity in Crystals-2 (CCG)	Metalloproteins: Structure and Dynamics (BSG)	
14:15								
14:30								
14:45						CCDC Prize Lecture		
15:00	Coffee 15.00-15.30	Coffee 15.00-15.30				Coffee 15.0		
15:15								
15:30	Lecture Theatre 1	Sessions 15.30-17.00				Sessions 15.3		
15:45	Young Crystallographers 2	Lecture Theatre 1	Lecture Theatre 2	Computer Rm	Lecture Theatre 4	Lecture Theatre 1	Lecture Theatre 2	
16:00		Dynamic Techniques (CCG/YC)	Complementary Techniques (BSG)	dSNAP Workshop	New Developments in Instrumentation and TXRF (XRF)	Temperature-Dependent Crystallography (CCG)	Dynamics at the Membrane (BSG)	
16:15								
16:30								
16:45								
17:00	Break	Break 15 minutes				Break 15 minutes		
17:15		Lecture Theatre 1			Lecture Theatre 4	Lecture Theatre 1		
17:30	Lecture Theatre 1	Exhibitors Forum 17.15-18.45			Exhibitors Forum (XRF)	Plenary (BSG)		
17:45	Young Crystallographers 3							
18:00						Lecture The		
18:15						BCA AGM 18.		
18:30								
18:45		Dinner, exhibition and posters						
19:00	Young Crystallographers' Dinner					Comfort		
19:15								
19:30								
19:45								
20:00						Conference Dinner		
20:15								
20:30								
20:45								
21:00								

ugh 2009

ESDAY 22nd April			Day 3 THURSDAY 23rd April				Day 4 FRIDAY 24th April
re Theatre 1			Lecture Theatre 1			Lecture Theatre 4	Frank Allen Symposium
IG (XRF/XRD)			Teaching Plenary (PCG) Martin Dove			XRF Keynote Method Validation	
9.45-10.15			Coffee 9.45-10.15				
sions 10.15-11.45			Sessions 10.15-11.45				
2	Lecture Theatre 3	Lecture Theatre 4	Lecture Theatre 1	Lecture Theatre 2	Lecture Theatre 3	Lecture Theatre 4	
ar	Crystallography Near the Edge (PCG)	Environmental Applications (Joint XRF/XRD)	Hydrogen Storage (PCG)	Dynamics of Radiation Damage (BSG)	Understanding API Phase Transitions (IG)	Method Validation (XRF)	
	PCG AGM 11.45-12.30	IG AGM 11.45-12.30	Break 15 minutes				
			Sessions 12.00-13.30				
			Lecture Theatre 1	Lecture Theatre 2	Lecture Theatre 3	Lecture Theatre 4	
/AGMs/exhibition 11.45-13.30			Dynamics in Framework Structures (PCG)	Snapshots of Dynamic Processes (BSG)	Crystallography in the Pharmaceutical Pipeline (IG)	Portable Instruments (XRF)	
s 13.30-15.00			Close 13.30				
2	Lecture Theatre 3	Lecture Theatre 4	Frank Allen Symposium				
s:	Monitoring Crystals, Crystallisation and Transformations-1 (IG/BACG)	Environmental Applications of XRF					
15.00-15.30							
s 15.30-17.00							
2	Lecture Theatre 3	Lecture Theatre 4					
	IG/YC Prize Lecture						
ne	Monitoring Crystals, Crystallisation and Transformations-2	Trace Analysis (XRF)					
es							
e 1							
)							
re Theatre 1							
M 18.00-19.00							
nfort time							
nner 19.30 for 20.00							

Scientific Programme: Dynamic Crystallography

PLENARY LECTURES

Lonsdale Lecture (CCG): **David Watkin** (University of Oxford)
Crystallography - Technology, Science or a Black Art?

Teaching Plenary (PCG): **Martin Dove** (University of Cambridge)
Dynamics from Diffraction: Information Beyond the Atomic Displacement Factor

Biological Structures Group: **Venki Ramakrishnan** (MRC, Cambridge) *Insights into Translation from Crystallography of Functional Complexes of the Ribosome*

XRF: **David Lowe** (United Kingdom Accreditation Service)
Method Validation to Achieve ISO 17025 Accreditation

Industrial Group: **Nick Marsh** (University of Leicester) *Environmental Analysis with XRF and XRD*

SESSIONS AND CONFIRMED SPEAKERS

New Synchrotron Instrumentation (BSG/CCG)
Chair: **Gwyndaf Evans**

Clemens Schulze-Briese (Paul Scherrer Institut, Swiss Light Source) *Protein crystallography with 6 million detectors: the PILATUS 6M*

Robin Owen (Diamond Light Source) *New tools for on-line UV-Visible and Raman spectroscopies at MX beamlines*

Complementary Techniques (BSG)
Chair: **Pierre Rizkallah**

Mike Hough (Liverpool University) *Monitoring gated electron transfer in crystals of nitrite reductase*

Sandor Brockhauser (EMBL Grenoble) *Tomography for Macromolecular Crystallography*

John Helliwell (University of Manchester) *Case studies of time-resolution and dynamics in protein crystallography*

Reactions in Macromolecular Crystals (BSG)
Chair: **Arwen Pearson**

Elena Kovaleva (University of Leeds) *Title: TBC*

Andrea Hadfield (University of Bristol) *Title: TBC*

Metalloproteins: Structure and Dynamics (BSG)
Chair: **Peter Moody**

Paul Ortiz de Montellano (University of California)
Cytochrome P450 enzymes and conformational dynamics

Emma Raven (University of Leicester)
Conformational mobility in a heme peroxidase

Mark Banfield (John Innes Centre, Norwich)
Structure/function studies of a metal binding loop

Dynamics at the Membrane (BSG)
Chair: **Liz Carpenter**

Dave Stuart (STRUBI, University of Oxford) *Title: TBC*

Alex Cameron (Diamond Light Source)
Structure and Mechanism of Mhp1, a Nucleobase-Cation-Symport-1 Family' Transporter

Dynamics of Radiation Damage (BSG)
Chair: **Elspeth Garman**

Colin Nave (Diamond Light Source) *Radiation damage - how much, how fast, how far*

Martin Weik (Institut de Biologie Structurale, Grenoble, France)
Temperature controlled crystallography and radiation damage

Snapshots of Dynamic Processes (BSG)
Chair: **David Stuart**

Rick Lewis (Newcastle) *Molecular architecture of the "stressosome", a signal integration and transduction hub*

Computational Crystallography (CCG/PCG)
Chair: **Richard Cooper**

Frank Leusen (IPI): *A breakthrough in crystal structure prediction.*

Mustapha Sadki (University of Oxford) A new framework for reliable refinement data types

Dynamic Techniques (CCG/YC)
Chair: **Lynne Thomas**

Robert Feidenhans'l (Copenhagen) *Structural Changes at Short Time Scales*

Robert Hammond (Leeds) *Title: TBC*

Reactivity in Crystals 1 and 2 (CCG)
Chairs: **Andrew Bond and Alex Griffin**

Marc Messerschmidt (SLAC/LUSI-Stanford) *Time-resolved diffraction studies on tetrathiafulvalene-p-chloranil (TTF-CA): new aspects from polychromatic experiments.*

Hazel Sparks (University of Durham)
[2+2] cycloaddition reactions in the spotlight

Stephen Moggach (University of Edinburgh)
Reactivity in crystals at high pressure

Ann Chippindale (University of Reading) *Bending, twisting and breaking: chain, layer and framework cyanides*

Stefanie Schiffers (University of Bath) *Crystal engineering and solid-state reactions*

Temperature-Dependent Crystallography (CCG)
Chair: **Andres Goeta**

Philippe Guionneau (Institut de Chimie de la Matière Condensée de Bordeaux and University of Bordeaux)
A temperature dependent metal co-ordination number change associated with a spin crossover

Andrew Goodwin (University of Cambridge) *Colossal positive and negative thermal expansion in extended Prussian Blue Analogues*

Simon Coles (University of Southampton) *Structural and physical characterisation of temperature-dependent single-crystal-to-single-crystal transitions*

Environmental Applications -1 (XRF/XRD)
Chair: **Richard Morris**

Peter Stacey (Health and Safety Laboratory) *New applications in the use of X-ray diffraction at the Health and safety Laboratory:- A case study using XRD to assess emissions across construction sites*

Monitoring Crystals, Crystallization and Transformations
Chair: **Nick Blagden** (BACG) and **Alison Burke** (IG)

Roger Davey (University of Manchester) *Monitoring nucleation of cocrystals: a solution chemistry perspective*

Paul Barnes (Birkbeck College) *Opportunities for observing the synthesis and behaviour of functional materials using synchrotron X-Ray diffraction*

Kevin Roberts (University of Leeds) *Application of Process Analytical Techniques in Monitoring and Controlling the Crystallization of Fine Chemical Products*

Speaker to be Announced *Industrial Group/Young Crystallographers Prize Talk*

Chick Wilson (University of Glasgow) *TBA*

Dermot O'Hare (University of Oxford) *A Retrospective of the Time-Resolved In-situ EDXRD Data We Collected At the SRS*

Understanding API Phase Transitions (IG)
Chair: **Brett Cooper**

Paolo Avalle (Merck Sharp & Dohme Development Laboratories) *The use of real-time variable temperature Raman microscopy to monitor temperature related API phase transitions*

Ji Yi Khoo (Imperial College) *Solid-solid phase transformations in channel hydrate during dehydration*

Russell Johnson (University of Edinburgh) *Identification of Driving Forces in High Pressure Phase Transitions Using the Pixel Method*

Crystallography in the Pharmaceutical Pipeline (IG)
Chair: **Matt Johnson**

Cheryl Doherty (Pfizer) *Crystallography for Drug Development*

David England (Sanofi-Aventis Deutschland GmbH) *The crystal structure is the gold standard for proof of structure of the API: What can be achieved for the drug product?*

Multiferroics (PCG)
Chair: **Andrew Wills / Peter Hatton**

Crystallography Near the Edge (PCG)
Chair: **Matt Tucker / David Allan**

Madeleine Helliwell (University of Manchester) *Methods and applications of anomalous dispersion in small-molecule crystallography*

Hydrogen Storage (PCG)
Chair: **Dave Keen / Ivana Evans**

Marco Sommariva (ISIS Facility) *Neutron diffraction studies and complementary techniques for H2 storage materials.*

Andrea Baldi (VU University Amsterdam) *Mg-Ti multilayers: nanostructured hydrogen-storage alloys*

Dynamics in Framework Structures (PCG)
Chair: **Andrew Goodwin / Matthew Tucker**

Richard Walton (Warwick University) *Time-Resolved Diffraction from Flexible Metal Organic Frameworks Interacting with Guest Molecules*

XRF: General Session (XRF)
Chair: **David Beveridge**

Stephen Davies (PANalytical) *Calibration Maintenance: Food for Thought.*

Simon. FitzGerald (HORIBA Jobin Yvon Ltd.) *The 10 Micron Innovation - Applications in Micro-XRF*

Luc Bérubé (Corporation Scientifique Claisse) *Minimizing time and manipulations for the preparation of ferroalloys by borate fusion for XRF analysis*

New Developments in Instrumentation and TXRF (XRF)
Chair: **Margaret West**

Christina Streli (TU Wien, Atominstitut der Österreichischen Universitäten) *Developments in TXRF analysis*

Armin Gross (Bruker AXS Microanalysis GmbH) *Trace Element Analysis of Pharmacological, Medical and Biological Samples by TXRF*

Environmental Applications-2 (XRF)
Chair: **Dave Taylor**

Christine Vanhoof (VITO - Environmental Analysis and Technology, Belgium) *How XRF fits into RoHS analyses.*

Trace Analysis (XRF)
Chair: **Mark Ingham**

Jamie Cutting (Scot Wilson) *TBA*

David Beveridge (HARMAN technology Ltd.) *Determination of traces of heavy metals in water by XRF*

Method Validation (XRF)
Chair: **Ros Schwarz**

Portable Instruments. (XRF)
Chair: **Margaret West**

Phil Potts (Open University) *Portable X-ray fluorescence analysis - new opportunities, new challenges*

TBA (British Geological Survey) *Analysis of Limestone & Dolomite*

dSNAP WORKSHOP

The Cambridge Structural Database is an enormously powerful resource, but with more than 450,000 entries, extracting meaningful information when there is a large number of hits when searching for a fragment of interest can be daunting.

dSNAP is a free computer program that assists in this by letting the user:

- Import structural information
- Correct for local chemical symmetry
- Perform cluster analysis in which similar fragments are easily identified
* Perform separate analysis on variables in which distance/ angle trends and outliers in search can be analysed
* Visualise and superimpose structures to understand the structural chemistry underlying the groupings

dSNAP also provides a series of graphical displays and options to allow the user to interpret the results quickly and easily. The workshop will present a series of hands-on examples of dSNAP in action, along with some of the theoretical background of what it is doing.

More information is available at
www.chem.gla.ac.uk/snap
or by emailing
dsnap@chem.gla.ac.uk

THE FRANK ALLEN SYMPOSIUM

The Symposium will take place at the Annual Spring Meeting on Thursday afternoon and Friday morning. It embraces talks by both established and younger scientists. There will also be a dinner in honour of Frank on the evening of Thursday 23 April.

Angelo Gavezzotti (University of Milan, Italy) *Thirty Years of Organic Crystal Polymorphism in the Cambridge Database*

Simon Parsons (University of Edinburgh) *High Pressure Phase Transitions in Molecular Crystals*

Lee Brammer (University of Sheffield) *Understanding Intermolecular Interactions involving Halogens in Molecular Crystal Structures*

Bob Docherty (Pfizer, Sandwich, Kent) *Application of Material Sciences in Pharmaceutical Research & Development*

Sally Price (University College, London) *Progress Towards Control and Prediction of the Organic Solid State?*

Peter Galek (CCDC, Cambridge) *Assessing Polymorphs through Hydrogen Bond Prediction*

Laszlo Fabian (CCDC, Cambridge) *Database-assisted Design of Co-crystals*

Peter Wood (CCDC, Cambridge) *Carbamazepine Co-crystals - New Insight from a Familiar Compound*

Kirsty Anderson (University of Durham) *Crystal Packing in Molecular Solids: Insights from Structures with Z'>1*

Robin Taylor (Scientific Software Consultant, Rickmansworth, Herts) *title to be confirmed*

Frank Allen (CCDC, Cambridge) *Publication of Crystallographic Results - the Future*

Colin Groom (CCDC, Cambridge)
The CCDC's Future Direction

Young Crystallographers Agenda

THE Young Crystallographers are proud to announce their next meeting: The YC2009 will take place in the afternoon of 20th April and in the morning of 21st April prior to the BCA Spring Meeting in Loughborough. As in previous years we will run three sessions of oral presentations, which are a superb opportunity for Young Crystallographers to discuss their work in a relaxed environment and practise their presentation skills. There will also be a poster session on Monday evening together with a buffet dinner and drinks.

Accommodation and registration for the YC2009 will be free once more and should be done through the BCA website (http://www.crystallography-meetings.org.uk, see also this page for further information on bursary applications.)

So all we need now is your abstracts! Deadline for abstracts to be considered for oral presentations is 26th January 2009 and deadline for poster abstracts is 2nd February 2009. Submission should be made through our
webpage www.chem.gla.ac.uk/yc/.

Like in the years previously there will be a range of prizes for outstanding contributions to be awarded at the main conference dinner so don't hold back!

Below is a preliminary programme and once all speakers are confirmed the full programme will be available on our website.

YC1 PLENARY (PHYSICAL)

Dominic Fortes (Planetary Ices Group, UCL) - "High-pressure neutron diffraction studies of ammonia hydrates, or how to spend five years indexing a powder pattern"

YC2 PLENARY (BIOLOGICAL)

tba

YC3

AGM
1 minute poster flash presentations
Poster Session with dinner and wine

YC4 PLENARY (INDUSTRIAL)

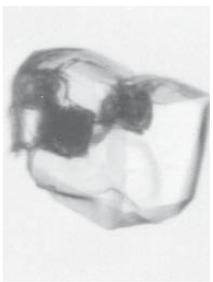
Frank Allen (Former Director of the CCDC) *"Energy Matters!"*

See you all in Loughborough!

Susanne Huth
YCG Chair

Kill or Cure?

Kill or Cure? Radiation damage in protein crystallography



Crystal of N9 neuraminidase from avian influenza virus isolated from a Great Barrier Reef Noddy Tern, damaged by 100K data collection at 3 positions. The beam was 100 microns x 100 microns at the ESRF 9ID14-4. When the crystal was allowed to warm up in its buffer after the experiment, the black beam spots became visible.

SINCE the advent of brighter synchrotron sources in the mid-nineties, radiation damage has re-emerged as a limiting problem in macromolecular crystallography (MX). Advances in dealing with radiation damage in the field are intimately intertwined with the development of cryo-crystallographic techniques. The first systematic study of the effects of X-rays on protein crystals was carried out at room temperature by **Blake** and **Phillips** in 1962 on myoglobin, of which at the time they did not even know the full sequence. In their landmark paper, they proposed an empirical model for the diffraction decay which could not account for all the changes in diffraction intensities that they observed. They postulated that this `may indicate structural changes due to indirect effects of the radiation'. This suggestion was subsequently confirmed for data collected at 100K a long time later (in 2000!), when it was found that particular amino acids were more susceptible to damage than others and that this specific damage occurred in a reproducible order in many proteins.

In 1970 **David Haas** and **Michael Rossmann** found that cooling lactate dehydrogenase crystals in 3M sucrose to 198K during irradiation prolonged their lifetime very significantly. By the late 1980s **Håkon Hope** was encouraging protein crystallographers to use cryo-techniques imported from small molecule crystallography. The loop mounting innovation of T-Y Teng made the method much more straightforward and involved using a thin (around 30 micron thick) loop of metal with a diameter matched to the crystal size. The crystal is `fished' from its liquid home, and surface tension forces hold it suspended in the loop in its mother liquor, which usually has to have a cryo-protectant agent added to avoid ice formation within the interstitial spaces between the protein molecules. The loop is swiftly flash cooled into liquid nitrogen or a gaseous nitrogen stream held at around 100K, and diffraction data are usually collected at temperatures between 90K and 120K. Researchers swiftly replaced the metal loops with lower diffracting material fibres from disparate sources such as fishing line, dental floss, babies' hair (including that of my own daughter...) and some spectacular pink mohair donated to us by **Louise Johnson**. This wool became famous when it was pinned to a poster at the BCA Spring meeting in Cardiff in 1995 and many pieces were cut off by passing attendees for subsequent use! The loop mounting method imposes much less physical stress on crystals, and thin plates can be mounted with more ease than when sealed glass or quartz capillaries were used for room temperature data collection.

The benefits of cryo-temperature data collection gradually became known, and the techniques were well developed by the mid-1990s. However, it was not long before high flux density synchrotron beams were observed to cause radiation damage even with the crystal held at around 100K, as predicted by **Richard Henderson** in 1990 from observations of the limiting dose in electron microscopy. Researchers started to try to understand the physical and chemical processes involved in this damage, which manifests itself in a number of different ways, including: changes in crystal colour, decreasing diffraction power with dose that is noticeable first in decreasing values of the signal to noise intensity ratios for the highest resolution reflections, a small but measurable linear increase in unit cell volume, and specific structural damage to covalent bonds in the protein molecules.

As mentioned above, the bonds are broken in a reproducible order: firstly delocalisation of the sulphur atoms in disulphides, secondly decarboxylation of glutamate and aspartate residues, followed by the disappearance of the -OH group on tyrosines and then the breakage of the C-S bond in methionines. This specific damage can lead to incorrect conclusions on biological mechanisms being drawn from crystallographic structures, especially since enzyme active sites and metalloproteins seem particularly sensitive to change by X-ray irradiation.

Thus in the last 5 years, the issue of radiation damage during diffraction experiments has come to the fore again as a concern for all structural biologists, and there is now considerable research effort being devoted worldwide to understanding and also on trying to mitigate the effects at cryo-temperatures. Starting in 1999 and then every two years or so, five International Workshops on 'X-ray Damage to Biological Crystalline Samples' have been held on the subject, resulting in 3 special issues of the Journal of Synchrotron Radiation in 2002, 2005, and 2007, and a fourth issue resulting from the fifth workshop is scheduled for March 2009.

The fact that the subject of radiation damage has become of widespread interest and almost 'mainstream' is reflected in the subject of the next CCP4 Study Weekend to be held at the University of Nottingham from 3rd-5th January 2009, which will be on "Experimental Phasing and Radiation Damage". The programme will be divided into sessions on 'Before the experiment', 'During the experiment', 'Using the experiment' and 'After the experiment', since the problem of radiation damage impacts all aspects of experimental phasing.

Radiation damage at 100K in MX has become an active area of ongoing research, and we hope that through this, we will better understand its effects on the quality of the biological information we obtain from three dimensional structures.

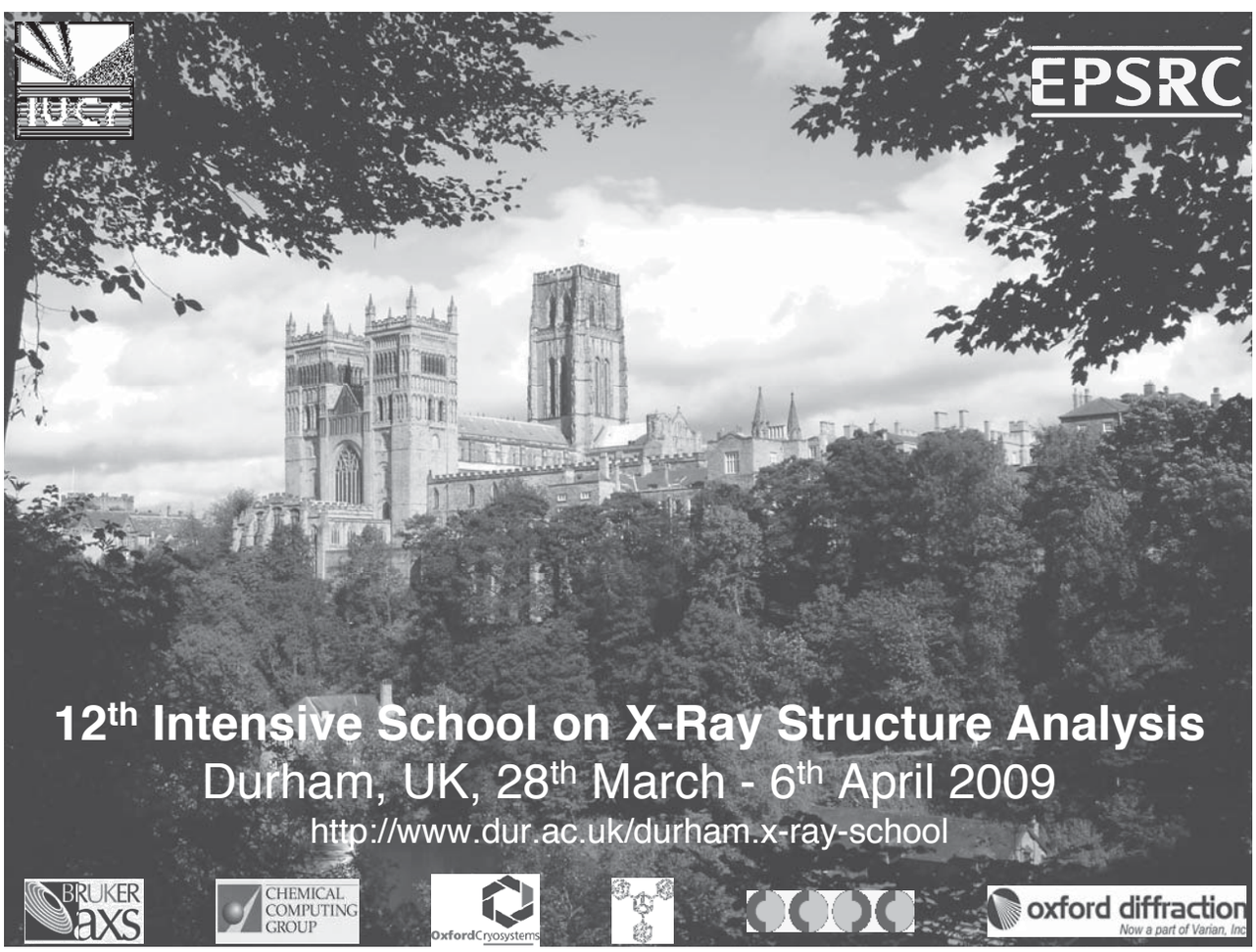
Elspeth Garman

CPOSS

Control and Prediction of the Organic Solid State - State of the Art and Challenges

THANKS to Basic Technology program funding, this project has developed the means of computing and archiving crystal energy landscapes, and an automated method of screening for new solid forms as a function of solvent crystallisation conditions. These technologies were combined with a range of diffraction and other experimental techniques to develop our understanding of polymorphism and crystallisation (www.cposs.org.uk). The project has received Translation Funding from EPSRC, to provide the manpower for small collaborative projects with academics and members of the CPOSS Industrial Alliance, and facilitate knowledge transfer and collaboration within the organic and pharmaceutical solid state community. We hope this will build on the generous involvement of so many UK groups in this research.

All academic groups with interests in the crystallisation or solid-state diversity (polymorphs, solvates, salts or co-crystals) of organic molecules are invited to a one-day meeting on Tuesday 31st March 2009, at UCL. The speakers illustrating "Control and Prediction of the Organic Solid State - State of the Art and Challenges" will be Alastair Florence (University of Strathclyde), Kenneth Harris (Cardiff University), Colin Pulham (University of Edinburgh), Jonathan Burley (University of Nottingham), Tomislav Friščis (University of Cambridge) and Sarah (Sally) Price (UCL). There will be ample time for networking, and contributions of posters from all related academic groups will be welcome. Registration, via our website, and lunch is free, thanks to sponsorship by members of the CPOSS Industrial Alliance.



IUCr Osaka, Japan 2008

XXI Congress and General Assembly of the International Union of Crystallography Osaka, Japan, 23rd - 31st August 2008

REPRESENTING 66 countries and territories, 2477 scientific participants and 140 accompanying members took part in 36 keynote lectures, 98 microsymposia, around 1500 poster presentations and many enjoyable social events. With so much competition it is indeed an honour that Helena Shepherd from Durham University won the Oxford Cryosystems Low Temperature prize for her poster "Structural studies of spin crossover compounds under extreme experimental conditions". Edited personal impressions from bursary recipients follow, ending with an account from your Editor.

Stephen Cairns - University of Glasgow

The 12 hour flight from London to Osaka may have been enjoyable in first class but was much more arduous in economy. Upon arriving in Osaka, the journey from the airport to the conference centre proved to be quite an ordeal, mainly due to the lack of signs in English. After much stumbling about, looking lost, I was fortunate enough to meet a couple of conference delegates, who were able to assist me in looking lost until we eventually could figure out which train we were meant to be getting.

The conference centre, known as the Grand Cube, is a massive 12 storey building situated on an island in the centre of Osaka. The conference was spread over rooms from the 3rd floor to the 12th floor of the conference centre, with the 12th floor offering spectacular views over Osaka. I was given student accommodation in the hotel NCB, which was only about 200m from the conference centre. The rooms were small but very clean and comfortable with excellent air conditioning. Breakfast in the hotel was not what I was used to back in Scotland, but instead consisted of soup and boiled rice, which is definitely healthier than a fry-up.

The conference kicked off with the 60th anniversary ceremony of the IUCr, followed by the opening ceremony of the XXI congress of the IUCr. During the opening ceremony, the Ewald Prize was presented to David Sayre, after which he gave the Ewald Prize lecture. The lecture focused on one of his most recent projects, the 3D imaging of the biological cell by single particle x-ray diffraction. He also discussed his memories of the first ever IUCr meeting and raised more than a few laughs when he asked for a show of hands from anyone else in the audience who had attended the first meeting. From my vantage it did not appear that anyone in the audience could responded to his request. It was very interesting to hear him talk about his memories of attending the first IUCr and how he listened to talks by people like W. L. Bragg and Dorothy Hodgkin.

The opening ceremony was followed by a welcome reception at the Rihga Royal Hotel next to the conference centre. We were treated to a fine buffet dinner, a plentiful supply of Japanese lager and music from the Osaka City University Concert Band. By 10 pm the evening was coming to an end, jetlag had finally caught up with me and I was as tired as I have ever felt in my life. So I was grateful that my hotel was only 200m down the road and my nice comfortable bed was there, waiting for me. Unfortunately I got caught in a very heavy and very sudden rain shower on the walk back to the hotel. I later learned this is typical for the region, prompting me to buy an umbrella to avoid similar soakings. I was soaked to the skin by the time I reached the hotel; and when I walked through the hotel lobby, I left a trail of puddles all the way to the elevator. I had never been so grateful to get to my bed in all my life.

The first full day of the conference started with a plenary lecture by Sumio Iijima on carbon nanotubes. He discussed the use of high resolution electron microscopy in combination with synchrotron x-ray diffraction to direct structure determination of single molecules such as higher fullerene molecules and metallofullerenes. This combination of techniques allows effects like the electro-migration and diffusion of atomic defects on the graphene sheet to be observed.

For me the highlight of the afternoon microsymposium titled "Growth of single crystals for neutron and x-ray investigation by the floating zone and other techniques" was a talk by Geetha Balakrishnan. He discussed the use of optical image furnaces at the University of Warwick for the synthesis of single crystals with sufficient size and quality for neutron diffraction experiments.

As the majority of my research has focused on powder diffraction studies, it is no surprise that my highlights of the week have a strong powder diffraction theme. Kenneth Harris gave a keynote talk titled "Advances in direct-space structure determination of molecular materials from powder diffraction data", which summarised the evolution of structure determination from powder data over the course of his career. He focused on the fundamental aspects of direct space structure determination using XRPD data to solve structures and presented a range of examples.

The Wednesday morning microsymposium on "Powder diffraction studies of hydrogen storage materials" provided an exciting introduction to a very topical subject. Of the five excellent talks during the morning session the highlight was the one by Toyoto Sato on structural investigations into metal borohydrides by XRPD and NPD, coupled with computational studies. He discussed the requirements of a good hydrogen storage material and demonstrated that none of the materials studied so far meet these requirements. He went on to discuss the methods of synthesis for the complex rare-earth aluminium phases under study and summarised the decomposition studies that had been carried out on these materials. This talk provided insight into the subject of hydrogen storage materials and a good summary of the work that had been carried out by his group.

Another microsymposium that I really enjoyed was "Developments in structure solution and refinement from powders" on Wednesday afternoon. This session had some excellent talks in it, particularly from Maria Burla and Kenneth Shankland, but the highlight had to be watching my supervisor, Chick Wilson, giving a talk on neutron powder diffraction. This is work that he has been doing with my colleagues Marc Schmidtmann, Paul Henry and Mark Weller and focuses on developing methods towards routine refinement of hydrogenous materials using neutron powder diffraction. Most of you will be used to watching Chick give talks on single crystal x-ray and neutron studies of hydrogen bonded materials, so it was fun to watch him talk about extending these studies into powder materials. There is hope for him yet.

The last couple of days of the conference were overshadowed and diminished by the sad news that Andy Parkin had died. Andy was a post-doc in Chick's group when I started doing my PhD and provided a lot of help and advice during the first 6 months, which continued after he had been made a lecturer within the chemistry department. The shock of the sad news about Andy quickly spread through the delegates at the conference and the level of distress at this news showed just how highly Andy was thought of by everyone in the Crystallography community. He will be sorely missed.

Susanne Huth - University of Southampton; Chair of the YCG

After Florence in 2005, this year saw the 21st congress of the IUCr in a marginally more exotic location: Osaka, Japan. Having gained a bit of conference experience at the national level with the last three BCA Spring Meetings and a couple of CCG autumn meetings I felt the time was right to start exploring the international stage. Full of ambition I submitted an abstract, which, very much to my surprise, was accepted for a talk – now I really had to think of a way to get myself to Japan! Luckily, due to the very generous support from my two sponsors, the CCDC and Pharmorphix Ltd., and thanks to the Durward Cruickshank Prize the funds for the long journey were secured and early on Thursday 21st August I found myself together with the rest of our group boarding a plane set for the land of the rising sun.

Slightly jet-lagged we arrived at the Grand Cube in Osaka and dived more or less straight into the Satellite meeting "New routes to crystallographic data publication" organized by Simon Coles. Despite being on the Saturday before the official opening of the IUCr08 a lot of delegates attended this workshop. In the morning sessions 10 talks introduced the audience to the different issues of (open) data archives and the actual publication process along with reuse of data and databases. First up was Brian McMahon presenting the IUCr's perspective and calling for a White Paper to set the framework for publishing crystallographic data in its own right without being associated to the standard publication routes through journal articles. Other speakers included the Acta E and Acta F Editors, Bill Clegg and Howard Einspahr, as well as database representatives John Westbrook (PDB) and Frank Allen (CCDC), whilst Ashley Buckle (TARDIS project, Australia) and Simon Coles (eCrystals Federation) presented new approaches to the data dissemination problem. Further details including talk abstracts and the major points that were raised during the open debate in the afternoon session can be found at **http://eprints.soton.ac.uk/63072/**.

For the following seven days we saw session after session packed with exciting science and excellent speakers. Considering myself a chemical crystallographer, I first went to "New algorithms for single crystal and powder diffraction", eager to hear Rob Hooft talk about absolute structure determination using Bijvoet pair differences. With this approach it is possible to determine the absolute structure even for light atom structures using Mo-radiation making this a very convenient alternative to Flack's method. The next talk by Luc Bourhis was about toolboxes for small molecules (smtbx) and common crystallography (cctbx), which are available to the crystallographer through the new Olex2 program. The third speaker in this morning session was Lukas Palatinus who showed how dual-space structure solution methods are utilised in the charge flipping procedure. Following that we heard from Henning Sorensen how the gap between single crystal and powder diffraction can be closed by examining polycrystalline materials through total crystallography. The session was closed by Carmelo Giacovazzo's presentation on EXPO2008, a program for structure solution and refinement from powder data.

After this fairly intense session my stomach was rumbling and so I was magically drawn to one of the lunch seminars organised by various manufacturers, who treated attendees to a free Bento box – the Japanese version of a lunch box. Sipping my cold green tea and battling with chopsticks I explored the contents of my Bento box, which contained a curious selection of sticky rice and all sorts of pickles and jellies, whilst listening to the latest developments in crystal diffraction equipment.

The following short paragraphs simply summarise my personal highlights of this conference.

On Sunday Juan Manuel M. Garcia-Ruiz was the afternoon plenary speaker and impressed the audience with beautiful movies showing the growth of silica biomorphs forming non-crystallographic morphologies that are observable in living organisms.

An aspect of my research is concerned with charge density experiments and so the sessions dealing with the determination of electronic structures were of particular interest to me. Most of the leaders in the field were to be found and oral contributions were made by Philip Coppens, Claude Lecomte, Piero Macci, Anatoli Volkov, Peter Luger, Dietmar Stalke, Dylan Jayatilaka and Tayur Guru-Row, to name just a few. The presentations revealed new findings and theories and it was quite inspiring to listen to (and hopefully learn from) all these highly reputed crystallographers.

On Tuesday evening a sizable group of primarily female crystallographers gathered for the Satellite meeting "The Future of Female Crystallographers". In a very nice and relaxed atmosphere we heard from Kazue Kurihara, Jenny Glusker, Judith Howard, Louise Johnson and Irene Margiolaki the different challenges women face in science and how each of them has managed to establish a career. The most interesting account for me was Jenny Glusker sharing her experiences all through her academic life and I was thrilled to have had the chance to talk to her personally in the following mixer session.

The ultimate highlight for me was Mark Spackman talking about intermolecular interactions from a purely electrostatic point of view. Mark set the scene with a highly convincing (at least in my opinion) demonstration of the mapping of the electrostatic potential onto a molecule's Hirshfeld surface and how the packing of these units reveals striking complementarity. Co-crystals of benzene and hexafluorobenzene provided an impressive example. In benzene the H atoms are positive while the pi cloud has negative potential. In hexafluorobenzene the F atoms acquire the negative potential at the expense of the pi cloud. It instantly becomes clear why their co-crystal is built from alternating molecules stacked like pancakes.

A conference wouldn't be such a splendid affair without the conference dinner. Looking forward to sampling some of the fine Japanese cuisine, we went to join our group at their table amongst all the other dinner guests, but found ourselves escorted to a rather deserted looking table. Upon closer inspection we discovered a small sign stating "Vegetarian" matching our own 'special' badges. Surely we were to be in for a treat! Slowly other branded vegetarians (in)voluntarily filled the other seats and the general consensus was that this was a rather odd form of quarantining. The actual dinner did not improve matters very much but soon a plentiful supply of drinks made us see the comical side. Catching up with other people from the BCA community it was soon decided to embrace Japanese culture even more and we headed for a Karaoke bar in town. It was a very merry round and nothing else shall be revealed, but the Japanese staff learned that night they should have charged per glass.

That encounter left me in perfect condition for Saturday, incidentally the day of my own presentation. Despite it being the final day of the IUCr08 the delegates showed some real endurance and the talks were still well attended.

And so the IUCr08 came to an end for me and whilst sitting on the bullet train to Tokyo I tried to digest the impressions of the long but thoroughly rewarding conference. I will always remember this congress for the people I was so fortunate to meet and see giving presentations. It was a truly overwhelming experience!

Stefanie Schiffers - University of Bath

The 2008 IUCr meeting held in Japan this year was for us a wonderful opportunity to combine a great meeting with the excitement of visiting Japan. Thanks to everyone who made this conference such a success. The kindness of the Japanese people was amazing; we missed the opening ceremony as we were invited by a random Japanese guy to a street festival, where we practised our Japanese dancing style.

The best talk I have ever heard was the keynote lecture of Masahiro Irie on Monday morning. His lecture with a lot of "exciting" experiments was like a TV program. He first irradiated diarylethylene derivatives during the lecture to show their colour change. And after pictures of single crystals which changed shape, he played Pinball with a single crystal needle and a metal ball, as the crystal was bending under irradiation .

There were two Photochemistry microsymposia on Monday, in which the talk by Leonard MacGillivray, about photoreactions on pyridylethylene derivates, was really good. Judith Howard's keynote lecture on Wednesday was really interesting, as she had shown so many possible methods (like high pressure, low temperature and magnetic switches) for non-ambient crystallography. An interesting talk with a good title (A molecular Legoland through halogen bonding) was given by Giuseppe Resnati, in which he cleverly organised the molecules over bonding modes.

The side program was just as well organised. On Monday we visited one of the evening sessions, a puppet theatre. The way we were led to concentrate on the puppets seemed like Black Light theatre, but there was no need for black light. The mix of tradition and humour made it an enjoyable show.

For the huge conference dinner on Friday evening I ordered a vegetarian dinner, which was served at one of the "out-of-the-way" tables. We had to have gallows humour, as our portions were so small that we had to steal some bread and ice cream from other tables. After the lights were switched off at 9:40, we went into town for a great Karaoke night with bad singers and a lot of beer.

Halina Mikolajek - University College London

As a biochemist, I attended mainly sessions that covered crystallography of biological macromolecules. My favourite sessions of the whole conference were the talks on crystallising macromolecular complexes and on teaching macromolecular crystallography. Crystallising macromolecular complexes had been one of my PhD projects, in which I had problems to produce crystals that diffracted well enough. This session was very useful for new ideas. The teaching session was very interesting as it discussed the difficulties in teaching macromolecular crystallography. In one of these talks Annette Faust informed us about an online tutorial for learning

and teaching macromolecular crystallography that has been put together recently. I wish this had been available when I started learning crystallography, and guess what I will be recommending to anyone starting out in crystallography?

Around 1500 posters were exhibited over the conference time period. I was glad that I could discuss my poster, "Ligand binding to pentraxins", with a number of people who provided good comments and advice.

On the last day of the conference I attended the structural informatics and database session, where the talk by Thomas Lutteke caught my attention. Thomas discussed the requirement for quality checks for carbohydrate structures in PDB entries and provided the solution with his program. The program Structure Suite automatically analyses features of carbohydrate structures contained in the PDB: characteristic torsion angles, glycoprotein sequences and carbohydrate–protein interactions. This talk was particularly useful to me as one of the proteins I work with is glycosylated and I always wanted to do a quality check on my structure.

I thank the BCA for the Arnold Beevers bursary, enabling me to attend such an amazing conference.

Alex Bowyer - University of Southampton

With help from the BCA and an Arnold Beevers Bursary my attendance at my first international conference in Osaka was not a disappointment. Everything from the scientific lecture programme to the social events was designed to delight and enthuse. My interest in the field of protein crystallography was treated to a host of talks detailing macromolecular structures of interest, such as flaviviruses by Michael Rossmann's group and macromolecular association by Wayne Hendrickson. Of particular interest was the stop-action movie presented by Wei Yang, in which we were shown UvrD helicase unwinding DNA one base pair per ATP hydrolysed. It was fantastic to see how multiple crystal structures of UvrD-DNA complexes could be combined to so effectively visualise a molecular mechanism.

The conference presented not only individual protein structures, but also the advances in X-ray methodology and a whole host of other complementary techniques, such as SAXS and neutron scattering. The pre-conference workshop chaired by Simon Coles looked at 'new routes to crystallographic data publication', in which speakers presented their ideas and methodologies, and the subject was then opened up for general discussion. It was interesting that the last talk of the conference by John Westbrook, representing the PDB, also examined this challenging area and informed us of some of the steps being taken to address the issue. This seven day conference has certainly influenced my research and was an experience that will stay with me throughout my career.

Alex Hamilton - University of Bristol

The highlights of the early part of the week for me were Artem Oganov's talk on evolutionary algorithms for structure prediction, Dietmar Stalke's talk on charge density studies of organolithium structures with interesting bonding types and Daisuke Hashizume's talk on strained and hypervalent molecules. By the middle of the week crystal engineering had become the topic of choice, with an excellent microsymposium featuring Pierangelo Metrangolo on the rational design of molecular solids with halogen bonds, and Guillermo Minguez on the design of metal-organic frameworks combining hydrogen bonds and halogen bonds. Interesting presentations on polymeric frameworks by Susumu Kitagawa and Michaele Hardie showed the intrinsic beauty held within a crystal.
The highlight of the week for me was the talk by Gautam Desiraju. He gave a thought-provoking discussion of what a crystal is and why we spend so much time looking at them; which led to further talk that night in the bar! The congress ended, as ever, with the social banquet. Approximately a thousand people sitting to a multiple course Japanese banquet is a sight to behold, let alone orchestrate!

Helena Shepherd - University of Durham

The 21st Congress of the IUCr in Osaka was the first international conference I have been to and the sheer size of the meeting was one of many things that impressed me. On the Sunday I particularly enjoyed the talk by Trixie Wagner who presented an entertaining (think Star Wars!) beginner's guide to modulated structures.

On Tuesday morning there was a session on the electric and magnetic properties of molecular crystals. I was especially pleased to hear Eugenio Coronado discuss his research into network based molecular magnetism. The afternoon session about crystallography of planetary materials under extreme conditions was of particular interest for the experimental techniques used by the scientists in this field, and the dramatic effects of these extreme sample environments on relatively simple molecules.

Michaele Hardie presented some very striking supramolecular structures in a talk focussed on host-guest chemistry at the beginning of a session dedicated to such architectures on Thursday. The session on Thursday afternoon concerning co-crystals featured talks from Gautam Desiraju and Christer Aakeroy who both gave very informative talks within the area.

A Keynote from Mohamed Eddaoudi on Friday morning explored strategies for obtaining porous functional materials, using the molecular building block approach. A following session on metal-organic frameworks included Matthew Rosseinsky discussing the potential for selective chiral sorption in MOFs, and Len Barbour who showed interesting results of frameworks that are flexible enough to remain intact during solvent removal.

Saturday's highlight was a session on space groups and the generalisations. The session was full of complex and fascinating interpretations of symmetry and its applications within crystallography.

Outside of the conference Osaka had much to offer and thankfully I had a bit of spare time to explore the city and even

enjoy a trip to Kyoto. The welcome from the Japanese people and the great food and culture were all wonderful additions to a great conference.

Vicky Fawcett - University of Manchester

Lectures given by Joel Bernstein, Sally Price and Lian Yu were highly relevant to my current research. Joel Bernstein highlighted the importance of controlling the crystallisation of a specific polymorph, particularly within the pharmaceutical industry. The talk presented a number of factors that can influence crystallisation of a certain polymorph. Sally Price illustrated the use of computation to predict crystal structures and calculate their energy. Examples of published predictions were given and these provided a number of useful references to follow up after the conference. Lian Yu presented work demonstrating how an understanding of polymorphism can be used to study the crystallisation process. This work is of great importance to the chemical industry, in particular pharmaceuticals, and highlighted many different mechanisms of growth. This presentation also gave me a number of ideas for new polymorphic systems to work with.

A lecture by Laszlo Fabian inspired me to investigate the use of statistical methods to determine which molecular descriptors are significant to my research; and Colin Pulham's presentation on high pressure crystallisation of polymorphs was of interest to me, as I had not previously considered changing the pressure in my crystallisation experiments.
I presented a poster entitled "Polymorphism from a solution perspective: Rationalisation at the molecular level". On the whole, people seemed interested in my results. This opportunity to discuss my current and future work with my peers led to the generation of new ideas and key contacts about potential collaborative projects using X-ray analysis within my work. I was also challenged with some questions that I had not previously considered, which I believe will allow my research to progress more effectively. From other posters I was able to pick up a number of ideas regarding my experimental work, although the computational techniques I use were not heavily represented.
I would sincerely like to thank the BCA for awarding me an Arnold Beevers Bursary which has allowed me to attend such a prestigious and informative conference.

Luca Russo - University of Newcastle

I arrived in Japan on Thursday 21/08, landing in the impressive setting of the Osaka airport. On the first night I had the chance of exploring the very lively Namba district, also having my first Japanese (crab) sushi.

On the Saturday I attended the workshop 'New routes to crystallographic data publication', with very intense discussions about the most suitable criteria to adopt towards a reasonable compromise between effective data dissemination and adequate data quality. Among the most interesting lectures on Monday afternoon was the one from Simon Coles, providing an update on the latest web resources available for teaching and outreach in crystallography, namely the eCrystal repository, also covering the related implications towards the peer review process. On the Tuesday, I chose the MS32, 'Nanostructure refinement and solution', providing interesting highlights on the analysis of partially ordered materials at the nanoscale. On Thursday I attended the MS59, about 'Chemical recognition and supramolecular architectures', where I found particularly interesting the summary given by Giuseppe Resnati on his extensive work on halogen bonding. I was also intrigued by the final talk by Roeland Boer, providing some examples of macromolecular-based supramolecular architectures at the end of a mainly small-molecule based symposium. In the same afternoon Armin Wagner provided an amazing video-demonstration featuring the manipulation of microcrystals with laser tweezers.

As usual, this was a great chance to keep in touch both with the ongoing development in and around my research area and with old friends. From this, my first visit to Japan, I shall remember the beautiful settings and temples in Nara and Kyoto, a dinner in a traditional (no English menu!) sushi bar and a well-planned culinary trip to try a Kobe steak.

Carl Schwalbe (Ed.)

The highlight of the session celebrating the 60th anniversary of the IUCr was an invited lecture by Ted Baker. Given the almost impossible task of surveying the whole field of crystallography, he achieved exactly that with a masterly lecture on "Crystallography and the world around us". He began by tracing the study of snow crystals from the 17th century to the present day. Saluting the contributions of great crystallographers including Lawrence Bragg, Linus Pauling and Dorothy Hodgkin, he proceeded to celebrate some of the greatest achievements in structural biology. He delighted the audience with a show of patterns that recurred in small-molecule and macromolecular structures alike.

The Ewald Prize was awarded to David Sayre. Remembering his key paper of 1952 on direct methods, we might have expected his prize lecture to contain purely historical reminiscences. Instead we were treated to an electrifying glimpse into a possible crystallographic future. Using data from the most modern synchrotron sources and applying concepts from remembered conversations with great scientists like Arthur Lindo Patterson, he and his team have obtained diffractive images of a single cell. In the future crystals may become redundant, but we crystallographers will still be employed because of our superior knowledge of diffraction. The International Union of Crystallography might have to change its name to the International Union of Diffraction; unfortunately those initials are already in use! Those of us who had hurried directly to the opening sessions now needed to return to our hotels to change clothes for the welcome reception. Unfortunately the food ran out within 20 minutes of the starting time. We who arrived late found empty serving dishes with neat labels suggesting that they had once contained delicious Japanese and western food. We became the unwitting subjects of a nutrition experiment testing whether soybeans and crackers, the only things left, were capable of sustaining human life.

The results of this experiment being positive, I was back

at the Grand Cube the next morning for a microsymposium on water clusters, which imaginatively juxtaposed results on hydrated proteins, nucleotides, metal polycarboxylates and polyoxometalates. Masayoshi Nakasako plotted water molecules from the Protein Data Bank, showing that their hydrogen bond partners cluster around the vertices of a tetrahedron. Molecular dynamics simulations suggest that surface hydrogen bonds between water and polar protein residues persist for a long time. As proteins at work change their conformation, e.g. to capture a substrate, their water framework adapts. Catalina Ruiz-Perez described several water motifs found embedded in metal polycarboxylate crystal hosts and demonstrated the interdependence of water clusters and crystal host. Yoko Sugawara reminded us that the change between A-DNA and B-DNA is driven by changes in humidity. Therefore it is worthwhile to study the water clusters in a series of nucleotide hydrates by X-ray and neutron diffraction as phase changes occur under variation of humidity and temperature. Tomaji Ozeki designed host-guest complexes with metals as joints and ligands as pillars, creating a host which leaves spaces for a primary guest and possibly water as a secondary guest. If the host and primary guest are well matched in both size and charge, there is no opportunity for water. Incompatibility in size, if limited, allows room for single water molecules; if major, it may provide for water channels. Incompatibility in charge leads to voids which can be occupied by clusters of up to of 14 water molecules.

We kept busy at lunchtimes attending presentations by commercial or non-profit organisations with a tasty Japanese Bento box lunch as the reward. These lunches consisted of a good-sized portion of boiled rice accompanied by a selection of meat and fish enlivened by piquant pickled vegetables. It would be invidious to mention the innovations of any of our excellent commercial suppliers while omitting their equally excellent peers. However, three presentations by non-profit organisations deserve special mention. The International Centre for Diffraction Data described the evolution of the Powder Diffraction File starting with a list of peaks, then adding atomic coordinates, and now beginning to store entire digitised traces. Experimental developments have enhanced the effectiveness of traditional phase analysis; with synchrotron radiation 10 phases comprising as little as 1% of the total composition have been found in vitamin pills! Another lunchtime presentation introduced the SPring-8 third-generation synchrotron with its very high energy of 8 GeV in its very large ring of 1436 m circumference. By around 2011 this facility will be complemented by an accelerator-based X-ray free electron laser, also of energy 8 GeV, featuring 2 x 10^{11} photons per pulse repeated at 10 to about 3000 pulses per second. Peak brilliance should be enhanced by 10^{10} compared to a third-generation synchrotron. A presentation by J-PARC set out with great clarity the advantages of neutron diffraction for structural research: if a wavelength of 1 Å is desired for a diffraction experiment, X-rays carry energy of 12.4 keV, electrons 150 eV, and neutrons only 81.8 milli eV. Thus with neutrons radiation damage is not a worry. J-PARC is open to international use, and proposal criteria follow the recommendations of the International Union of Pure and Applied Physics.

The keynote lecture by Judith Howard on “Some structure-property relationships” had a starting time of 8:30 on Wednesday morning, the midpoint of the conference. Fatigue had set in. Fortunately Judith’s talk was as stimulating as a big cup of coffee. Beginning with conductivity and superconductivity in organic compounds, Judith showed a correlation between structural and electrical properties: kinks on a plot versus temperature of cell parameters matched kinks on the resistivity curve. Other studies related thermochromism, photochromism and gas absorption to structure. Once again Judith’s attitude to apparatus was noteworthy: if what she needed was not commercially available, she would design it herself and then cheerfully offer it for collaborative use.

The Friday sessions were topped and tailed by two exciting keynote lectures dealing with opposite ends of the pharmaceutical discovery and development process. Tom Blundell began with the search for suitable protein targets. Biological space, defined by gene products, is huge but finite. Chemical space (the space of compounds) is potentially infinite. The traditional use of structural data to relate chemical compounds to biological targets is by optimisation of a lead compound, retaining key hydrogen bonds and efficiently filling pockets. High-throughput X-ray crystallography now makes it possible to screen weakly binding small-molecule ligands and elaborate them into lead compounds.

Michael Zarowotko illustrated the use of co-crystals to improve the properties of a drug. The important anti-epileptic drug carbamazepine forms a variety of polymorphs and solvates including a poorly soluble dihydrate, leading to variable oral bioavailability. Co-crystals of carbamazepine and saccharin show improved reproducibility and solubility. The solubility of fluoxetine hydrochloride (Prozac) is improved by making co-crystals with succinic acid. Homochiral co-crystal formers may lead to the resolution of enantiomers. The hierarchy of hydrogen bonds embodied in the Cambridge Structural Database can be exploited to design co-crystals.

A “first” for most delegates was the chance to see Osaka by amphibious bus. This surprisingly successful Japanese technology gave us a two-phase sightseeing trip, starting with a street-level view of the city. We then had a brief opportunity to stretch our legs while the bus reconfigured its propulsion system, after which we re-boarded, the bus glided into the water, and we enjoyed a mini-cruise on the river.

My impression of the conference banquet Friday evening differs from some of the other reports here, possibly because Joan and I were seated at a non-vegetarian table. I have been a long-term sashimi- and sushi-refuser, partly because I regard the discovery of fire as one of mankind’s greatest achievements and partly because I imagine fish parasites seizing with delight on a new flavour of host. However, after a certain amount of liquid refreshment and a degree of arm-twisting by my companions I tried these dishes and lived to tell the tale. There followed a variety of delicious cooked food and salads, which we washed down with excellent Japanese lager that had the versatility to complement all these flavours.

AmphiBus

The strong UK delegation at the General Assembly of the IUCr. Their happy smiles have been attributed to knowledge that the meeting was about to finish. An alternative explanation relating their facial expressions to the canned drink in the foreground cannot be fully evaluated. Examination of the label at high resolution reveals the words "Premium" and "Suntory", a manufacturer of good whisky (though not as good as Scotch!) but also of juice drinks.

Dr Andy Parkin (1975-2008)

Andy Parkin at the BCA meeting in Manchester 2004. Photo kindly provided by John Warren

Dr Andy Parkin (1975-2008) - an Appreciation

IT was my privilege to know Andy Parkin for around 10 years, and to work with him for five successful, productive and in all senses rewarding years in Glasgow. Andy was a Lecturer in Structural Chemistry at the University of Glasgow, appointed in September 2006 after a period of three years as PDRA with me; we continued to work closely together until his untimely passing on 28 August 2008.

Andy approached his work with determination, enthusiasm, generosity and enormous good humour. As a friend and colleague we had so many good times together both inside and outside science; he helped me drink gallons of coffee, and more than the occasional touch of something stronger; bailed me out whenever I had forgotten something, which was often; helped generate so many ideas and shared the cowboy hat we put on when a particularly crazy one was being discussed, and was like a kindly older brother to so many in our research group.

Andy was trained in crystallographic techniques and applications working with **Simon Parsons**, **Peter Tasker** and **Len Lindoy** during his PhD at the University of Edinburgh and subsequent post-doctoral positions in Edinburgh and Sydney. As a researcher he was both enthusiastic and innovative, taking basic crystallographic techniques and pushing them in new directions, for example in looking at small or difficult crystals, developing methods for growing crystals and interfaces *in situ* using electrocrystallisation, and making high profile advances in the area of structural comparison of solid-state molecular materials, in work with **Chris Gilmore**. Andy drove the development of a software package in this area, *d*SNAP, which has over a hundred users around the world, and his development of the concept of "Structural Genetic Fingerprinting" for the quantitative comparison of whole crystal structures was a genuine breakthrough that had a high impact in the scientific community.

He was popular with staff and students in the Department of Chemistry and in the wider community, reflecting his enthusiasm, his willingness to give generously of his expertise and energy, and recognition of both a passion for, and expertise in, his area of science. He was also, although still early in his career, already influential in the community. He had very significant involvement with the BCA, including being the inaugural Chair of the Young Crystallographers' Group, the winner in 2007 of the CCDC Young Scientists Award and a member of the Committee of the Chemical Crystallography Group. He organised a very successful meeting of the CCG here in Glasgow in Autumn 2006.

Andy was also involved more widely in contributions to Chemistry and science in general. He was instrumental in establishing the partnership we have with Rigaku in an innovative and challenging diffraction development programme, and made the initial contact with **Ann McKechin** MP that led to her accepting our invitation to inaugurate the Cruickshank Diffraction Laboratories, opened in the presence of Durward in a ceremony in Glasgow in 2006. Andy was also very active in outreach programmes; in partnership with **Gordon Barr** he designed and displayed the "Chemistry Cow" at the 2006 Cow Parade in Edinburgh; Chemistry on a Cow? What a bizarre idea, but what an inspired idea! Subsequently this educational and publicity vehicle for Scottish chemistry was unveiled in the Department by the Chief Science Advisor for Scotland, Professor **Ann Glover** (at Andy and Gordon's invitation), and has been on display since then at the Glasgow Science Centre.

Outside science, Andy was an enthusiastic climber, cricketer and kayaker, with a love for all sports. He met his wife **Kylie Schumacher** during his time as a post-doc in Sydney, and they were married in January 2006, making their home

in Glasgow. Kylie shared Andy's passion for sport and they were regularly to be found kayaking both inshore and offshore.

Andy is a great loss and will be sorely missed by colleagues and friends alike. His popularity, and the sadness at his sudden and tragic passing, has been reflected in the many messages received since the announcement of his untimely death. He leaves a legacy of initiating innovative and challenging research, and of contributing in the broadest, most human sense to the success of Chemistry and Crystallography in the University, the BCA and more widely

Chick Wilson
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Dr Andy Parkin

THE first time I met Andy Parkin was at the Young Crystallographers' Satellite Meeting in Lancaster in 2006, incidentally being my first ever BCA Spring Meeting, and immediately his vibrancy and enthusiasm were striking. This was the second YC gathering after Andy had successfully organised the first ever YC satellite meeting prior to the BCA Spring Meeting in Manchester in 2004. Throughout the conference Andy stressed the importance of giving young people starting off in the field the chance to present their work in a relaxed and friendly environment without the pressure of scrutinizing questions from more senior crystallographers. The full lecture theatre and the variety of many excellent talks were direct proof of how right he was. The YC meeting ended with Andy calling for people to make this satellite a permanent feature and I was very tempted to become involved in this good cause.

Over the following year Andy moved on from YC activities and quickly became a significant contributor to BCA proceedings. At the CCG Autumn Meeting in Glasgow that same year Andy was not just engaged in hosting the event but was also one of the speakers presenting his work on using Hirshfeld surfaces and fingerprint plots to extract information about packing similarities of molecular crystals. This novel approach clearly demonstrated forward thinking and was soon recognized with Andy being awarded the CCDC Prize for Younger Scientists by the CCG at the BCA Spring Meeting in Canterbury in 2007.

Andy was also interested in actively promoting chemistry to the wider public and as part of this outreach the chem-oo-stry.org project evolved. The design of a chemistry cow to go on exhibit during the 2006 Edinburgh Cow Parade was an extremely creative effort that turned out to be very successful and attracted a lot of attention. The picture below shows the cow and Andy together with friend and co-chem-moo creator **Gordon Barr**.

Andy's career carried on to develop fast with more appearances at conferences and a lectureship in structural chemistry at the University of Glasgow and naturally he was scheduled to present his research at the IUCr08 in Osaka. However, shocking news reached the UK delegates on the morning of the penultimate day of the IUCr08 that Andy had passed away after short illness.

When standing for the post of chair of the YCG earlier this year I felt very grateful and honored to take on Andy's legacy to ensure the continuity of the YC community and associated events. Thanks to his initial efforts the YCG became the official fifth group of the BCA in April this year and we will seek an appropriate way to acknowledge Andy's immense contribution to the Young Crystallographers. It is still incomprehensible how a person so full of energy and compassion is not with us any more and in Andy the BCA community as a whole has lost one of its most original and promising members.

Susanne Huth
(on behalf of the YCG)

Andy and Gordon Barr with the chemmoostry.org cow at the launch of the cow parade in 2006

A Request from Havana for Help

In late August and early September Cuba was affected by two huge hurricanes barely a week apart: Gustav in the west and Ike in the east. Although Havana was not in the path of the highest winds, the city and the university still received costly damage.

In our institute we are assessing damages and discussing what to do. Our buildings did not suffer too much but some items of our scientific equipment, already poor and outdated, will not survive this blow as they have been soaked in water and in our tropical climate corrosion will unavoidably render them useless in no time and the electronic parts are also heavily damaged. Parts of the ceiling were blown away in one of our buildings and air conditioning and acclimatization equipment was partially damaged. Rain was our worst enemy.

We would like through the IUCr, to request all our colleagues and friends in crystallography around the world to help us as much as they can. Any help in infrastructure, equipment or financial resources is welcomed.

The goal is to rebuild our crystallography laboratory that is the only one in Cuban universities. Today we do not know if we will be able to recover our old diffractometers, and the country is putting all its resources into much more urgent needs than ours. Some may think that trying to make science in our condition today makes no sense and we should instead concentrate on other efforts. We instead strongly believe that the capability of a country to raise itself depends in its ability to see beyond the urgent and project itself to the future. There is much more than buildings and houses to be reconstructed. To lose our ability to make science, our ability to teach students in science and build skillful human resources, is to renounce the ability to build a better country. We cannot do that, and we will not do that. At least that much we owe to our youngest sons. Everything needed to make this possible will be done. We know we are not alone and we can count on our friends all over the world. We also ask if the IUCr could help us to channel any help that friends are willing to give us.

We have also decided to go on as planned with our crystallography school for July 2009. As you know we organize every two years an international school on crystallography where students mainly from Cuba and Latin America come and get first hand state of the art lectures by invited renowned professors. Over the years this school has been an important part in the curricula of our students in physics, material science, chemistry, engineering and life science. This school is attended by students from all over the country and from all universities in the country. We will submit the proposal for support to the IUCr in the next days. We also ask for professors willing to come to our school covering their cost and give lectures to please contact me so we can arrange the school program. We would like this year to give emphasis in protein crystallography, from single crystal to recent developments in powder methods. Yet as usual the school is open to other subjects. I take the opportunity to thank you personally for the friendly support over the years.

Kind regards

Ernesto

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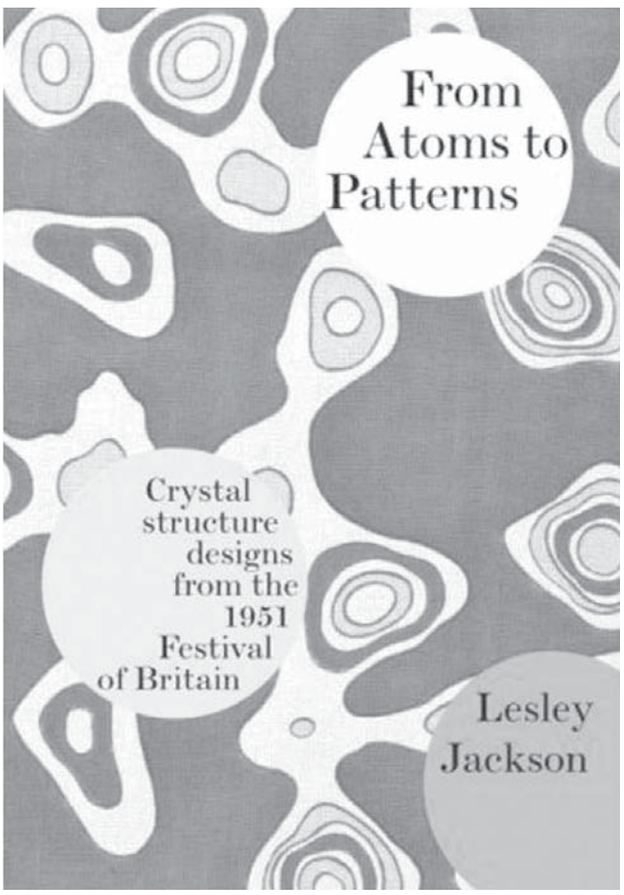
Books

From Atoms to Patterns: Crystal Structure Designs from the 1951 Festival of Britain

by Lesley Jackson



IN 1943, at the height of the Second World War, proposals were first mooted in the press that Britain should plan to stage a festival marking the centenary of the Great Exhibition of 1851. Though wildly optimistic at the time, this idea was in fact taken up by the post-war Labour government and by 1949 plans were well advanced for a national festival which would celebrate British achievements in science, industry and the arts. A derelict bomb-site on the south bank of the Thames - where today crowds queue for the London Eye - was chosen for the main exhibition buildings. These eventually included the enormous Dome of Discovery which was to house many of the science and technology exhibits, pavilions devoted to "The Land" and "The People", and most strikingly the Skylon, a 300 foot vertical feature which, like the British economy at the time, was said to have no visible means of support. Despite virulent criticism ahead of its opening, especially from right-wing newspapers such as the Evening Standard, the Festival of Britain was a huge success, attracting more than eight and a half million visitors over the summer of 1951.

The Royal Engineers built a footbridge across the Thames (alongside Hungerford Railway Bridge) to bring people directly onto the Festival site, where they were greeted - astonishingly - by a profusion of crystallographic design. Carpets, curtains, wallpapers, glassware, silverware, porcelain, furniture and even Nottingham lace were all manufactured for the Festival using designs adapted from crystal packing diagrams, mineral structures, electron density maps and Patterson projections. Many of the leading crystallographers of the day - **Lawrence Bragg**, **Dorothy Hodgkin**, **Max Perutz**, **John Kendrew**, **Monteath Robertson**, **Gordon Cox** and **Charles Bunn** - contributed structures to the project, as did **Helen Megaw**, who first had the inspiration to apply crystallographic patterns to industrial design. She in fact raised the possibility as early as 1946, in a letter to the director of the Design Research Unit, but it was not until 1948 that her idea was taken up by the architect **Mark Hartland Thomas** who, with Megaw as chief scientific consultant, founded the "Festival Pattern Group". This comprised some 28 manufacturing companies who would ultimately produce no fewer than 80 crystallography-based designs for the Festival. Many of these were only ever manufactured in small, prototype quantities, but a number went on to full commercial production - notably the "Festival" glass from Chance Bros., with a pattern based on the structure of the mineral apophyllite.

In the summer of 2008 the Wellcome Trust held an exhibition "From Atoms to Patterns" in which the Festival Pattern Group's creations, now held by the V&A and the Science Museum, were brought together for the first time since 1951. The exhibition was curated by design historian Lesley Jackson, and her book (A4, 124 pages), published in conjunction with the Wellcome Exhibition, provides a wonderfully complete and beautifully illustrated account of the achievements of the Festival Pattern Group. Chapter 1 comprises an extended introduction to the origins of the Group (including the delightful story that Dorothy Hodgkin's 1937 wedding present from Helen Megaw was a linen cushion embroidered with the crystal structure of aluminium hydroxide); Chapter 2 is a full-colour, facsimile reproduction of the 1951 "Souvenir Book of Crystal

Designs" published at the time of the Festival; and Chapter 3 provides an illustrated catalogue of the designs produced and their manufacturers (I especially liked the "Beryl" china from Wedgwood, the "Insulin" lace from A.C. Gill, and the "Haemoglobin" and "China Clay" ties from Vanners & Fennell). These Chapters are followed by short essays from Helen Megaw on "Pattern in Crystallography" and "Crystal Sructure Diagrams", a Chapter entitled an "A-Z of Crystal Structures" (showing not only the actual structures used by the Festival Pattern Group but also the dyeline prints from these, which were used to develop the industrial designs), and finally a Chapter containing brief biographies of all the crystallographers who contributed their structures to the design project. An extensive bibliography is provided for those wishing to read more deeply on the subject.

The book is produced to a very high standard and is a must-have for anyone interested in any or all of (i) the history of crystallography, (ii) the Festival of Britain, and (iii) British design and manufacturing. It would make an excellent Christmas present for any crystallographer!

Howard Colquhoun
University of Reading

Personal X-ray Reflections

Uli Arndt

Athena Press, London, 2006
Price £6.95
ISBN 1-84401 694 3, 177 pages

THIS INFORMAL autobiography introduces a talented, well-liked and much travelled physicist who developed widely-used X-ray crystallographic equipment. Including retirement projects, his active research career at Cambridge, the Royal Institution and elsewhere spanned 60 years. He was a former Secretary of the X-ray Analysis Group, precursor to the BCA.

Uli (strictly Ulrich) Wolfgang Arndt FRS (1924-2006) devoted a long and effective career to designing and developing apparatus for the observation and collection of data on the X-ray reflections of crystals. Much of this research, including his post-retirement activity, was carried out at Cambridge, either at the Cavendish or the MRC's Laboratory of Molecular Biology (LMB), but for most of 1950-1963 he was based at the Royal Institution (RI). Many crystallographers outside the fields of instrumental development ("finding an elegant solution tomorrow to yesterday's problems") and biological structures will recall his dapper and perceptive presence at conferences. Fortunately, his views and wit, as well as his happy family life, are evident in his autobiography, seen to completion by his daughters.

Arndt was born in Berlin to parents with German, Dutch and Russian backgrounds. Payment in guilders by his Dutch-German employers enabled Arndt's father Ernst, an engineer, to support his family in reasonable comfort during the 1920s German inflation. They moved to Darmstadt in 1930 when Ernst Arndt became a manager of a company making weighing and balancing machines. By becoming the British agent for his company, Ernst was able to extract the family from Nazi Germany in 1936, the same year that Uli's future boss Max Perutz (born 1914) moved from Vienna to the Cavendish. However Arndt experienced none of the privations of internment as enemy aliens or impoverishment suffered by Perutz and his parents. Indeed, Ernst Arndt, who had served throughout World War I in the German army, helped the British aviation industry in World War II, while Uli, although barred from the Services by the graduate Joint Recruiting Board, was able to engage in wartime research in the crystallographic laboratory under Henry Lipson at the Cavendish, headed by W.L. Bragg.

Uli's move to England at age 12 evidently enabled him both to retain his fluency in German and yet rapidly to lose his German accent in English. He was also able to compare education at the strictly disciplined German Gymnasium, with its emphasis on Latin, with that in England, first at Dulwich College and then from early 1939 at King Edward VI School, Birmingham. Having taken Greek and Classics for the School Certificate, his first science lessons were in September 1938 (against the school advice to do Classics). For 1939-1940, the school was evacuated to Repton, where Uli took his first Higher School Certificate (A-level analogue).

As a natural sciences (physics, chemistry, mathematics and electronics) undergraduate on a college scholarship at Cambridge, 1942-1944, Uli recalls teaching by W.L. Bragg, P.A.M. Dirac and G.F.C. Searle, and notes the advantages for meals and accommodation of his membership of the college fire brigade. His research at the Cavendish, nominally on the crystallography of magnetic alloys, soon involved overhauling an electron microscope and using surplus military components to construct X-ray tubes and a novel Geiger-counter X-ray powder spectrometer.

This experience set his course – he greatly enjoyed sailing on the Broads and in the North Sea – on the design of crystallographic instruments and the development of new techniques. Arndt reflects on the attraction of a scientific field in which competition was sufficient to be interesting but not so great as to promote cut-throat rivalry (except, perhaps, over area detectors). Such a choice, together with a fluency in languages and a liking for travel, contributed to an above-average participation in international summer schools. Conversely, as a scientist in non-university research institutions, he was happy to be free of academic teaching and administration. Also, although on the edge of the development of large-scale instrumental facilities, he contrived to minimise participation in the many international committees, so as to continue working at the bench. He quotes the disarming technique of Fred Sanger (winner of two Nobel prizes) in responding to invitations to serve by saying he was not very good at that sort of thing.

Having experienced working at several large national and international scientific laboratories, Arndt makes clear his preference for smaller, less bureaucratic and hierarchal institutes.

Arndt claims that he never applied for but was always offered new jobs. In 1950, D.P. Riley invited him into the Davy-Faraday Laboratory of the RI. Arndt's proportional-counter apparatus soon enabled much more data to be collected on biological material. Under resident professor E.N. da C. Andrade, the RI administration was in some disarray until W.L. Bragg was persuaded to leave the Cavendish and head the RI in 1954.

Arndt describes a memorable sabbatical year, 1957, beginning and ending in deep midwinter, at Madison, Wisconsin; apart from much air travel, he drove 12,000 miles over 7 months in a $170 Pontiac. Back at the RI, successful development of the three-circle X-ray diffractometer (as the spectrometer was now called) helped confirm Arndt in the opinion that he was more suited to single-crystal instrumentation design than the extraction and X-ray scattering of biological materials. Collaboration with B.T.M. Willis over two summers at AERE on the parallel design of X-ray and neutron diffractometers (constructed by Hilger and Watts and Ferranti) led to the book Single crystal diffractometry (Cambridge UP, 1966). In 1958, Arndt had married Valerie, a languages graduate who had spent time in China and Spain. They first met in 1955 on a skiing holiday; the book is partly a remembrance for Valerie, who died in late 2004.

In 1963, Arndt was invited by Perutz to join the MRC's LMB; he soon became involved with the screenless oscillation camera, subsequently marketed by Enraf-Nonius. Although sceptical about the effort expended on neutron beams for biology, Arndt was reluctantly persuaded to spend a trial year from 1972 at the ILL, Grenoble, as a UK representative. Returning to the LMB, he resumed work on the area detector, partly in conjunction with Enraf-Nonius, and produced a series of papers on the X-ray television diffractometer. In retirement, with the help of Retired Worker's (or "shoe-leather") and other grants, Arndt continued at LMB 1989-2004, improving micro-focus X-ray tubes, collaborating on optics with commercial manufacturers, and doing even more travelling. He reflects that many of the laboriously acquired skills for building electronic circuits from scratch, memorising valve or transistor details, or applying vacuum techniques, are no longer relevant.

Arndt is fairly frank in his observations about colleagues at the Cavendish, RI and LMB. From the experience of a year in each of the USA and France, as well as many shorter spells at institutions in several countries, he has perceptive comments about national attitudes to familiarity, status, specialisation and engineering. He emphasises that his reactions relate to individual workplaces at specific times in recent history.

This is not a formal autobiography in that there are no references or footnotes and there is no index, although the simple contents page neatly summarises Arndt's dates. Unusually in a scientific biography, the penultimate chapter is effectively an annotated list of remembered books, from children's stories to the classics. One regrets that Arndt was not spared time to write the second volume of his memoirs of a modest, accomplished and influential scientist. Durward Cruikshank, in our last telephone conversation, highly recommended Arndt's charming little book as an entertaining read. I suggest that other crystallographers would enjoy following this advice.

Derry W Jones
University of Bradford

Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to list please send them to the Editor, c.h.schwalbe@aston.ac.uk. The help of the IUCr listing is gratefully acknowledged.

3-6 March 2008
16th Annual meeting of the German Society of Crystallography, Erlangen, Germany
www.conventus.de

1-4 December 2008
GISAXS (Grazing Incidence Small Angle X-ray Scattering) Symposium, Boston MA USA
http://www.mrs.org/s_mrs/

16 December 2008
Biological Structures Group Winter Meeting: Protein:Nucleic Acid Interactions, University of Newcastle
http://conferences.ncl.ac.uk/BCA_BSG_Winter_2008/

3-5 January 2009
CCP4 Study Weekend: Experimental Phasing and Radiation Damage, University of Nottingham
http://www.cse.scitech.ac.uk/events/CCP4_2009/

19 January 2009
High Spatial Resolution Neutron Reflection Methods for the Study of Gold Supported Biomembranes, Cosener's House, Abingdon
http://www.isis.rl.ac.uk/largescale/LSS/MCM/MCM_main.htm

26-30 January 2009
2nd ILL Annual School on Advanced Neutron Diffraction Data Treatment using the FullProf Suite, Grenoble, France
http://www.ill.eu/news-events/workshops-events/fpschool/home/

10-13 February 2009
9th International Conference on Quasielastic Neutron Scattering, Paul Scherrer Institut, Villigen PSI Switzerland
http://qens2009.web.psi.ch/

15-19 February 2009
TMS Symposium on Emerging Applications of Neutron Scattering in Materials Science and Engineering, San Francisco, California, USA
http://www.tms.org/meetings/annual-09/AM09home.aspx

25-27 February 2009
Workshop "Neutrons and X-rays meet biology", Helmholtz Zentrum Berlin, Germany
http://www.iucr.org/news/notices/meetings/meeting_2008_124

2 March - 3 April 2009
Course in Neutron and Synchrotron Radiation for Condensed Matter studies, Grenoble, France
http://hercules.grenoble.cnrs.fr/accueil.php?lang=en

9-12 March 2009
17th Annual Meeting of the German Crystallographic Society, Hannover, Germany
http://www.conventus.de/dgk2009

19-20 March 2009
Polymorphism & Crystallization, Chemical Development Issues, Brussels, Belgium
http://www.scientificupdate.co.uk/conferences/polymorphism/index.php

28 March - 6 April 2009
12th Intensive School on X-ray Structure Analysis, Durham
http://www.dur.ac.uk/durham.x-ray-school

29 March - 3 April 2009
European Workshop on Self-Organized Nanomagnets, Aussois, France.
http://nanomagnets2009.neel.cnrs.fr/

31 March 2009
Control and Prediction of the Organic Solid State - State of the Art and Challenges, University College London
http://www.cposs.org.uk/

5-8 April 2009
Recent Advances in Characterization, Processing, Design and Modelling of Structural and Functional Materials, Lisbon, Portugal
http://www.demat.ist.utl.pt./materiais2009/

15-24 April 2009
PHARE 2009, a modular workshop on global PHAse REtrieval, Martina Franca, Italy **http://phare.ic.cnr.it/**

21-23 April 2009
BCA Annual Spring Meeting: Dynamic Crystallography, University of Loughborough
http://www.crystallography-meetings.org.uk/

3-7 May 2009
2009 International Conference on Neutron Scattering (ICNS2009), Knoxville, Tennessee, USA
http://www.iucr.org/news/notices/meetings/meeting_2008_125

24-30 May 2009
Seventh European Workshop in Drug Design, University of Siena, Italy
http://www.unisi.it/EWDD/

4-14 June 2009
High Pressure Crystallography: from Novel Experimental Approaches to Applications in Cutting-Edge Technologies. Erice, Italy
http://crystalerice.org erice2009/2009.htm

8-12 June 2009
X-ray Techniques for Advanced Materials, Nanostructures and Thin Films: from Laboratory Sources to Synchrotron Radiation. Strasbourg, France
http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=272

14-19 June 2009
Eleventh International Workshop on Physical Characterization of Pharmaceutical Solids, Stamford, Connecticut, USA
http://www.assainternational.com/

22-24 June 2009
ICNX-2009, International Conference on Neutron and X-Ray Scattering, Kuala Lumpur, Malaysia
http://icsd.ill.fr/ICNX2009.pdf

22-26 June 2009
Goldschmidt 2009 'Challenges to our Volatile Planet', Davos, Switzerland
http://www.goldschmidt2009.org/

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

27-30 July 2009
Energy materials research using neutron and synchrotron radiation, Helmholtz Zentrum Berlin, Germany
http://www.helmholtz-berlin.de/events/emns2009/

2-7 August 2009
SAGAMORE: Charge Spin and Electron Density, Santa Fe NM USA
http://www.sagamoreXVI.org

3-5 August 2009
Polarized Neutrons and Synchrotron X-rays for Magnetism 2009, Bonn, Germany
http://www.fz-juelich.de/iff/pnsxm2009

14-16 August 2009
Symmetry and Crystallography in Turkish Art and Culture: Satellite Conference of ECM-25, Istanbul, Turkey
http://www.lcm3b.uhp-nancy.fr/mathcryst/istanbul2009.htm

16-21 August 2009
25th European Crystallographic Meeting, Istanbul, Turkey
http://www.ecm25.org

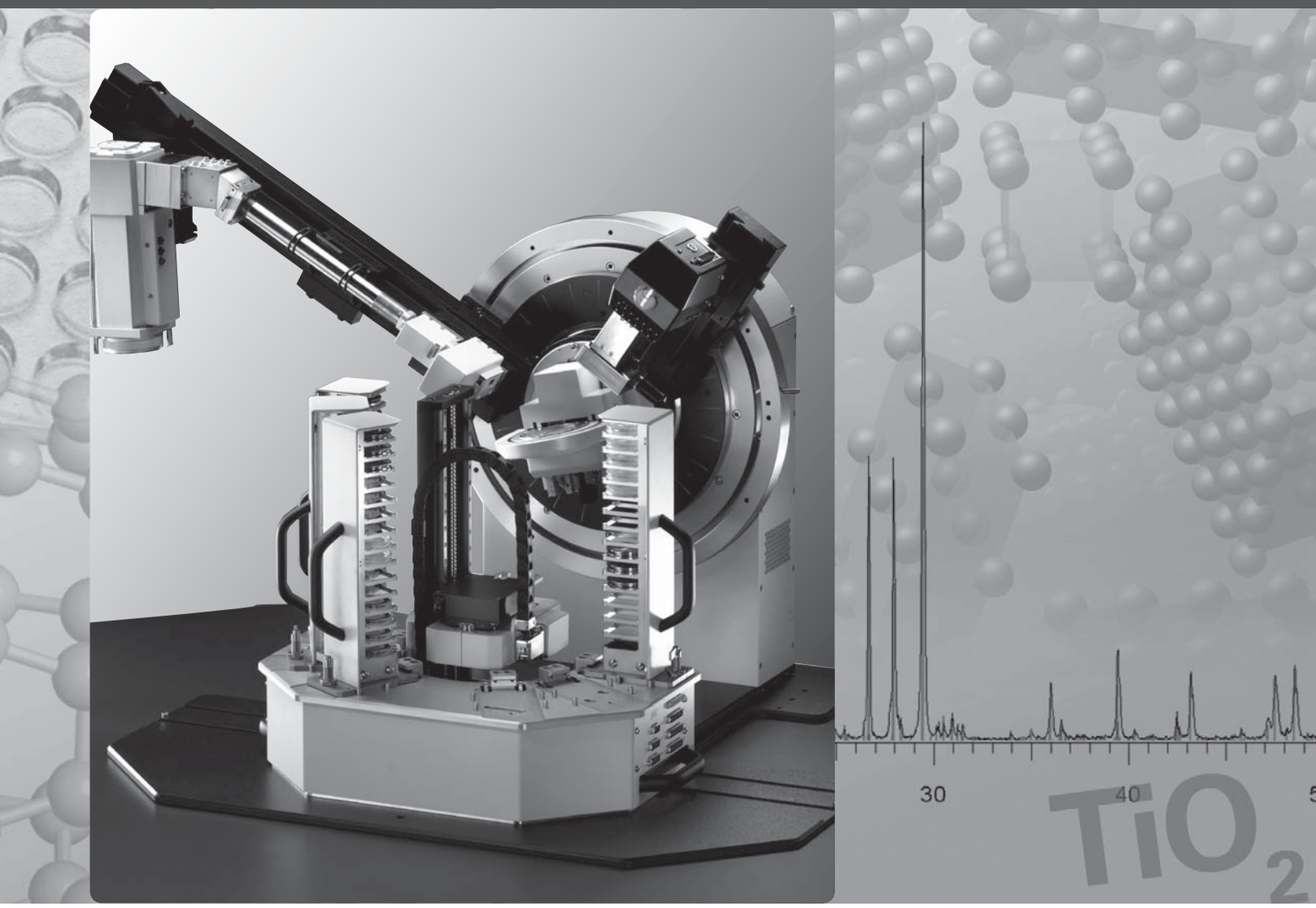
13-18 September 2009
Aperiodic09, University of Liverpool
http://www.aperiodic09.org

20-23 September 2009
European Conference on Solid-State Chemistry, University of Münster, Germany
http://www.gdch.de/vas/tagungen/tg/5585__e.htm

20-23 September 2009
Grazing Incidence Small Angle Scattering (GISAS) Conference DESY, Hamburg Germany
https://indico.desy.de/conferenceDisplay.py?confId=797

27 September - 2 October 2009
SRI2009: 10th International Conference on Synchrotron Radiation Instrumentation, Melbourne, Australia
http://www.sri09.org/

Bruker AXS



D8 DIFFRACTION SOLUTIONS – Manage your Analytical Challenges

D8 DIFFRACTION SOLUTIONS stands for continual progress in all X-ray core technologies: X-ray sources, X-ray optics, sample handling, detectors and software – all on a common platform. Two innovations for higher data quality and sample throughput enhance the D8 capabilities:

- Auto Changer for large sample batches
  - Effective instrument usage without user intervention
  - Reflection and transmission investigations without conversion
- LynxEye™ and VÅNTEC-1™ linear detectors
  - Large 3° 2Theta coverage for 150 times faster measurements
  - Huge 12° 2Theta coverage for 1 second Snap-Shot recording of kinematic processes

Contact us for more details and system demonstration! www.bruker-axs.com