

# *Crystallography News*

British Crystallographic Association



Issue No. 108 March 2009

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## **Loughborough 2009** p7-13



**CCP4** p21

**Aperiodic'09** p25

**25th European Crystallographic Meeting** p26

**Cueva de los Crystales** p29

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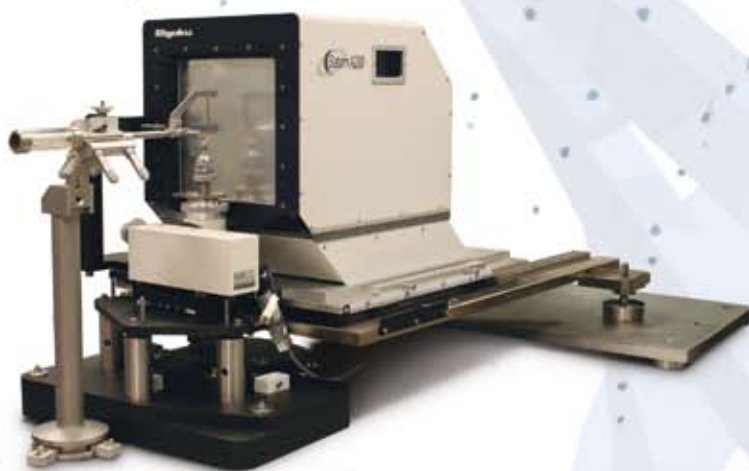
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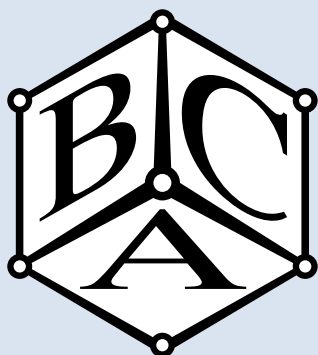
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***This month's cover:***  
Gigantic crystals  
in Mexico;  
springtime in  
Loughborough



# From the President



**BY** the time this column appears in print it will almost be time for the **Loughborough Spring Meeting**. As usual the Meeting commences with the **Young Crystallographers satellite meeting on Monday 20th April** and, this year, runs on until **Friday, 24th April**, with a special symposium in honour of **Frank**

**Allen**, the recently retired Director of the Cambridge Crystallographic Data Centre.

This year the theme is *dynamic crystallography* and **Simon Parsons** and the Programme Committee have done an excellent job in producing a wide ranging scientific programme that should appeal to the whole community. In addition, this year we have great pleasure in welcoming back the XRF community who will be running parallel sessions throughout most of the meeting. The full details of the programme appear later in this issue of *Crystallography News* and I would like to take this opportunity to thank Simon and his team for all their hard work in attracting such an impressive list of speakers. At the Spring Meeting my term as BCA President comes to an end so that this is my last column. I would very much like to thank all those who have helped and supported me throughout my term. In particular, I am most grateful to all the Officers and members of the Council, past and present, for all their hand work. I would also like to thank the current editor of *Crystallography News*, **Carl Schwalbe**, and his predecessor **Bob Gould** for all their patience with me and for their editing skills during the preparation of my columns.

I wish the next President all the very best for the next three years and can assure them that they will have a very strong team to support them.

Also coming to the end of their terms on Council are the three Ordinary Members, **Richard Cooper**, **Elsbeth Garman** and **Bill Clegg**. The Officers and I are most grateful to them for their dedication to their duties over the past three years and look forward to their continued input into the BCA.

In the context of vacancies on Council, may I, therefore, remind you that nominations for the new president and for the three new ordinary members of Council are now open and the Secretary, **Georgina Rosair** ([G.M.Rosair@hw.ac.uk](mailto:G.M.Rosair@hw.ac.uk)), is looking forward to receiving your nominations in the near future.

During my term it has been a pleasure to watch the BCA develop. During the last three years the Young Crystallographers have become firmly established as a Group within the BCA and their constitution is now being developed. The new BCA website has been launched recently, and I am very grateful to **Sandy Blake**, **Simon Coles**, **Mike Probert**, **Will Bisson**, and particularly **Richard Cooper** for all the hard work that they have put in over the last few months. It is also a pleasure to announce that **Richard Cooper** has kindly agreed to act as webmaster. We invite you to visit the website <http://www.crystallography.org.uk/> which also contains information about the Spring Meeting.

One of my final pleasurable duties as President is to be able to announce the results of the new Honorary Membership election. This year the Officers received five very strong nominations and after lengthy deliberations have recommended the election of two new Honorary Members of the BCA, **Frank Allen** and **David Watkin**, in recognition of their outstanding services to crystallography and the BCA. They will receive their letters of election at the Loughborough Meeting.

Finally, I close by wishing all the members of the BCA all the very best for the future, and I look forward to seeing as many as possible of you at the Loughborough Meeting.

**Paul Raithby**

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# From the Editor



**WRITING** this column on a dark January evening, I look forward to the brighter days of March when this issue will appear, and to the conference season it heralds. This year's BCA meeting will take place April 21-23 at the University of Loughborough, which we know from past experience will

provide a convenient and congenial venue. Under the theme of "Dynamic Crystallography" the Programme Committee has devised an exciting mixture of topics that will appeal to all types of crystallographers. This issue also contains reports on several fascinating group meetings that were held late last year. They should provide an added stimulus to meet the participants in Loughborough for further discussions.

Readers are reminded that other conferences have imminent deadlines for submission of abstracts. This year's European Crystallographic Meeting will combine up-to-the-minute crystallography with a dash of the exotic in Istanbul. The conference dates are August 16-21, but the abstract deadline is already March 15, and the deadline for cheap early registration is April 15. Details can be found at [www.ecm25.org](http://www.ecm25.org). Last November **John Helliwell**, as president of the European Crystallographic Association, led a site visit to Istanbul. If you will pardon the mixed metaphors, John is a high-flying jet-setting scientist who has wide experience of conferences, and he is a down-to-earth Mancunian who would readily detect and reprove incipient failures of organization if there were any. This issue contains a lightly edited version of his report, which describes with enthusiasm the palatial conference venue and the well-planned scientific sessions and support facilities. It is followed by the list of focus areas and microsymposium topics.

With the same impressive regularity as planetary motion, Aperiodic'09 will follow Aperiodic'06, 03, 00, 97, 94. Although this sequence is imposed by the calendar of meetings of the International Union of Crystallography, perhaps it is a metaphor for the way crystallographic brainpower can extract systematic knowledge even from such unruly subject matter. This year's International Conference on Aperiodic Crystals, conveniently sited in Liverpool, has May 1 as the deadline for abstracts. Crystallographers who, like me, have a particular interest in pharmaceuticals will find two more meetings to their liking: Pharmaceutical Powder X-ray Diffraction in Glasgow in May, and the British Association for Crystal Growth in Bristol in September. More details of all these meetings are given in this issue.

Our cover photograph shows the largest crystals any

crystallographer could aspire to see, up to 11 m in length. However, the estimated induction time for detectable crystals to appear is 1 million years, which might exhaust the patience of our collaborators and the Research Councils if we tried this in our home lab! I thank **Stanley Nyburg** for encouraging me to describe the origin and nature of these gypsum megacrystals in Naica, Mexico.

There is a story behind the picture, too. I had formed the idea that explorers were people like **Livingstone** and **Stanley** who lived in Victorian or Edwardian times, and the Earth had been well explored by the time **Amundsen** reached the South Pole in 1911. However, our cover picture was taken by **Richard D. Fisher**, a genuine 21st-century explorer. Having a particular interest in canyons, he is a gifted photographer who knows about anthropology as well. In 1992 he was the first foreigner to explore the Yarlung Tsang Po in Tibet, the world's deepest canyon. He will soon be returning to the most remote region in Tibet with a geology professor as his guide interpreter to do anthropological and geological research. It seemed almost inevitable that Rick would be drawn to the Cave of the Crystals after its discovery in 2000. This beautiful cave is full of perils for the photographer. At its ambient temperature around 54°C with 100% humidity a human can only function for six to ten minutes before severe loss of mental functions occurs. Electronic devices in cameras suffer too, so there are few sources of really high-quality pictures of these crystals. More stunning photographs taken by Rick can be found on his website, <http://www.canyonsworldwide.org/>.

Last year's "From Atoms to Patterns" exhibition at the Wellcome Trust showing the influence of crystal structures on design at the 1951 Festival of Britain delighted many visitors, and the book based on it received highly favourable comments in our December issue. **Lindsay Sawyer** has now found a supplier willing to re-create cloth in one or two of the patterns displayed. However, the minimum order quantity of 50 m exceeds the requirements for curtains in the Sawyer residence, and Lindsay is hoping that other crystallographers would like to join in and make up a sufficiently large order. In this issue the patterns are displayed and the colours are described.

With St. Patrick's Day approaching it seems appropriate to salute our Irish members. The American Crystallographic Association includes a sizeable number of Canadians, and this year's annual meeting will take place in Toronto. Perhaps the shamrock has traditionally taken a more modest place in the BCA than the maple leaf in the ACA, but we do have a contingent of Irish members, and more would be very welcome!

**Carl H. Schwalbe**



# Puzzle Corner

**THE puzzle in this issue has not been set by a question-master with a definite answer in mind. Rather, it is a feature of the English language that has puzzled me, and I hope readers will be able to supply answers.**

Sometimes a person's name is turned into an adjective. Mathematicians, physicists and musicologists seem particularly keen to do this, and "-ian" is the usual ending. It may be applied as a simple suffix:

Bohm - Bohmian  
Freud - Freudian  
Keynes - Keynesian  
Lagrange - Lagrangian  
Laplace - Laplacian

*Sometimes the accent is changed:*

Darwin - Darwinian  
Mozart - Mozartian

*Along with the change of accent, the pronunciation of the final vowel may be lengthened:*

Abel - Abelian  
Beethoven - Beethovenian  
Hamilton - Hamiltonian  
Mendel - Mendelian  
Wagner - Wagnerian

*The adjective may end with -c instead of -n:*

Galvani - Galvanic  
Napoleon - Napoleonic  
Ptolemy - Ptolemaic  
Volta - Voltaic

We crystallographers don't seem to do this. We discuss the Bohmian interpretation of quantum mechanics but not the Braggian interpretation of diffraction. We use the Hamiltonian to calculate our wave functions but not the Pattersonian to calculate our vector maps. So I ask our readers:

- (1) Can you name any crystallographers-turned-adjectives?
- (2) Can you name other important people-turned-adjectives, especially if their suffix has a different structure?
- (3) Can you formulate rules for the whole business?



## 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:

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# From the Secretary

## Announcement of Election to Council - President and three Ordinary members of Council

**THIS** year we have a vacancy on BCA Council for the Office of President, as **Paul Raithby** will have come to the end of his three-year term. We also have three

vacancies for ordinary members of Council since **Bill Clegg, Richard Cooper** and **Elsbeth Garman** have come to the end of their three year terms. Please send your properly seconded nominations for this position to me as soon as possible. I will accept nominations until two weeks before the date of the AGM on 22nd April 2009. If you nominate someone, please confirm that that the person you nominate is willing to stand for election.

**Georgina Rosair**  
Secretary to Council

## Puzzle Corner... ...SEPTEMBER ANSWER

**RESEMBLING** the algebraic notation on a chessboard, the columns will be assigned letters from "a" at the left to "t" at the right, and the rows will be assigned numbers from "1" at the bottom to "20" at the top. The International Union of Crystallography and its conference cities and countries run in straight lines starting and ending as follows:

Amsterdam n17-f9  
Australia i7-q15  
Beijing t5-n5  
Bordeaux i5-b5  
Cambridge r19-j19  
Canada j9-e4  
China d1-h1  
Crystallography o20-a6  
Florence i20-p20  
France c19-h14  
Geneva a2-f2  
Germany d20-j14  
Glasgow s15-m15  
Hamburg a18-a12  
International e6-e16  
Italy e6-a6  
Japan f7-j11  
Kyoto a5-a9  
Montreal t18-t11  
Moscow g19-l14  
Netherlands q8-q18  
Of b19-c19  
Osaka d14-d10, h20-l16, j2-f2, s12-s8  
Ottawa d8-i8  
Paris o2-s6  
Perth r10-n6  
Poland a20-f15  
Rome q13-t13

P	K	Z	G	E	N	E	O	F	L	O	R	E	N	C	E	L	L	B	D
S	O	F	V	E	S	M	Q	S	E	G	D	I	R	B	M	A	C	I	F
H	O	L	R	L	R	S	O	W	A	H	E	Y	Q	O	W	S	V	O	M
A	R	K	A	A	P	M	E	S	A	K	S	O	A	Y	F	D	I	L	O
M	B	O	N	N	N	C	A	T	C	T	A	M	E	C	I	N	F	O	N
B	Y	S	J	O	D	C	I	N	A	O	S	W	O	G	S	A	L	G	T
U	N	N	O	I	N	U	E	L	Y	T	W	H	P	F	I	L	B	Y	R
R	O	C	S	T	W	E	L	V	E	P	S	C	Y	L	J	R	O	M	E
G	T	M	A	A	F	O	D	R	H	O	W	D	A	D	Z	E	E	O	A
O	S	A	K	N	G	B	D	E	N	T	I	R	E	M	R	H	E	S	L
I	S	Y	A	R	X	A	V	A	W	H	T	R	Q	T	S	T	P	A	G
O	X	Y	A	E	M	G	P	I	C	S	Z	M	S	Y	I	E	C	K	U
T	W	P	O	T	T	A	W	A	U	Q	E	P	H	S	R	N	D	A	R
O	H	B	V	N	J	E	N	A	C	E	R	P	E	T	U	Z	U	X	D
Y	L	A	T	I	H	A	E	L	O	M	L	O	H	K	C	O	T	S	W
K	X	U	A	E	D	R	O	B	Y	Z	A	T	G	N	I	J	I	E	B
I	P	Q	F	A	N	O	R	T	U	E	N	I	T	H	G	R	F	E	O
F	U	N	I	T	E	D	K	I	N	G	D	O	M	A	A	P	J	W	N
G	E	N	E	V	A	K	A	S	O	M	A	R	A	P	E	G	I	F	D
G	U	R	C	H	I	N	A	T	O	M	V	E	T	W	A	S	R	A	W

Seattle q1-k7  
Stockholm s6-k6  
StonyBrook b11-b20  
Sweden k9-f14  
Switzerland l13-l3  
Union g14-c14  
UnitedKingdom b3-n3  
United States r7-g18  
USSR p7-m10  
Warsaw t1-o1

How many times does Osaka occur? 4, plus a few mutated forms.

The prizewinner this time is **Jim Trotter**.

# Loughborough 2009

**THE Annual General Meeting of the British Crystallographic Association will be held on Wednesday 22nd April 2009 at p.m. at 18.00 in Lecture Theatre 1 at the University of Loughborough. At this meeting we will elect a new President and three ordinary members of Council.**

## Draft Agenda

1. Approval of Agenda.
2. Apologies for absence.
3. Minutes of the last AGM (published in Crystallography News).
4. President's Report.
5. Secretary's Annual Report.
6. Northern Networking Events Report.
7. Report of the Treasurer to include Presentation of the Accounts for 2008 and the Examining Accountant's Report.
8. Acceptance of the Accounts.
9. Appointment of Examining Accountant for 2009.
10. Updating the BCA statutes and by-laws
11. Elections to Council.
12. Any other business.

**Georgina Rosair**  
Secretary to Council

## Scientific Programme: Dynamic Crystallography

### PLENARY LECTURES

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

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

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

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

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

### PRIZE LECTURE

CCG Prize: **Hazel Sparkes** (University of Durham) *Exploiting Charge Density - Insights into Structure, Bonding and Reactivity*

### 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**

**Andrea Mozzarelli** (University of Parma) *Single crystal absorption microspectrophotometry and X-ray crystallography: the perfect marriage*

**Elena Kovaleva** (University of Leeds) *Trapping Intermediates in the O<sub>2</sub> Activation Mechanism of an Extradial Dioxygenase in Crystals*

**Andrea Hadfield** (University of Bristol) *Towards a Complete Structure-function Description of a Polyaromatic Hydrocarbon Degradative Pathway*

#### 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*

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### **Dynamics at the Membrane (BSG)**

Chair: **Liz Carpenter**

**David Stuart** (STRUBI, University of Oxford)

*Title TBC*

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

**Steve Prince** (Manchester Interdisciplinary Biocentre) *Ion Channels, Scaffold Proteins and their Interaction*

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### **Dynamics of Radiation Damage (BSG)**

Chair: **Elsbeth 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*

**John McGeehan** (University of Portsmouth) *Radiation Damage Of Nucleic Acids and Nucleoprotein Complexes*

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### **Snapshots of Dynamic Processes (BSG)**

Chair: **David Stuart**

**Rick Lewis** (Newcastle University) *Molecular Architecture of the "Stressosome", a Signal Integration and Transduction Hub*

**Jasper van Thor** (Imperial College, London) *Experimental Challenges of Protein Dynamics in the Incoherent and coherent time-domains*

**Daan van Aalten** (University of Dundee) *Structural Snapshots of Glycosidases*

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### **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*

**Philippe Aeberhard** (University of Oxford) *Exploring Hydrogen Storage Materials Using Density Functional Theory Calculations*

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### **Dynamic Techniques (CCG/YC)**

Chair: **Lynne Thomas**

**Robert Feidenhans'l** (University of Copenhagen)

*Structural Changes at Short Time Scales*

**Robert Hammond** (University of Leeds) *Solution-Mediated Nucleation, Growth and Phase Transformations of Polymorphs: Combining On-line X-ray Diffraction and Molecular Modelling*

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### **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*

**Stephen Moggach** (University of Edinburgh) *Reactivity in Crystals at High Pressure*

**Stefanie Schiffers** (University of Bath) *Crystal Engineering and Solid-State Reactions*

**Lee Brammer** (University of Sheffield) *Flexibility and Dynamics in Metal-Organic Frameworks*

**Ann Chippindale** (University of Reading) *Bending, Twisting and Breaking: Chain, Layer and Framework Cyanides*

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### **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*

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### **Monitoring Crystals, Crystallization and Transformations 1 and 2 (IG/BACG)**

Chair: **Nick Blagden** (BACG) and **Alison Burke** (IG)

**Chick Wilson** (University of Glasgow) *Exploring Crystallisation Phase Space - Expect the Unexpected?*

**Paul Barnes** (Birkbeck College) *Opportunities for Observing the Synthesis and Behaviour of Functional Materials Using Synchrotron X-Ray Diffraction.*

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

**Roger Davey** (University of Manchester) *Monitoring Nucleation of Cocrystals: A Solution Chemistry Perspective*

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

#### **Speaker to be Announced at Meeting**

*Industrial Group/Young Crystallographers Prize Talk*

#### **Understanding API Phase Transitions (IG)**

Chair: **Brett Cooper**

**Paolo Avale** (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 Johnstone** (University of Edinburgh) *Identification of Driving Forces in High Pressure Phase Transitions Using the Pixel Method*

#### **Crystallography in the Pharmaceutical Pipeline (IG)**

Chair: **Matthew 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?*

**Jeremy K. Cockcroft** (University College London) *From the Industrial via the Academic Laboratory to the Court Room: Cyclovirs - A Pharmaceutical PXRD Case Study*

#### **Multiferroics (PCG)**

Chair: **Andrew Wills/Peter Hatton**

**Michel Kenzelmann** (PSI-ETH) *Multiferroics*

**Neil Alford** (Imperial College) *Ferroelectric Thin Films*

**John Claridge** (Liverpool)  
Title TBC

#### **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*

**Gopinathan Sankar** (University College London) *Application of Anomalous Scattering Methods in Determining the Structure of Active Sites in Complex Oxides*

**Alison Davenport** (University of Birmingham) *Dynamics of Salt Films on Dissolving Metal Surfaces*

#### **Hydrogen Storage (PCG)**

Chair: **David Keen/Ivana Evans**

**Marco Sommariva** (ISIS Facility) *Neutron Diffraction Studies and Complementary Techniques for H<sub>2</sub> Storage Materials*

**Andrea Baldi** (VU University Amsterdam) *Mg-Ti Multilayers: Nanostructured Hydrogen-Storage Alloys*

**Neal Skipper** (UCL) *Molecular and Atomic Hydrogen in Graphite Intercalates*

#### **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*

**Robert Bell** (UCL) *Simulating Adsorption Phenomena in Microporous Frameworks*

**Ashleigh Fletcher** (Strathclyde) *Title TBC*

#### **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*

**Y. Kataoka** (Rigaku, Japan) *Micro Spot Analysis of Electronic Components using Polycapillary Lens in Standard WDXRF*

#### **Portable Instruments (XRF)**

Chair: **Margaret West**

**Phil Potts** (Open University) *Portable X-Ray Fluorescence Analysis - New Opportunities, New Challenges*

**Mark Ingham** (British Geological Survey) *Analysis of Limestone & Dolomite*

**Deborah Cane & Duncan Slarke** (Birmingham Museum and Art Gallery) *Penguins & Precious Metals, the Use of the Hand Held XRF at Birmingham Museum & Art Gallery*

#### **Environmental Applications -1 (XRF/XRD)**

Chairs: **David Taylor** and **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*

**Clive Roberts** (Wolverhampton University) *Heavy Metals in Sediments of the Canal Network in the Black Country*

# Timetable, AGM Loughborou

	Day 0 Monday 20th April	Day 1 TUESDAY 21st April				Day 2 WEDNESDAY 22nd April	
9:00		Lecture Theatre 1				Lecture Theatre 1	
9:15						Plenary IG	
9:30		Young Crystallographers 4				Coffee 9.30-10.00	
9:45						Parallel Sessions	
10:00						Lecture Theatre 1	Lecture Theatre 2
10:15							
10:30		Registration/Exhibition 10.30-11.30			Lecture Theatre 4	Reactivity in Crystals-1 (CCG)	Reactions in Macromolecular Crystals (BSG)
10:45					XRF General (XRF)		
11:00		Lecture Theatre 1					
11:15		Lonsdale Lecture 11.30-12.30					BSG AGM 11.45-12.30
11:30							
11:45							
12:00							
12:15							
12:30							
12:45		Lunch/Exhibition/Registration 12.30-13.30				CCG AGM 12.30-1.15	Lunch/AGM
13:00	Lecture Theatre 1						
13:15							
13:30		Sessions 13.30-15.00			Sessions 13.30-15.00		
13:45		Lecture Theatre 1	Lecture Theatre 2	Lecture Theatre 3	Lecture Theatre 4	Lecture Theatre 1	Lecture Theatre 2
14:00	Young Crystallographers 1	Calculating Dynamic Properties (CCG/PCG)	New Synchronisation Instrumentation (BSG/CCG)	Multiferroics (PSG)	XRF Applications Workshops (XRF)	Reactivity in Crystals-2 (CCG)	Metalloproteins: Structure and Dynamics (BSG)
14:15						CCDC Prize Lecture	
14:30							
14:45							
15:00	Coffee 15.00-15.30	Coffee 15.00-15.30			Coffee 15.00-15.30		
15:15							
15:30	Lecture Theatre 1	Sessions 15.30-17.00			Sessions 15.30-17.00		
15:45		Lecture Theatre 1	Lecture Theatre 2	Computer Rm	Lecture Theatre 4	Lecture Theatre 1	Lecture Theatre 2
16:00							
16:15	Young Crystallographers 2	Dynamic Techniques (CCG/YC)	Complementary Techniques (BSG)	dSNAP Workshop	Portable Instruments (XRF)	Temperature-Dependent Crystallography (CCG)	Dynamics at the Membrane (BSG)
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						
17:45						Plenary (BSG)	
18:00		Exhibitors Forum 17.15-18.45			Exhibitors Forum (XRF)	Lecture Theatre 1	
18:15	Young Crystallographers 3					BCA AGM 18.30-19.00	
18:30							
18:45							
19:00						Conference Dinner	
19:15							
19:30							
19:45							
20:00	Young Crystallographers' Dinner	Dinner, Exhibition and Posters					
20:15							
20:30							
20:45							
21:00							



WEDNESDAY 22nd April		Day 3 THURSDAY 23rd April				Day 4 FRIDAY 24th April	
Theatre 1		Lecture Theatre 1		Lecture Theatre 4		Frank Allen Symposium	
(XRF/XRD)		Teaching Plenary (PCG) Martin Dove		XRF Keynote Method Validation			
9.45-10.15		Coffee 9.45-10.15					
Sessions 10.15-11.45		Sessions 10.15-11.45					
Lecture Theatre 3	Lecture Theatre 4	Lecture Theatre 1	Lecture Theatre 2	Lecture Theatre 3	Lecture Theatre 4		
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)		
13.30-15.00		Close 13.30					
Lecture Theatre 3	Lecture Theatre 4	Frank Allen Symposium					
Monitoring Crystals, Crystallisation and Transformations-1 (IG/BACG)	Environmental Applications of XRF						
15.00-15.30							
15.30-17.00							
Lecture Theatre 3	Lecture Theatre 4						
Monitoring Crystals, Crystallisation and Transformations-2 YC Prize Lecture	Trace Analysis (XRF)						
Theatre 1							
18.00-19.00							
Short time							
After 19.30 for 20.00							

**Ravi Yellepeddi** (Thermo Fisher Scientific) *Matching XRF and XRD Solutions with Analytical Needs For Cleaner, Safer and Healthier Environment*

## Environmental Applications-2 (XRF)

Chair: **David Taylor**

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

**Richard C. E. Morris** (Morris Analytical X-ray Ltd) *Where There's Muck There's Brass and Iron and Lead and Chromium....*

**Ian Croudace** (University of Southampton) *ItraX micro-XRF Core Scanner: Just What the Environmental Sciences Needed*

## Trace Analysis (XRF)

Chair: **Mark Ingham**

**Jamie Cutting** (Scott Wilson Ltd) *On Site Analytics: The Application of XRF to Contaminated Land Remediation*

**David Beveridge** (HARMAN Technology Ltd) *Determination of Traces of Heavy Metals in Water by XRF*

**Phil Russell** (PANalytical) *Trace Analysis on Alternative Fuels by Polarised EDXF*

**Mike Dobby** (Bruker AXS) *XRF - the new Trace Technique*

**Yoshiyuki Kataoka** (Rigaku Corporation, Japan) *A Simple and Rapid Method for Trace Element Analysis of Waters Using Benchtop Polarized Edxf Spectrometer*

**Chris Calam** (Thermo Fisher Scientific Niton Analyzers) *Trace Analysis using a Geometrically Optimised Large Area Drift Detector(GOLDD)in Portable XRF*

## Method Validation (XRF)

Chair: **Ros Schwarz**

**Debra Schofield** (Oxford Instruments Analytical Ltd.) *Method Validation - Working Our Way Through the ASTM Process*

**Eddie Birch** (CIQ Audit) *A Practical Approach to ISO 17025 Accreditation*

**Paul Thomas** (University of Loughborough) *Some Statistics Useful in Method Evaluation*

## New Developments in Instrumentation and TXRF (XRF)

Chair: **Margaret West**

**Christina Strelj** (TU Wien, Atominstitut der Österreichischen) *Developments in TXRF Analysis*

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

**Malcolm Haigh** (Spectro Analytical UK Ltd.) *Energy Dispersive XRF - Its Diversity and Capabilities*

## DSNAP WORKSHOP

dSNAP is a free computer program that assists the user to extract meaningful information from the Cambridge Structural Database by the following operations:

- \* 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

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](http://www.chem.gla.ac.uk/snap) or by emailing [dsn timer@chem.gla.ac.uk](mailto:dsn timer@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 Meeting 20th -21st April 2009

### MONDAY 7TH APRIL:

**12.00-13.00: Registration**

**13.00: Welcome: Susanne Huth** (University of Southampton)

**13.00-15.30: Session YC1: Chair: Graham Findlay**

**13.00-13.30: Plenary: Dominic Fortes** (Planetary Ices Group, UCL) *High-pressure neutron diffraction studies of ammonia hydrates, or how to spend five years indexing a powder pattern*

**13.30-13.45: Edward Bilbe** (University of Reading) *Mixed-Metal Copper, Silver and Gold Cyanides: Order/Disorder in 1-D systems*

**13.45- 4.00: Karthik Paithankar** (University of Oxford) *X-Ray Diffraction Studies On Multiple Single-Crystals*

**14.00-14.15: Craig Robertson** (Durham University) *Structure and Bulk Properties of Sulfur and Selenium Containing Neutral Radicals*

**14.15-14.30: Jeppe Christensen** (University of Warwick) *Crystallographic Adventures in Binary Intermetallics: Sb-Sn Revisited in (3+1)D Space*

**14.30-14.45: Arefeh Seyedarabi** (Queen Mary, University of London) *Domain swapping in Shigella flexneri IpaH9.8*

**14.45-15.00: James Haestier** (University of Oxford) *Effects of Cell Errors on Derived Parameters*

**15.00-15.30: Coffee & Tea**

**15.30-17.30: Session YC2: Chair: Arefeh Seyedarabi**

**15.30-16.00: Plenary: John Helliwell** (University of Manchester) *The Structural Chemistry and Structural Biology of Coloration in Marine Crustacea*

**16.00-16.15: David Millar** (University of Edinburgh) *The Crystal Structures of Two Polymorphs of RDX*

**16.15-16.30: Ivan Campeotto** (University of Leeds) *Structural Analysis of Engineered N-acetyl-D-neuraminic Acid Lyase*

**16.30-16.45: Kirsten Christensen** (Diamond Light Source Ltd.) *Open-Framework Germanates - Structures and Building Units*

**16.45-17.00: Adam Cowell** (University of Birmingham) *Co-Crystal Structure from Powders: Yes, We Can!*

**17.00-17.30: Break**

**17.30-19.00: Session YC3: Chair: Helena Shepherd**

**17.30-18.00: Annual General Meeting**

**18.00-19.00: Flash Presentations for Poster**

**Contributors:** You have 1 minute to make your poster sound the best!

**19.00-21.00 Poster Session with dinner and wine**

### TUESDAY 21ST APRIL:

**09.00-11.00: Session YC4: Chair: Suzanne Buttar**

*A themed session in special recognition of Dr Andy Parkin's contributions to chemical crystallography*

**09.00-09.05: Opening Remarks**

**09.05-09.35: Plenary: Frank Allen** (Former Director of the CCDC) *Energy Matters!*

**09.35-09.50: Anna Stevenson** (University of Bath) *Increase in Pore Size of Newly Synthesised Metal-Organic Frameworks*

**09.50-10.05: Andras Kallay** (University of Glasgow) *Studies of Unusual Proton Behavior in DMAN Proton Sponge Complexes*

**10.05-10.20: Samantha Callear** (University of Southampton) *Preparation, Characterisation and Structural Assessment of Solid Form Organic Compounds*

**10.20-10.25: Graham Findlay** (University of Glasgow) *Investigation of the Effects of Substituents on the Conformation of 5-Carbon Chains using CSD Search Results & dSNAP*

**10.25-10.50: Graham Tizzard** (University of Southampton) *Characterisation and Investigation of Structural Relationships of 4,4'-Disubstituted Chalcones*

**10.50-11.05: Craig Martin** (University of Glasgow) *Controlling the Formation of Co-Crystal Polymorphs*

**11.05-11.30 Registration for Main Meeting**



# Minutes of BCA AGM 2008

## BRITISH CRYSTALLOGRAPHIC ASSOCIATION

Minutes of Annual General Meeting held on 9th April 2008 at 18:00 in the University of York. The President (Paul Raithby) was in the Chair.

More than 100 voting members were present

### 1. Approval of Agenda

The agenda was proposed by Carl Schwalbe and seconded by Paolo Radaelli. The President had one item of AOB.

2. Apologies for absence: Christine Cardin, Judith Howard, David Watkin.

### 3. Minutes of the last AGM (published in Crystallography News)

These were accepted as a true and accurate record (proposed by Mike Glazer, seconded by Moreton Moore).

### 4. President's Report

The President announced that we were in the middle of a very successful meeting in an excellent venue and he thanked the speakers, poster presenters, exhibitors, sponsors, all those attending and particularly thanked John and Ivana Evans for assembling an excellent scientific programme. He also thanked Gill Moore and David Massey (his first BCA meeting) of Northern Networking for administrative support and the University of York Conference Office. Next year's meeting will be at Loughborough (20th - 23rd April) starting with the Young Crystallographers meeting. Simon Parsons (Edinburgh) will be the programme chair and the theme is dynamic crystallography. The provisional 2010 programme chair is Simon Coles (Southampton).

After due and careful consideration by Council, Paul Fewster and Bob Gould have been Elected as Honorary Members of the BCA. The nominations deadline for the next round is 31 October (nominations to the President). Bob Gould retires as Editor of Crystallography News and the President thanked him for his sterling efforts over the past 6 years. His worthy successor is Carl Schwalbe who will be producing his first issue in June. Sheila Gould has come to the end of her term as Treasurer so he asked for a vote of thanks for serving as Treasurer over the past 3 years, leaving the BCA on a very stable financial footing. Both Bob and Sheila Gould have been an enormous support to himself and his predecessors. Education Coordinator Chick Wilson regretfully resigned due to many other commitments. He has served Council for 11 years and the President thanked Chick for all his hard work and enthusiasm. Mike Probert (Durham) is his proposed successor and the President requested that this be ratified: those present agreed and wished Mike well in his new post. A new version of BCA website is being trialled, it is more flexible, with members of Council including the President able to add their own content. The website will be going live soon. Thanks were expressed to Jeremy Cockcroft for all his work on the previous website.

The President regretfully announced the passing of three eminent crystallographers since the last AGM; Durward Cruickshank, Keith Prout and Geoff King (a minute's silence was held). He was pleased to announce that there was a bequest from Durward Cruickshank's will for the BCA, and Council has used the money to set up the Durward Cruickshank Young Crystallographer's Prize, the first of which will be awarded at this meeting.

The IUCr meeting is in Osaka this August and the BCA nominated 21 respective members for committee membership and Chris Gilmore has been nominated for President of the IUCr. There will be 5 voting members representing UK crystallography at the General Assembly in Osaka. A bid is being prepared for the 2013 ECM meeting to be held in Edinburgh. The President also reminded members of the "From Atoms to Patterns" exhibition at the Wellcome Collection on Euston Road, London which runs until 10<sup>th</sup> August.

There were no questions on the President's report.

## 5. Secretary's Annual Report

The Secretary also thanked her predecessor Christine Cardin for her assistance and Sheila Gould for her role as Treasurer and Bob Gould for serving as Editor of Crystallography News and she wished Carl Schwalbe all the best in his new role.

The website is also undergoing changes and there was on-line registration again this year. There are online payment facilities for IG and CCG Group meetings which is important since cheques are becoming progressively obsolete. The PCG now have a wiki for their webpage to enable more rapid updating.

The Council has discussed email usage and recommend using compiled email lists or BCC so as not to disclose addresses to others as once an email is sent you have no control over it. She reminded members who have changed their email addresses to inform Northern Networking through the BCA Website and their Group secretaries. On a related matter the IUCr's World Directory of Crystallographers which is accessible via the IUCr website needs to be kept up to date to be useful so she encouraged members to add their entry or update it if they are already in the directory.

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

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

Chris Gilmore encouraged members to sign up with the World Directory of Crystallographers as they are then eligible for a 20% discount on IUCr and OUP books. Mike Glazer asked what happens with the WDC entries for people who have

passed away. Chris Gilmore said he will raise this matter in Osaka, while Sandy Blake suggested Chester (IUCr) remove their email addresses from their entry.

## 6. Northern Networking Events Report

Gill Moore reminded members that Northern Networking Events do the

administration for the BCA and look after the annual conference. The Association has 723 paid members. She asked that those who pay by standing order ask their banks to identify the transaction by the member's surname so the member can be identified. Some members are still paying £12 by standing order and they need to notify their bank to change this to the correct amount. Online payment has been very successful; it is much easier to trace payments. Gill also thanked Sheila Gould very much for serving as Treasurer with tireless assistance and patience.

Recently the 104th issue of Crystallography News was produced and Incoatec GmbH joined as a new advertiser; she thanked the 18 advertisers and listed them, thanking them for their valuable contribution to the BCA. She thanked Bob Gould for his excellent editorship of Crystallography News and looked forward to working with Carl Schwalbe in the future.

At this meeting there were 339 registrations and 75 for the Young Crystallographers meeting. She thanked John and Ivana Evans with their programme committee for putting together the scientific programme and onerous task of checking and signing off the abstract book. 178 delegates used online payment and these records can be downloaded straight into the BCA database. She thanked David Massey for undertaking the administration for this meeting and asked members to inform David of any suggestions for improvements to the website.

John Warren mentioned that in the list of sponsors, CCLRC should now be STFC

#### 7. Report of the Treasurer to include Presentation of the Accounts for 2007 and the Examining Accountant's Report

Sheila Gould provided a summary of financial statements to the meeting. The 2007 Durham school (£30K funding) accounts for differences between 2006 and 2007. Crystallography News is covering its costs by advertising. The IUCr fund has increased in value; it is now £26.8K but it is a restricted fund. She thanked Chick Wilson, Paul Raithby, all members of Council, Gill Moore and the accountants for their support and assistance.

Mike Glazer asked about the payment for the IUCr Congress and she replied that Osaka had not requested the offered funds, but Madrid (the venue for 2011) will be offered these funds.

#### 8. Acceptance of the Accounts

These were proposed by Mike Glazer and seconded by Harry Powell.

#### 9. Election to Council

There was one nomination for Treasurer, Harry Powell, nominated by Christine Cardin, seconded by Bob Gould therefore Harry Powell was elected unopposed.

#### 10. Appointment of Examining Accountants for 2008

The Young Company have been accountants for the BCA since 1996. They will charge £3450 + VAT for next year. Edward Bilbé asked why this is more than last year. The Treasurer replied that inflation was the main factor. She recommended that the Young Company be reappointed as examining accountants; proposed by Mike Probert, seconded by John Helliwell and therefore this was accepted by the AGM.

#### 11. AOCB

Simon Coles raised the issue of the extension of student membership from 3 to 4 years. Currently this is £27.50 for 3 years but most PhD's now last for 4 years and membership is particularly beneficial in the final year when a student is looking to make connections for job opportunities. The new proposal (£35 for 4 years) will be cost neutral with the existing system.

The President mentioned that Council has discussed this and was supportive of the suggestion. Ratification of this proposal was nominated by David Allan and seconded by Chick Wilson. Therefore this proposal was accepted by the AGM

There being no further business the meeting closed at 18:45.

Georgina Rosair, Secretary to Council



# News from the Groups

## Report on the Biological Structures Group Winter Meeting, University of Newcastle, December 16<sup>th</sup> 2008

**THE Biological Structures Group Winter 2008 meeting was held on 16<sup>th</sup> December in Newcastle - a city well known for its ship-building past as well as its nightlife, evocative weather and, of course, the river Tyne. Motorists get splendid views of the city's famous landmark, the Angel of the North, from the A1 or Great North Road. In fact, A1 is a perfect phrase to describe both the content and the organisation of the meeting which was hosted by Rick Lewis (Newcastle) and had the theme of 'Protein-nucleic acid interactions'.**

First to speak was **Ehmke Pohl** (Durham) who described the gene regulator protein clgR from *Corynebacterium glutamicum* which is involved in regulating expression of proteolytic complexes. The clgR protein itself consists of 107 amino acids and was solved by MAD phasing using selenomethionine-substituted protein. The structure consists of a 5-helix bundle with a long C-terminal helix and a model for the interaction of the protein with DNA was presented.

**John McGeehan** (Portsmouth) began his talk on a bacterial restriction-modification system by mentioning that there are around  $10^9$  phage particles per ml of seawater - something very poignant for molecular biologists who spend much time trying to eradicate these nasties. Bacteria try to protect themselves against phage by the action of endonucleases that cleave foreign DNA and they protect their own DNA by methylating it. John described the structure of a regulatory C-protein, which controls the expression of the restriction endonuclease gene. The C-protein, which consists of 5-helices, binds as a dimer to the DNA at two adjacent operator sites. Binding to the left-hand, high-affinity operator activates expression of the C-protein gene and the associated endonuclease. As the level of C-protein increases, binding to the right-hand, low-affinity operator switches off gene expression. John described the structure of the C-protein-DNA complex and outlined how mutagenesis experiments had confirmed a model of how the dimers assemble co-operatively on the DNA, thus opening the major groove and activating transcription of the genes.

**Malcolm Walkinshaw** (Edinburgh) then spoke on the recognition of methylated DNA by the protein MeCP2 which

recognises methylated C bases in CpG island promoters. This protein possesses a 'methyl-binding domain' along with 'AT hooks' and mutations in it are associated with the neurodevelopment disorder Rett syndrome. To determine its structure by the selenomethionine MAD method, methionine residues had to be mutated into the sequence and the protein was co-crystallised with a synthetic oligonucleotide. The crystals had to be soaked with PEG and magnesium chloride to improve diffraction quality. The resulting structure showed that water molecules play an important role at the protein-DNA interface and, surprisingly, that the methyl groups in the DNA are recognised by polar groups in the protein. A number of conserved threonine residues in turn regions, which are important in recognising the phosphates of DNA, are mutated in Rett syndrome. Next to speak was **Susan Firbank** (Newcastle) who enlightened us on the structure and function of archaeal DNA polymerases. The occurrence of uracil in DNA due either to its errant incorporation or to the deamination of cytosine is a well-known cause of mutations. Structural and other studies showed that archaeal DNA polymerases stall DNA replication in response to uracil due to the presence of a uracil binding pocket which causes the 'thumb' domain of the polymerase to move significantly and this ultimately initiates a repair process. The morning session was followed by the BSG AGM and then lunch during which many acquaintances were remade and much-needed Phyllosan flowed in abundance.

The afternoon sessions began with a talk by **Anne-Cécile Déclais** (Dundee) who spoke on the recognition of branched DNA junctions by T7 endonuclease I. Holliday junctions are of great importance in homologous recombination and play major roles in DNA repair and the generation of genetic diversity. Anne-Cécile's lecture covered a fascinating crystal structure of the endonuclease in complex with a synthetic four-way DNA junction. The next lecture was by **Panos Soultanas** (Nottingham) who spoke about the protein DnaB which is involved in the opening up of compacted DNA. The C-terminal domain of the protein, for which an NMR structure exists, binds DNA whereas the N-terminal domain, which forms tetramers in the crystal structure, has the ability to aggregate and form scaffolds. DnaD interacts with its partner protein DnaA for remodelling of OriC segments via DNA looping. Next, **Fred Antson** (York) spoke about the portal protein of the DNA translocating motor of phage SPP1 which packages DNA into the phage capsid. The portal protein forms 13-mers with a central tunnel that is lined by the 'tunnel loop' of each monomer and concerted movement of these loops is pivotal to pushing the DNA through the hole, as emphasised by an impressive movie. The negatively charged surface of the

tunnel is probably important for stopping the DNA getting stuck.

After coffee, **Ahmed Ibrahim** (Manchester) spoke about an RNA-activated protein kinase which is involved in innate immunity and has a double-stranded RNA-binding domain as well as a kinase domain, each of known structure. Double-stranded RNA is a replication intermediate in virally infected cells and adenovirus VARNA is a potent inhibitor of PKR and forms a 1:1 complex with it probably by virtue of binding to its RNA-binding domain. Adenovirus produces a number of such RNA transcripts to counteract the host cell defense system. Ahmed reported that various truncated forms of VARNA retained activity against PKR. Next, **Nicola Stonehouse** (Leeds) explained how phage  $\phi 29$  uses RNA as part of its capsid packaging motor (pRNA) and described studies of phage MS2 into which small RNA fragments were soaked and co-crystallised for structural studies along with studies of the pRNA-connector protein complex from  $\phi 29$ . Last but not least, **Jon Marles-Wright** (Newcastle) described cryo-electron microscopic studies of a complex between RNA polymerase and the transcription factor NusA at 25 Å resolution. NusA is well-known for its solubility-enhancing properties and its N-terminal domain binds to RNA polymerase whereas its C-terminal domain resembles the sigma-factor. Jon described how initiation occurs when sigma-factor binds to RNA polymerase and it had been thought that the elongation complex is formed when the sigma factor leaves and NusA then binds to at the same site. However, new data suggests that both proteins can bind simultaneously to the polymerase. This concluded a very interesting and memorable meeting and the organiser **Rick Lewis** (Newcastle) is thanked by the BSG for compiling an excellent and well-organised programme.



**Jon Cooper**  
UCL



## Chemical Crystallography Group Meeting Report

**12TH November 2008, University of Newcastle**  
The 2008 BCA CCG Autumn Meeting, “New Methods in Chemical Crystallography” was chaired by **Dr Andrew Bond** and featured six speakers presenting current research in crystallographic techniques.



*Natalie Fey, Lynne Thomas, Susanne Huth, Trixie Wagner, Sarah Lister & Rob Hooft*

The first lecture, “*Advancing into higher dimensions: a practical approach to modulated structures*”, was given by **Dr Trixie Wagner** (Novartis). In this very engaging talk, Trixie gave an introduction to what modulated structures are, and how they can be dealt with in practice using a reciprocal lattice viewer and the program Jana to refine the necessary extra parameters associated with this type of problem.

Next to speak was **Dr Rob Hooft**, (Bruker AXS) who gave a lecture on “*Reliable Determination of Absolute Structure Using Small Bijvoet Differences*”. Within the lecture he argued that a Gaussian distribution does not fully account for legitimate outliers, and instead showed that by using Student t-distribution, the determination of absolute structure using Molybdenum radiation can be made more reliable.

After lunch **Dr Lynne Thomas** (University of Glasgow) spoke about thermal diffuse scattering in the lecture “*Bragg Scattering and Beyond... Getting More from Diffraction Patterns*”. She described the process in which observed scattering patterns are

compared with those calculated from a simulated model in order to determine the most likely model for the disorder present in a structure.

**Sarah Lister** gave some nice examples of how techniques other than diffraction have been used to gain insight into unknown phases in a talk entitled *"The Use of Complementary Techniques in Structure Solution from Powders"*. Solid state NMR, IR and thermal gravimetric analysis proved invaluable to her in determining the behaviour of molybdenum phosphate.

**Susanne Huth** (University of Southampton) gave a talk about *"Understanding the Crystal Chemistry of Organic Solids"*. She showed how she has used structural systematics to study the 1, 2 and 3 dimensional similarities and differences of families of compounds. The molecular packing motifs and hydrogen bonding of substituted anilides and anthraquinones were examined in detail. Susanne pointed out that structural systematics can be used to select samples on which to perform charge density experiments, often resulting in chemically interesting results.

*"Building Knowledge Bases from Structural Data"* was the final talk of the meeting, given by Dr **Natalie Fey** (University of Bristol). The talk highlighted some of the challenges and opportunities that arise when combining results from experimental crystallography and computational chemistry. Searches through databases reveal compounds that are outliers in terms of expected structural features. These outliers often can be either rationalised through combining these complementary approaches, or improved to become more accurate.

**Helena Shepherd**  
Durham University

## Pharmaceutical Special Interest Group - Report 5th November 2008 AstraZeneca, Charnwood



Speakers: Left to Right are - Matt Tucker (ISIS), Graeme Day (University of Cambridge), Xue Wang (University of Leeds), Robert Docherty (Pfizer), Claire Thompson (GSK), Frank Leusen (IPI, University of Bradford), Amy Robertson (AstraZeneca), Matthew Johnson (GSK), Talbir Austin (AstraZeneca)

The Pharmaceutical Special Interest Group held its Autumn meeting on the 5th November 2008 at Astra Zeneca, Charnwood. Seven speakers presented an excellent range of topics including computational techniques such as polymorph prediction, Process Analytical Technology (PAT) focusing particularly on in-situ monitoring of crystal growth and finally techniques for characterising amorphous materials in the pharmaceutical industry, introducing Pair-wise Distribution Functions (PDF) for the understanding of amorphous structure at a molecular level. The chairs for the morning and afternoon sessions were **Matthew Johnson** (GSK) and **Brett Cooper** (MSD) respectively.

**Bob Docherty** (Pfizer) started the morning session with a review of the Pfizer vision for computational techniques within the pharmaceutical pipeline, highlighting a molecule to market approach which starts at the molecular level and builds up with each stage of development through formulation to manufacture and launch. Computational techniques, he explained, linked the crystal structure of the drug product to the physical properties of the drug, its surface characteristics and therefore the interaction characteristics of that surface to other materials, which will directly influence such processes as milling, drying and formulation. By utilising computational techniques he believes it will be possible to produce a stable drug product faster and cheaper than ever before.

**Graham Day** (University of Cambridge) followed Bob's review by focusing on polymorph prediction and the benefits this could have on the pipeline. Polymorph prediction can be used to generate otherwise unknown crystal structures of a molecule and rank them by energy to determine the most stable polymorph.

This has obvious benefits to the pipeline in that allows more focused screening to be developed to crystallise, via certain solvent combinations, the stable polymorph. He presented the case study of Carbamazepine, a combination of experimental and computational approaches, where he identified that Form 2 could only be stabilised during crystallisation by the addition of toluene in the channels of the crystal structure. This was independently confirmed by Fabbiani et al in 2007 by the collection of the single crystal structure containing channel toluene.

**Frank Leusen** (IPI, University of Bradford) followed on from Graham on the topic of polymorph prediction, summarising the CCDC blind tests from 1999-2007, particular highlighting the large Dutch movement in this field! Frank described the new approach and results obtained by himself and Marcus Neumann of Avant-garde Materials Simulation. In the 2007 CCDC blind test they predicted four out of four structures, with each of the structures being ranked as the first structure prediction. This talk really highlighted the level of complexity involved in polymorph prediction, but also showed the current state of the art and the potential for the future.

Moving away from computational chemistry **Xue Wang**



(University of Leeds) gave an excellent talk summarising the use of PAT for morphological population balance modelling and 2D/3D on-line monitoring of crystal growth. The case studies he presented demonstrated the effect of size and shape on bioavailability and processing and that once defined it is possible to control these variables on large scale (e.g. 200L reactors) by completing the suggested simulations to produce an optimised cooling regime.

In the first presentation after lunch **Amy Robertson** (Astra Zeneca) gave a fascinating overview of how AZ applies PAT to really understand the crystallisation process. She highlighted the importance of monitoring the crystallisation process to ensure the correct particle size and morphology, which are key to the final product performance within the Quality by Design framework. She described the application of Focus Beam Reflectance Measurement (FBRM) and Particle Vision Monitoring (PVM) to show how crystal size, shape and growth could be monitored during the process. Finally, she described the use of FTIR and Raman probes to demonstrate how form turnovers could be monitored and how processing could be controlled to ensure delivery of the correct form with the desired properties.

In the second afternoon presentation **Claire Thompson** (GSK) highlighted the importance of monitoring how much amorphous material was present in batches of API, especially when developing inhalation formulations. She highlighted how amorphous material can form during milling and what could happen to the particle size distribution should the amorphous material crystallise and fuse together particles of API. Claire then highlighted the "Plethora" of analytical techniques that could be used to study amorphous content. She discussed their relative sensitivities

and discussed the approaches for quantifying amorphous content in the API batches.

In the last talk of the afternoon session **Matt Tucker** (ISIS) highlighted the benefits of total scattering or PDF method. Matt described how synchrotron X-ray or neutron data could be normalised to an absolute scale to provide information on local, medium and long range atomic structure. He then went on to describe how this could be applied to monitor pressure induced amorphisation in the negative thermal expansion of  $ZrW_2O_8$  at the molecular level, identifying the structure of the amorphous nano-zones. Finally he challenged the Pharma audience to think of ways this technique could be applied to the challenges faced during pharmaceutical development.

We would like to thank **Anne Kavanagh** (Astra Zeneca) and **Tal Austin** (Astra Zeneca) for all their help organising the event at Astra Zeneca, Charnwood.

## Conference Feedback

When asked about the meeting overall, the content, organisation and the venue the rating assigned by responders was "Excellent". When asked if they would attend future Pharma meetings or the BCA Spring meeting the majority of responders said "definitely" or "probably". When asked how far people had come or where they prefer to have meetings, it seemed clear that the Midlands to the South would be the best location to hold meetings. When asked what they would like to see at future meetings the majority of responses were "more of the same please". So we will try to do our best next year.

**Matthew Johnson** (GSK) and **Brett Cooper** (Merck)



**THE** 40th annual BACG conference will be held at Wills Hall, Bristol University from Sunday 6th to Tuesday 8th September 2009 with a workshop on Computational Pharmaceutics on Wednesday 9th September. As in previous years the Conference will include the BACG Annual lecture, the BACG Young Scientist Award, keynote lectures and contributed presentations in a number of dedicated symposia. A dedicated poster session will also be held. Instrument vendors will exhibit their products throughout the event. This year a reception will honour some of the key British scientists who have led the field of crystal growth and crystallisation in the UK over the last 40 years. These people will be present throughout the meeting and will be involved in scientific discussion. A list of those attending will be published when confirmed.

## Conference Programme & Call for Papers

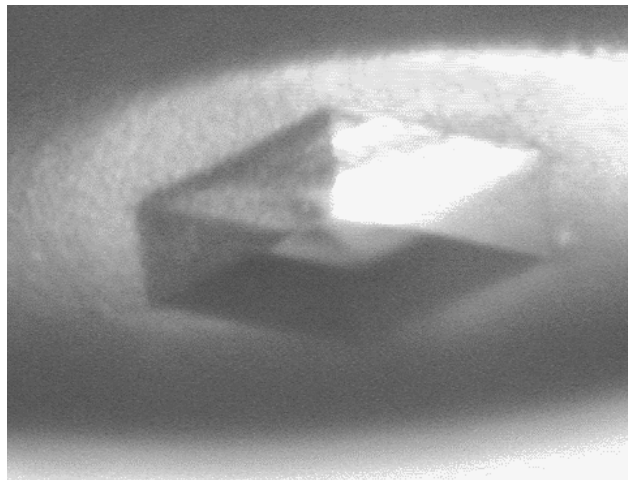
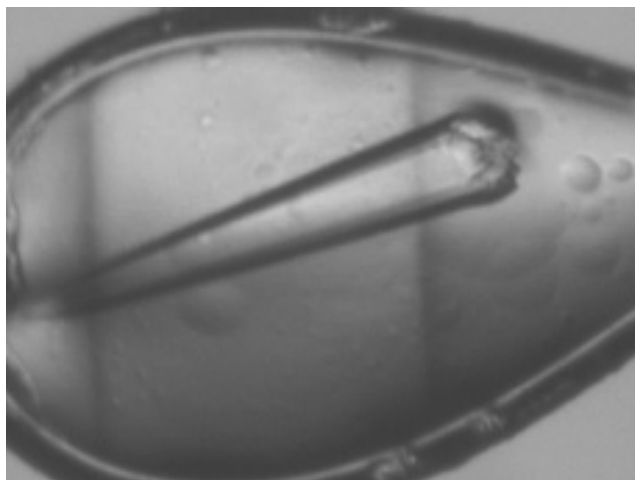
The conference will be based around symposia covering the following subjects and themes:

*Pharmaceuticals, Food, Polymers, Fine Chemicals, Biominerals, Polymers and Macromolecules -*  
·process analytical and in situ techniques; crystal growth and nucleation, polymorphism; crystal shape,  
·morphological stability & habit control; formulation & product design.

There will be a special issue of Crystal Growth and Design published based on material presented at the meeting. Attendees at the meeting are invited to consider submitting material for publication in this special edition.

Further information is available at [www.bacg.org.uk](http://www.bacg.org.uk)





*Cryo-cooled protein after exposure to third generation synchrotron X-ray beams: the discoloration is often blueish in hue, and this is caused by hydrated electrons which absorb at the red end of the visible spectrum. (Image provided by Elspeth Garman, University of Oxford; see Garman and Owen (2006), Acta Cryst D62, 32-47)*

## CCP4 at Nottingham

**THE** annual Collaborative Computational Project in Macromolecular Crystallography (CCP4) Study Weekend was held at the East Midlands Conference Centre at the University of Nottingham meeting on January 3-5, 2009. The meeting, "Experimental Phasing and Radiation Damage", took a highly focused look at the influence of radiation damage upon phasing and how experimental and computational methods can be optimised to yield structure solutions. The scientific programme was organised by **Clemens Vornrhein** (Global Phasing Ltd, Cambridge, UK), **Elspeth Garman** (University of Oxford, UK) and **Arwen Pearson** (University of Leeds, UK). Participants, numbering 325 this year, came from a range of academic and industrial institutions in the UK and eleven other European countries, as well as the United States, China, India, Japan and Brazil.

The chairman of CCP4 Working Group 1, **Jim Naismith** (St Andrew's University) issued his usual reminder of the open and collaborative nature of CCP4, and encouraged everyone to use and contribute to the package. He also announced that he will be stepping down as chairman of WG1, the post to be taken up by **Martin Noble** (University of Oxford) from next year. **Peter Moody** (University of Leicester) became a new member of the executive. All PIs, actual and prospective, were invited to register as members of WG1. **Clemens Vornrhein**, one of the programme organisers, also welcomed the attendees and explained how the programme sessions were set out as an Introduction, Before the Experiment, During the Experiment, and After the Experiment.

The first session opened with **Garry Taylor** (University of

St Andrews) who explained crystallography as a diffraction experiment where samples are exposed to X-rays, and the diffraction pattern recorded. The aim of the experiment is to estimate the value of the electron density,  $\rho$ , at every point in a unit cell. The experiment records intensities only, and the phase is lost due to the nature of the experiment. Phases have to be determined in order to be able to reconstruct the electron density. As diffraction occurs in waves, the various waves need correct phase relations for a Fourier transform to succeed in reconstructing the object. A demonstration with a hypothetical structure was used to emphasise the importance of phases. Phases can be derived with different techniques: 1) Direct Methods use theoretical phase relations between reflections to calculate the whole set, but the method is not reliable at resolutions below 1.2Å, 2) Molecular Replacement has become a popular technique to use models of known structures as seed for determining new structures, 3) MIR & SIRAS have also gained importance as experimental methods to derive phases, although they are very sensitive to radiation damage. Although the isomorphous difference signal could be as much as 25%, a small non-isomorphism of 0.5% in cell-dimensions gives rise to 15% isomorphous difference. 4) Anomalous scatter via MAD & SAD exploit the energy tunability of modern synchrotron sources to determine a substructure of anomalous scatterers from very small signals between 1 and 5% of the total scatter. Tutorials prepared by Garry Taylor are available at <http://www.st-andrews.ac.uk/~glit2/CCP4>. Despite the difficulties in all the above techniques, researchers have used them routinely to obtain a starting set of phases. An array of mathematical tools then allows phase improvement to a degree where model building becomes possible: solvent flattening, phase extension to higher resolution, histogram matching, NCS averaging, DMMULTI using the non-isomorphism of different crystals. The damage induced by

radiation absorption has also become the latest tool in phase determination.

“Radiation Damage in macromolecular Crystallography: What is it and why do we care?” was **Elsbeth Garman**'s (University of Oxford) theme, describing radiation damage as a re-emerging problem with new high-brightness SR sources. At room temperature, the beam often leaves a track of discoloration where it had shone through the crystal, and the effect continues post exposure. Elspeth did not recommend this as a method for imaging the beam! Radiation damage was described as arising from primary and secondary ionisation induced free electrons and free radical products. Direct events occur when X-rays are absorbed by protein atoms, while indirect events occur in the solvent channels where electrons can eventually reach lattice contacts that get broken. According to Blake and Phillips (1962), one 8 keV photon absorbed would ionise some 70 molecules, and affects another 90. Their model was able to fit observations made during collecting several data sets from 1 crystal at room temp: a part of the crystal order was completely destroyed, another part was damaged and a third part was unaffected. At cryotemperatures, it has been found that di-sulphide bridges are the first to succumb, where the bridge is broken, followed by decarboxylation events of glutamate and aspartate side chains, OH release from tyrosines and then methionine destruction. Some symptoms of radiation damage were discoloration, loss of diffraction, cell dimension expansion, and higher Wilson B factors. Of the X-rays (at 1 Å) that interact with crystals, around 8% contribute to elastic (Thompson) scatter that gives the diffraction pattern, another 8% contribute to inelastic (Compton) scatter, and the remaining 84% generate primary photo-electrons, resulting in secondary ionisation events. A stark statistic was presented, as native HEWL absorbs 1.6% of IO, while a Pt derivative absorbed 4%. Heavier element containing samples, e.g. Holo-Ferritin, suffer radiation damage more quickly with the same incident flux because of the increased absorption. The experimental investigations give a maximum recommended dose of 30 MGy, which could be translated into time windows at various SR facilities in which data may be collected before the effects of radiation damage alter the biological fidelity of the sample. Cooling to 100 K has been the method of choice to counter the effects of X-ray absorption, e.g. to immobilize OH radicals, as they start to become mobile above 110 K. Future work was aimed at devising ways of extending the time window for data collection, in order to extract maximum information about a biological sample: perhaps cooling below 100 K to see if that further immobilises free radical species, investigating using shorter wavelengths where the absorption but also the diffraction is reduced, adding radical scavengers, and using very small crystals so that the primary photoelectron might escape.

In the second session **Helen Walden** (London Research Institute) presented a highly informative and light-hearted contribution on “Selenium Incorporation using recombinant techniques.” The pro's and con's of a range of expression hosts (bacteria, insect cells, yeast, mammalian cells) were contrasted along with costs of each system related to pints of beer. Importantly, she presented a number of strategies which could be used to optimise the levels of selenium incorporation. She emphasised that many protocols are available which provide options for even the seemingly most recalcitrant proteins. She also recommended <http://www.doe-mpi.ucla.edu/local/protocols/> for protocols on the preparation of selenomethione-substituted proteins.

<http://www.doe-mpi.ucla.edu/local/protocols/> for protocols on the preparation of selenomethione-substituted proteins.

**Peter Sun** (NIAID, Rockville, MD, USA) followed with a methodological talk entitled “Toward a Rational Approach to Conventional Heavy Atom Screening.” In a nutshell, the goal of his work in this area is to try to obtain a heavy atom derivative of a protein without using a crystal. In this regard procedures were described which use mass spectrometry to rapidly screen for derivatisation of proteins in solution. Data obtained from these studies, which assessed an enormous number of reactive conditions, have been compiled into a database of heavy-atom reactivity tables ([http://sis.niaid.nih.gov/cgi-bin/heavyatom\\_reactivity.cgi](http://sis.niaid.nih.gov/cgi-bin/heavyatom_reactivity.cgi)) which highlights in a more systematic way how parameters such as buffer and pH influence the chemical reactivities of residue side chains with heavy atoms. A quick soak method was also described for reducing non-isomorphism in protein crystals (typically involving soaking in a 10 mM solution of the heavy atom compound for about 10 minutes). The success of this methodology was illustrated with examples including lysozyme and FcγRIII receptor crystals. Given the sometimes vanishingly small amounts of protein samples one has to contend with, methods like this offer new ideas for obtaining samples suitable for use in phasing in an efficient manner with a reduced amount of traditional empirical crystal screening.

**Douglas Juers** (Whitman College, Walla Walla, WA USA) gave a very informative talk “Rational Approaches to Crystal Cooling” He presented a critical perspective of the technical problems which can arise in cryo-cooling protein crystals and the strategies which can be used to optimise cryo-cooling methods. He described how the effects of cryo-cooling can be understood in terms of considering a protein crystal as an assemblage of domains, where interactions of the domains with the bulk solvent at cryo-temperatures can alter spot shapes and widths in collected data. He described how attention to selection of the cryo-buffer, the equilibration process and the method of transfer to the cryo-stream can minimise the negative effects of cryo-cooling upon data quality. Although the use of cryo-cooling is effectively ubiquitous amongst protein crystallographers, this talk was a good reminder that even small changes to well established protocols can yield measurable improvements.

The session concluded with two short presentations by young scientist. **Tobias Beck** (Georg-August-Universität, Göttingen, Germany) presented his work on compound called I3C (5-amino-2,4,6-triiodoisophthalic acid) in a talk entitled “The Magic Triangle: a New Phasing Tool.” He described how I3C, which contains three anomalous scatterers in a triangular arrangement, was used for both SAD and SIRAS phasing using SHELXD. Restraints for I3C for use with SHELX or remlac are available at <http://shelx.uni-ac.gwdg.de/~tbeck/i3c.html>. The second presentation, “Know your dose: RADDPOSE”, given by **Karthik Paithankar** (University of Oxford), described the factors influencing radiation damage and how these are taken into account in the programme RADDPOSE. This programme can be used to calculate the absorbed dose of radiation (in Gray units) absorbed by crystals and provides a means for assessing radiation damage. Particularly interesting was the explanation of how X-ray

fluorescence can influence radiation damage, particularly in the collection of MAD data.

The session before dinner on Sunday night brought three speakers, starting with **Zbigniew Dauter** (Argonne National Laboratory, Argonne, IL, USA) talking about "Carrying out an Optimal Diffraction Experiment". He made the point that it is hard to satisfy all possible requirements for the perfect data set at the same time, well measured intensities at all resolutions, good redundancy throughout the data, and maximum resolution possible from the crystal. A few minutes spent at the beginning of a data collection experiment, even in these days where synchrotron data collection can be so fast, are well spent if they result in data being collected that are more useful for the planned purpose. He strongly advocated the use of strategy programmes, which can take into account the orientation of the crystal, the intensity of the diffraction and the requirements for high resolution data, maximum completeness, or accuracy throughout the data set. For molecular replacement, strong reflections are of utmost importance because of their effect on Patterson functions and therefore care should be taken to avoid overloading any of the reflections, whereas for high resolution refinement completeness and low resolution reflections are less crucial and may need to be sacrificed a little to achieve maximum resolution. Experimental phasing, especially involving anomalous measurements requires the most precision of data, and therefore the most care with data collection to ensure optimal completeness and to minimise the effects of radiation damage.

**Gerard Bricogne** (Global Phasing Ltd, Cambridge) followed with a discussion of "Interleaved Data Collection Protocols for Optimally Exploiting Anomalous Scattering and its Anisotropy for Phase Determination". It followed a thread that ran throughout the meeting about dealing with radiation damage, proposing two strategies to deal with the phenomenon in data sets collected at third generation X-ray sources. Taking the traditional approach, the effect is minimised by collecting related reflections at times when the radiation damage should be similar, e.g. using the data collection strategies outlined by Hendrickson and others when the "MAD" phasing strategy was first described. He also made the case for using scaling methods that not only allow for radiation damage but take advantage of "creeping nonisomorphism" and anisotropy of anomalous scattering to give extra phase information, which has been achieved using the programme PHASER.

**James Holton** (Lawrence Berkeley Laboratory, Berkeley, CA, USA) rounded up the session with his debate on "The Theoretical Limits of Macromolecular Crystallography." His talk centred around the problem of striking a balance between data quality and x-ray dose. He put to rest any idea that we can all collect data well already by quoting some statistics from his analysis of data sets collected at US beamlines, suggesting that only 2% of the data sets collected lead to a deposited structure in the PDB. He described his programme MLFSOM (MOSFLM in reverse) which can simulate an entire data collection experiment, and that he has used to look at the major sources of error in a diffraction experiment, coming to the conclusion that the optimal strategy for MAD/SAD data collection is very many short exposures, with the brevity

determined by the shutter response at the beamline and the stability of the X-ray beam but not the detector.

The first session on Monday morning started at 9am with a presentation by **Alexander Popov** (ESRF, Grenoble, France) entitled "BEST Data Collection". The BEST software package allows the modelling of data collection strategy to obtain the optimum strategy in terms of I/SigI, data completeness, resolution and radiation damage. Alexander described how new algorithms for this optimization had been implemented and demonstrated how a gradual increase in exposure time could compensate the loss of signal due to intensity decay. The latest version of BEST is available in which the user is able to optimise the parameters to obtain the lowest possible noise in anomalous difference data in high dose data collection. Based on two collected images at 90 degrees to each other, the user can choose what is the most important requirement for the data, e.g. resolution, completeness etc. and calculate the most appropriate strategy. The program can also determine the best crystal orientation for the collection of Friedel pairs and high redundancy.

**Susan Lea** (Sir William Dunn School of Pharmacy, Oxford) then gave a presentation entitled "With Phases - Two Wrongs Can Sometimes Make a Right". Here, Susan told us a story where reproducible native crystals were grown and experimental phases were obtained, but the structure still remained elusive. The protein contained two methionines. When a selenomethionine-substituted version of this protein was purified and multiple data sets collected from the crystals grown, a good Patterson map was calculated, but she could not get distinction between the possibilities for the hand. Very poor electron density maps were obtained. The middle of three domains was solved using NMR and used as a model for molecular replacement. This domain was correctly placed, but still the other two domains could not be built. Finally, these data were combined with the selenomethionine data to produce an interpretable map from which the whole structure could be built.

The final speaker in this session was **Zbyszek Otwinowski** (Southwestern Medical Centre, Dallas, TX, USA). His presentation was entitled "Correcting for Radiation Damage". Zbyszek outlined how 'Scalepack' corrected for radiation damage; first he described the decay correction, where diffraction intensities are corrected in a resolution dependent manner by B-factors. This correction cannot take into account non-decay changes which are initially linear with dose. Zbyszek explained how these changes could be analysed for their significance by comparing their normalised expectation to estimated experimental errors. Finally, examples were given showing this process in action and where the correction of radiation damage was critical for structure determination.

The fifth session opened with **Martin Weik** (IBS, Grenoble, France) who gave an overview of temperature controlled X-ray crystallography combined with spectroscopic techniques. He provided a few examples to show as to how catalytic intermediates could be captured at various temperatures. These experimental conditions are influenced by a number of factors, including the solvent content of the crystal and the size and shape of the solvent channel.



**Marc Schiltz** (École Polytechnique Fédérale de Lausanne, Switzerland) then gave two examples about the broken symmetry between equivalent reflections. One of those, namely the presence of anomalous scatterers, is a phenomenon which has been exploited for many years to gain phase information. The other contributing factor is X-ray induced radiation damage, which provides extra phasing information. This is exploited in the program SHARP.

**Arwen Pearson** (University of Leeds) closed out the session with a general introduction about recent developments in synchrotron sources in the instrumentation to complement X-ray diffraction experiments. These included single crystal UV-visible, fluorescence, Raman and infrared spectroscopic techniques. She demonstrated the 'extra' information generated by the combination of these various techniques on a few biological systems, such as methylamine dehydrogenase.

The final session of the meeting had four talks. First we had the real McCoy, with **Airlie McCoy** (CIMR, Cambridge) explaining what to do with your first electron density map. She explained that density modification and model building are part of the same thing. She then went on to lucidly explain Hendrickson-Lattman coefficients and probability density functions. She then explained the problems of centrosymmetric heavy atoms, the use of Log likelihood gradient maps to improve the substructure and that it is worth throwing out bad derivatives.

**Kevin Cowtan** (University of York) then followed by talking about his density modification programme Parrot and automated model-building programme Buccaneer, which is particularly good at low resolution structures. These are based around Maximum Likelihood Hendrickson-Lattman coefficients. I am sure many of the audience were keen to get back to the lab to apply these to their problems.

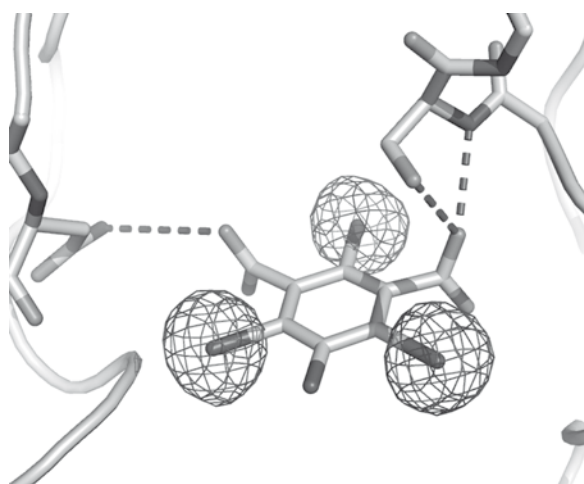
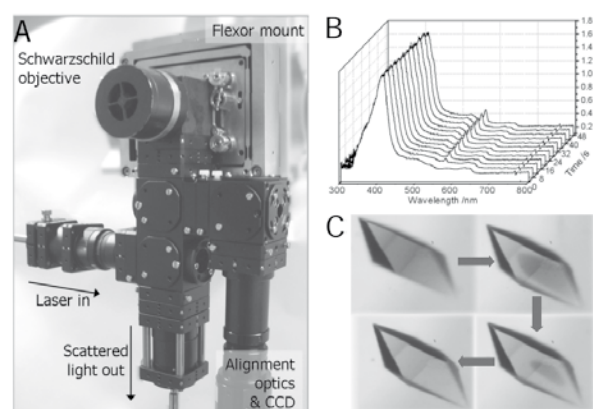
**George Sheldrick** (Georg-August-Universität, Göttingen, Germany) talked about his main chain tracing in SHELXE which is a useful way of improving the maps and resolving the correct enantiomorph. It also incorporates the "free lunch" algorithm where if the data are better than 2 Å then extending the map calculation to 1 Å using the calculated F and phase clearly gives better maps and subsequently better refinement against the real data. Much debate was held as to why this works.

Finally **Sean McSweeney** (ESRF, Grenoble, France) summarised a decade of radiation damage studies, what are now the known knowns, the known unknowns and what might be the unknown unknowns under the title "The Cheshire Cat's Smile". The radiation damage leaves faint traces behind in the density. An important issue that we do not yet know how to deal with is how to monitor the site specific radiation damage during the experiment so as to know how quickly we need to collect the data and when to discard the data as too damaged. Even monitoring general radiation damage is hard in real time. All this has to be examined after the event at present. There are experimental problems to be overcome. Crystal freezing is still trial and error; there are still instrumental limits in some experiments which would be nice to transcend such as reverse beam experiments and collecting small wedges at different wavelengths to get dispersive differences close in time. There are also issues of accuracy of goniometers

for very small crystals. The software needs modifying to deal with unmerged data and the data points need a radiation dose measurement attached to them. Understanding and dealing with radiation damage has come a long way in the ten years or so since third generation sources started burning frozen crystals, but there are still challenges ahead.

Finally, a meeting of this size and scope demands an excellent support team and in this regard we are truly indebted to the great work of the CCP4 organisation which includes **Shirley Miller, Damian Jones, Laura Johnston, Tracey Kelly** and **Stuart Eyres** (photography). Special thanks also to "The Funtime Frankies", the band who kept the dance floor full throughout the night at the conference dinner - Rock on!!

Prepared by the Biological Structures Group Committee and edited by **Kate Brown**, Imperial College London



A) SLS single crystal spectrometer, (B) myoglobin reduction by X-rays, (C) substrate reduction of methylamine dehydrogenase/amicyanin crystals. Reference Owen et al. (2009) *J. Synch. Rad.*, in press. (Image provided by Arwen Pearson, University of Leeds).

The MAD triangle B3C (5-amino-2,4,6-tribromoisophthalic acid) in proteinase K. This new phasing tool is suitable for MAD phasing. It features three bromine atoms arranged in an equilateral triangle and three functional groups for hydrogen bonding to biomolecules. Hydrogen bonds are depicted as dashed lines and MAD density is shown in wireframe. (Image provided by Tobias Beck, Georg-August-Universität, Göttingen, Germany).



# Aperiodic'09

**APERIODIC'09** is the sixth international conference on aperiodic crystals, organized under the auspices of the Commission on Aperiodic Crystal of the International Union of Crystallography (IUCr). It follows Aperiodic'94 (Les Diablerets), Aperiodic'97 (Alpe d'Huez), Aperiodic'2000 (Nijmegen), Aperiodic'03 (Belo Horizonte) and Aperiodic'06 (Zao). The conference aims to provide an up-to-date research progress in the field of aperiodic systems and encompasses quasicrystals and incommensurately modulated materials.

The conference will be held in Sherrington suite at the University of Liverpool from 13th-18th September 2009. It will be co-chaired by **Ronan McGrath** of the University of Liverpool and Uwe Grimm of the Open University. The main conference will consist of several sessions with invited and contributed talks. In addition there will be a number of poster sessions. A tutorial session will be held on 13th Sept. which is aimed at newcomers to the field. The proceedings will be published in the Journal of Physics Conference Series.

For enquiries, please contact the conference secretary Mrs. **Angie Reid** at [angie@liv.ac.uk](mailto:angie@liv.ac.uk)

Further information is available on the conference homepage: <http://www.aperiodic09.org>



APERIODIC '09

## The 8th Pharmaceutical Powder X-ray Diffraction Symposium - PPXRD-8

**GLASGOW, SCOTLAND, U.K.  
4-7 MAY 2009**

*Sponsored by the International Centre for Diffraction Data.*

**THE ICDD** is pleased to present this unique symposium focusing on cutting-edge topics surrounding the combined fields of Pharmaceuticals and X-ray Powder Diffraction. The deadline for registration is 15 March 2009. The symposium sessions include discussions on the following topics.

- Formulation, Product Development, Drug Delivery and Polymorph & Salt Screening.
- Patent and Regulatory Issues.
- Complementary Techniques and Process Analytical Technology.

- Amorphous, Activated and Nanomaterials.
- New Frontiers in XRD in Pharmaceutical R&D.
- XRPD Structural Techniques (Acquisition and Use of XRPD Data, Indexing, Structure Determination, Rietveld Refinement).
- Organic Crystal Structure Prediction

An optional workshop on Characterization of Pharmaceutical Solids will be held 4 May 2009.

Contact: **Leah Mooney**, ICDD

E-mail: [ppxrd@icdd.com](mailto:ppxrd@icdd.com)  
[www.icdd.com/ppxrd](http://www.icdd.com/ppxrd)



# Crystallographic Meeting

## Twenty-Fifth European Crystallographic Meeting Istanbul, Turkey, 16-21 August



**AN** extract follows from the report of **John Helliwell** to the European Crystallographic Association on this forthcoming meeting.

The Past President of the ECA, **Hartmut Fuess**, and I made a site visit to Istanbul last November.

We joined **Engin Kendi**, Chair of ECM25, and the local organisers to make a Working Group. We firstly toured the Harbiye Museum and Cultural Centre (see pictures below), which will serve as the conference venue. It adjoins the Military Museum. This centre is in the Ottoman 19th century style and has views of the Bosphorus Sea. There are various hotels nearby, notably the large Istanbul Hilton Hotel straight opposite. Functionally, as a Conference Centre, it comprises two large lecture-auditoria (seating 600 and 300 persons) and four of approximately 100 persons each (i.e. two of 100 persons, one of 120 persons and one of 80 persons). The Centre has leather armchair seating areas and is best described as being like a palace. Huge mirrors feature in the entrance hall and sweeping staircase. There are views of the Bosphorus Sea linking Europe and Asia (more of this later). A second building, about 100 metres away, provides the Exhibition, poster, internet, coffee and lunch areas split over two floors. The Conference Plan is near convergence with 16 Keynotes and 48 Microsymposia now defined.

The Conference Dinner will be held at the magnificent Dolmabahce Palace. Hartmut and I walked there from the Istanbul Technical University Guest House in about 20 minutes, the Guest House in turn being about 15 minutes walk from the Conference Centre. Sadly we were just too late to go into the Palace. Instead we sat drinking hot lemon tea at the sea's edge looking one way at the Palace, in Europe, and in another direction at Asia across the 'straits of Constantinople'. Our walk allowed for a picture across the water to Asia and of the Besiktas Soccer stadium. Of course these few anecdotes are no replacement for reading up-to-date tourist guide books or webguides.

On the end of the first day we were treated to a theatre

outing to see the Anatolian Legend 'Dance Show from its Native Land: Troy' ([www.fireofanatolia.com](http://www.fireofanatolia.com)). This was not a simple dance show but a true extravaganza culminating, of course, in the appearance of a Trojan Horse. The great feats of dancing, individually and in formation, were breathtaking. The performance received a standing ovation.

Our Conference Plan, as well as this being our 25th ECM, as well as the rich cultural heritage, the close linkage of Europe and Asia, some fantastic historical and touristic destinations before or after the Conference (such as Cappadocia, Ephesus, Pamukkale, Bodrum, Fethiye and Antalya) all promise a stimulating and nostalgic experience within a historic and cultural setting of unique geopolitical placement. I commend all European crystallographers to come to Istanbul and enjoy the ECM25 experience.

We are indebted already to the hard work and enthusiasm of Prof Engin Kendi and her local team. We look forward to seeing you at ECM25.

**John R Helliwell**  
ECA President



*View of the Conference Centre*



*The palatial interior*



One of those huge mirrors and leather armchair meeting areas



View of the Dolmabahçe Palace Gate



The coffee lounge



From left to right Engin Kendi, Suheyla Ozbey and Semra Ide



View of the Military Museum side



View of the Bosphorus

## Focus Areas and Microsymposia

- FA1: Biological and Macromolecular Crystallography**
- FA2: Materials and Minerals**
- FA3: Physical Including Fundamental Crystallography**
- FA4: Chemical Crystallography**
- FA5: Experimental and Computational Techniques**

### **FA1: Biological and Macromolecular Crystallography**

- MS 1 Large Macromolecular Complexes
- MS 2 50 Years of Globins
- MS 3 Novel Enzyme Mechanisms
- MS 4 Molecular Transport and Recognition
- MS 5 Structural Basis of Pathogenesis
- MS 6 Emerging Structural Systems Biology
- MS 7 Molecular Recognition and Drug Design
- MS 8 Membrane Proteins: Frontiers and Challenges
- MS 9 Practical Protein Production, Purification and Crystallization
- MS 10 Computational Methods in Macromolecular Crystallography
- MS 11 Complementary Biophysical Techniques
- MS 12 High Throughput and Model Validation in Macromolecular Crystallography
- MS13 NMR, Crystallography and Macromolecular Structure
- MS 14 Very High Resolution Protein Structures

### **FA2: Materials and Minerals**



- MS 1 Mineralogical Crystallography: Layered and Framework Structures
- MS 2 Minerals as Treasury for Advanced Materials
- MS 3 Crystallography in Art and Archaeology
- MS 4 Crystallography of Functional Materials Under Challenging Experimental Conditions
- MS 5 Ferroc Materials
- MS 6 Surfaces and Interfaces
- MS 7 Optoelectronic Materials
- MS 8 Coherent X-Ray diffraction and Imaging of materials
- MS 9 Combination of Synchrotron and Neutrons in Magnetic Materials
- MS 10 Electron Microscopy on Functional Materials
- MS 5 Structure and Reactivity in Molecular Crystals by Crystallographic, Spectroscopic and Computational Methods
- MS 6 Structure and Reactivity in Metal Complexes
- MS 7 Weak interactions in Chemical Processes or Properties
- MS 8 Metal Organic Frameworks - Away Through Pores and Holes
- MS 9 Crystallography in Pharmaceutical Sciences
- MS 10 Indirect Structural Information: Use of Data Bases
- MS 11 Crystal Energy Landscapes : Computation and Uses
- MS 12 The Future of Small Molecule Software

**FA3: Physical Including Fundamental Crystallography**

- MS 1 Coherent X-ray Diffraction and Imaging in Biology
- MS 2 Accuracy in Experimental Charge Density Determination
- MS 3 Quantitative electron crystallography
- MS 4 Time Dependent and In-situ Analysis

**FA4: Chemical Crystallography**

- MS 1 Organic and Inorganic Modulated Crystal Structures
- MS 2 Design and Properties of Functional Molecular Materials
- MS 3 Multicomponent Crystals
- MS 4 Supramolecular Architectures: From Structure to Function

**FA5: Experimental and Computational Techniques**

- MS 1 Structure Solution and Refinement From Powder Diffraction Data
- MS 2 Crystallography with EXAFS and XANES Spectroscopy
- MS 3 Remote Experimentation , Telepresence and Automation
- MS4 Synchrotron Radiation Based Crystallography and Spectroscopy in Middle East
- MS 5 Scattering Studies of Non-crystalline Systems
- MS 6 Nanocrystallography
- MS 7 Crystallography at High Pressure
- MS 8 Transient Structures: Observation vs. Prediction

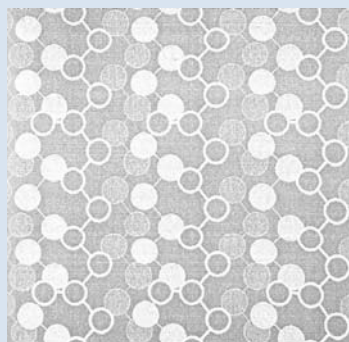
## Festival Pattern Group material available

**SINCERE** apologies for the considerable sloth in getting back to you about the Festival Pattern Group material we saw at the end of the summer. I attach pictures of the two for which I have a quote provided we order at least 50 m. I assume that if we order significantly more the cost might come down a bit! Part of the hold-up was my getting the width which I now have - it is 130 cm which is just over 4'. The cost per m for the 'ball-and-stick' of nylon ('Hemsley') is £32.00 in the various colours that are in stock. The afwillite Patterson map ('Surrey') is a richer material and is £48.00 per m + VAT + delivery at cost.

I am not sure how much of which people were interested in, but I would propose if there is sufficient interest to order some - my preference is for the more expensive one - and divide the cost per m. I would be most grateful if you think you know of others who might be interested, if you could let me know - or simply pass on this e-mail in a pyramid selling operation.

Best wishes

**Lindsay Sawyer**  
l.sawyer@ed.ac.uk



*The structure of nylon as seen by Marianne Straub for Warner's of Braintree based upon the structural work of Charles Bunn for ICI. This pattern came in a variety of colours: pale green, brown, rust, yellow, blue-green/ turquoise.*



*An electron density map of the mineral afwillite also by Marianne Straub for Warner's based upon her own crystal structure analysis.*

*This is available in green and gold; there was also an orange and gold.*



# Cueva de los Crystales

**OUR** cover carries a picture of a cave in a silver and lead mining area of northern Mexico containing huge crystals [reproduced with permission given by **Richard D. Fisher**]. As can be seen by comparison with the image of a man, these crystals are up to 11 metres long. They are mainly perfectly formed crystals of selenite, the quite colourless form of gypsum, calcium sulfate dihydrate; and although we recognise that our mineralogical readers may already know all about them, we thought there are probably many other readers who would also have an interest. A cave containing large crystals was also discovered in northern Spain in 2000, but the crystals are far smaller than those illustrated here. It is generally recognised that these crystals are the result of exceptionally stable temperature and humidity conditions, and it is suggested that the crystals may well be 500,000 years old. A scientific study of the cave and its contents has been published by Garcia-Ruiz et al.<sup>1</sup>

Gypsum<sup>2</sup> belongs to the monoclinic system, space group C2/c, with  $a = 5.679(5)$ ,  $b = 15.202(14)$ ,  $c = 6.522(6)$  Å,  $\beta = 118.43(4)^\circ$ . The authors of ref. 1 regard the long beam-like crystals as extended along the  $c$  axis with prismatic faces of form  $1k0$ . This does not appear to be in complete agreement with the Bravais-Friedel-Donnay-Harker principle whereby the shorter  $d(hkl)$  the more extended the crystal normal to  $hkl$ :  $d(100)$ ,  $d(010)$  and  $d(001)$  calculate as 4.99, 15.24 and 5.74 Å and thus the lengths of the crystals should be  $L(100) > L(001) > L(010)$ . However,  $L(001)$  seem to be longest. It should be noted that this habit is unusual, the characteristic habit of gypsum being platy or tabular. Figure 1 shows a  $z$ -projection of the crystal structure. Each  $\text{Ca}^{2+}$  ion is coordinated by eight oxygen atoms, of which six come from  $\text{SO}_4^{2-}$  ions and two from water molecules; Ca and O are closest together in the  $[001]$  direction<sup>3</sup>. In the same cave some gypsum crystals take on a blocky habit (Figure 2). Faces have been indexed for a representative example (Figure 3).

How did these remarkably large crystals form? A plausible hypothesis<sup>1</sup> was developed from analysis of the very scarce fluid inclusions in the megacrystals together with interpretation of the local geological features. Magma intruded into faults in a mass of limestone at Naica, Mexico, carrying the minerals that eventually became the object of mining activities. Sulfide ores underwent oxidation, acidifying the ground water with sulfuric acid. The acid attacked the limestone, raising the concentration of dissolved  $\text{Ca}^{2+}$  and  $\text{SO}_4^{2-}$  until  $\text{CaSO}_4$  began to precipitate. At this early high-temperature stage the anhydrous form was stable, and

beds of anhydrite were laid down inside caves within the limestone. Gradual loss of heat allowed the temperature to drop slightly below 58 °C, whereupon  $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$  (gypsum) became the thermodynamically stable phase. Ground water with  $\text{Ca}^{2+}$  and  $\text{SO}_4^{2-}$  concentrations in equilibrium with anhydrite thus became slightly supersaturated with respect to gypsum, and conditions for a phase transition were established.

Next, the question of nucleation was addressed<sup>1</sup>. The Cueva de las Espadas (Cave of Swords), located in the same area about 120 m below the surface and discovered in 1910, features numerous gypsum crystals about 1 m long sticking out like swords from the walls of the cave. The Cave of Crystals lies much deeper at about 290 m and contains fewer much larger crystals. Classical crystal growth theory states that the logarithm of the induction time (time taken to form detectable crystals) is inversely proportional to  $T^3 \log^2 S$ , where  $T$  is absolute temperature and  $S$  is the supersaturation<sup>1</sup>. Homogenisation temperatures for the fluid inclusions in the large crystals cluster around  $54 \pm 1$  °C. Under the very slight degree of supersaturation provided by the dissolution of anhydrite at this temperature the induction time for gypsum exceeds  $10^6$  years<sup>1</sup>. Thus only a few crystals would form, which would subsequently grow to enormous size. Nearer to the surface, the ground water in the Cave of Swords would have been cooler. At a temperature of 47 °C the induction time comprises thousands of years, enabling more crystals to form but limiting the size of any one.

Crystals coexisting in the same cave are described<sup>1</sup> as beam-like (see cover picture) and blocky, the latter sometimes aligned to form “shark’s teeth” (Fig. 2). An explanation of the development in close proximity of these two unusual forms does not yet appear to be forthcoming. Laboratory crystal growth experiments show that pH is an important influence on the habit of gypsum, but impurity ions and organic solutes also have an effect<sup>4</sup>.

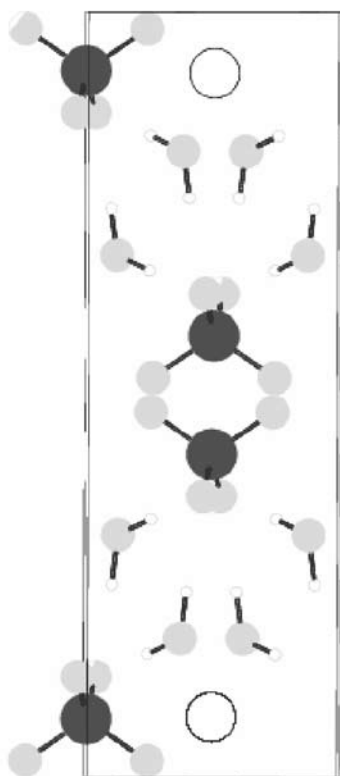
Following **Garcia-Ruiz** et al.<sup>1</sup> we conclude by posing a question about the future of this natural wonder. It has only become accessible because ground water has been intensively pumped out to facilitate mining. The heat and humidity within the Cave of Crystals remain life-threatening. A few attempts have been made to steal crystals, and one thief perished. Should the cave be made into a tourist attraction, properly lit, air-conditioned and guarded? There is concern that the soft crystals, deprived of the buoyant support from ground water, may begin to collapse; and

further changes in conditions may exacerbate this problem. On the other hand, when mining has been completed, should the water pumps be switched off, allowing the cave to flood and the crystals perhaps to resume their slow growth?

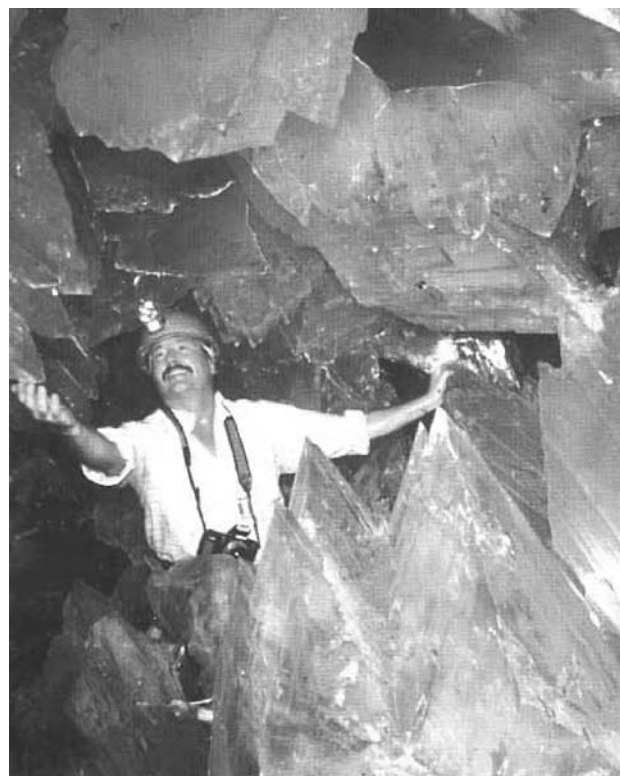
References:

1. J. M. Garcia-Ruiz, R. Villasuso, C. Ayora, A. Canals & F. Otálora
2. B. F. Pedersen & D. Semmingsen (1982) Neutron diffraction refinement of the structure of gypsum,  $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ , *Acta Crystallographica, B* 38, 1074 - 1077.
3. L. L. Y. Chang, R. A. Howie & J. Zussman, (2001) *Rock-forming minerals*, 2<sup>nd</sup> ed., Geological Society, London, p. 42.
4. *Ibid.*, p. 57

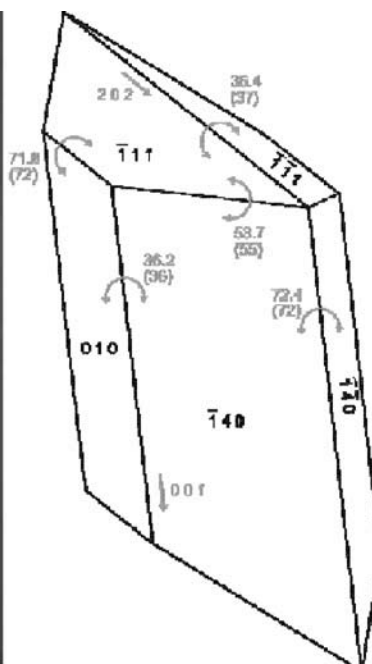
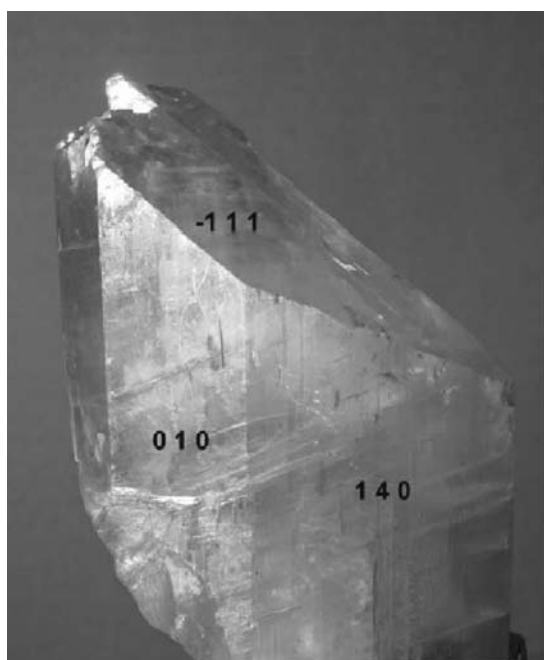
(2007) *Formation of natural gypsum megacrystals in Naica, Mexico*, *Geology*, 35, 327 - 330.



**Figure 1.** The unit cell of gypsum in z-projection. Symbols for the elements are: Ca, large open circles; S, dark shaded circles; O, light shaded circles; H, small open circles.



**Figure 2.** Examples of blocky crystals and "shark's teeth" aggregates in the Cave of Crystals [reproduced with permission given by Richard D. Fisher].



**Figure 3.** Face indices for a blocky crystal [reproduced from Supplementary Material for ref. 1]. In the vertical direction this crystal is 12 cm long.

# 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](mailto:c.h.schwalbe@aston.ac.uk). The help of the IUCr listing is gratefully acknowledged.

## 1-4 December 2008

GISAXS (Grazing Incidence Small Angle X-ray Scattering) Symposium, Boston MA USA  
[http://www.mrs.org/s\\_mrs/](http://www.mrs.org/s_mrs/)

## 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>

## 23-27 March 2009

ICDD Annual Spring Meeting, Newtown Square, PA, USA  
<http://www.icdd.com/profile/march09.htm>

## 26 March - 3 April 2009

30th Berlin School on Neutron Scattering Berlin, Germany  
<http://www.helmholtz-berlin.de/events/nschool2009/>

## 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/>

## 9-10 April 2009

Challenges in Protein Structure Prediction and Drug Design, La Jolla, CA, USA.  
<http://www.molsoft.com/meet09.html>

## 13-17 April 2009

2009 Materials Research Society Spring Meeting San Francisco, CA, USA  
[http://www.mrs.org/s\\_mrs/sec.asp?CID=10891&DID=201200](http://www.mrs.org/s_mrs/sec.asp?CID=10891&DID=201200)

## 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/>

## 25-29 April 2009

Protein folds in infectious and neurodegenerative diseases, Aussois (Savoie) France  
[http://www.cnrs.fr/insb/cjm/2009/steven\\_e.html](http://www.cnrs.fr/insb/cjm/2009/steven_e.html)

## 3-7 May 2009

2009 International Conference on Neutron Scattering (ICNS2009), Knoxville, Tennessee, USA  
[http://www.iucr.org/news/notices/meetings/meeting\\_2008\\_125](http://www.iucr.org/news/notices/meetings/meeting_2008_125)

## 4-6 May 2009

2009 Users Week at Argonne National Laboratory, Argonne National Laboratory, IL, USA  
<http://www.aps.anl.gov/Users/Meeting/2009/>

## 4-7 May 2009

The 8th Pharmaceutical Powder X-ray Diffraction Symposium, Glasgow, UK  
[http://www.iucr.org/news/notices/meetings/meeting\\_2009\\_32](http://www.iucr.org/news/notices/meetings/meeting_2009_32)

## 10-14 May 2009

EMAS 2009 - 11th European Workshop on Modern Developments and Applications in Microbeam Analysis, Gdansk, Poland  
<http://www.emas-web.net/>

## 14-15 May 2009

International Workshop on Anomalous Small Angle X-ray Scattering (ASAXS), BESSY Synchrotron, Berlin, Germany  
<http://www.helmholtz-berlin.de/aktuell/events/asaxs-workshop/>

## 16-21 May 2009

ESF--EMBO Symposium. Spatio-Temporal Radiation Biology: Transdisciplinary Advances for Biomedical Applications, Sant Feliu de Guixols, Spain  
<http://www.esf.org/activities/esf-conferences/details/2009/confdetail287.html?conf=287&year=2009>

## 18-22 May 2009

Practical X-ray Fluorescence, Newtown Square, PA, USA  
<http://www.icdd.com/education/xf.htm>

## 18-22 May 2009

Second International School on Biological Crystallization, Granada, Spain  
<http://www.isbcgranada.org/index.html>

## 24-27 May 2009

Neutron Scattering for the Geosciences, Toronto ON, Canada  
<http://www.agu.org/meetings/ja09/>

## 24-30 May 2009

Seventh European Workshop in Drug Design, University of Siena, Italy  
<http://www.unisi.it/EWDD/>

## 25 May 2009

FRM II User Meeting, Garching, Germany  
<http://www.frm2.tum.de/en/events/user-meeting-2009/index.html>

## 25-29 May 2009

International School on Crystallization. 2009: Drugs, Foods and Agrochemicals, Granada, Spain  
<http://lafactoria.lec.csic.es/iscgranada>

## 30 May - 3 June 2009

92nd Canadian Chemistry Conference and Exhibition, Hamilton, ON, Canada  
[http://www.csc2009.ca/index.cfm/ci\\_id/5144/la\\_id/1.htm](http://www.csc2009.ca/index.cfm/ci_id/5144/la_id/1.htm)

## 4-14 June 2009

High Pressure Crystallography: from Novel Experimental Approaches to Applications in Cutting-Edge Technologies. Erice, Italy  
<http://crystaleric.org/erice2009/2009.htm>

## 8-12 June 2009

ICDD X-ray Diffraction Clinic. Session I -- Fundamentals of X-ray Powder Diffraction Newtown Square, PA, USA  
<http://www.icdd.com/education/xrd.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](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/>

**14-19 June 2009**

Liquid Crystals, New London, NH  
<http://www.grc.org/programs.aspx?year=2009&program=liqcryst>

**14-20 June 2009**

ICC14: XIV International Clay Conference, Castellana, Italy  
<http://www.14icc.org/>

**14-22 June 2009**

2nd school and workshop on X-ray micro and nanopores (XMNP2009), Palinuro (Salerno), Italy  
[http://www.ifn.cnr.it/XMNP2009/scientific\\_motivation.htm](http://www.ifn.cnr.it/XMNP2009/scientific_motivation.htm)

**15-19 June 2009**

ICDD X-ray Diffraction Clinic. Session II -- Advanced Methods in X-ray Powder Diffraction Newtown Square, PA, USA  
<http://www.icdd.com/education/xrd.htm>

**18-20 June 2009**

4th TOPAS Users Meeting, University of Trento, Italy  
<http://www.fkf.mpg.de/xray/html/topas.html>

**21 June 2009**

Crystallography online: International School on the use and application of the Bilbao Crystallographic Server, Lekeitio, Spain  
<http://www.crystallography.fr/mathcryst/bilbao2009.php>

**21-26 June 2009**

Goldschmidt 2009 'Challenges to our Volatile Planet', Davos, Switzerland  
<http://www.goldschmidt2009.org/>

**22-24 June 2009**

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

**25-26 June 2009**

Workshop on Diffuse Scattering in Crystalline Materials, Grenoble, France  
<http://www.esrf.eu/events/conferences/DiffScatt09/diffuse-scattering-in-crystalline-materials>

**12-17 July 2009**

Thin Film & Crystal Growth Mechanisms, New London, NH, USA  
<http://www.grc.org/programs.aspx?year=2009&program=thinfilm>

**19-24 July 2009**

Clusters, Nanocrystals & Nanostructures, South Hadley, MA, USA  
<http://www.grc.org/programs.aspx?year=2009&program=clusters>

**25-30 July 2009**

Annual Meeting of the American Crystallographic Association 2009, Toronto, ON, Canada  
<http://www.cins.ca/aca2009/>

**27-30 July 2009**

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

**27-31 July 2009**

2009 Denver X-ray Conference, Colorado Springs, CO, USA  
<http://www.dxcicdd.com/>

**31 July - 4 August 2009**

The SYMMETRY Festival 2009, Budapest, Hungary  
<http://conferences.hu/symmetry2009/>

**2-7 August 2009**

X-ray Science, Waterville, ME, USA  
<http://www.grc.org/programs.aspx?year=2009&program=xray>

**2-7 August 2009**

SAGAMORE: Charge Spin and Electron Density, Santa Fe NM, USA  
<http://www.sagamoreXVI.org>

**2-8 August 2009**

8th PSI Summer School on Condensed Matter Research on Functional Materials, Zuz, Switzerland  
<http://sls.web.psi.ch/view.php/about/index.html>

**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>

**30 August - 4 September 2009**

GRC Solid State Chemistry Conference: New Frontiers in Materials Synthesis and Characterization, Oxford, UK  
<http://www.grc.org/programs.aspx?year=2009&program=sschem>

**30 August - 12 September 2009**

The Zurich School of Crystallography: Bring Your Own Crystal, Zurich, Switzerland  
[http://www.oci.uzh.ch/diversa/xtal\\_school/](http://www.oci.uzh.ch/diversa/xtal_school/)

**31 August - 12 September 2009**

11th Oxford School on Neutron Scattering, University of Oxford, UK  
[http://www.iucr.org/news/notices/meetings/meeting\\_2009\\_30](http://www.iucr.org/news/notices/meetings/meeting_2009_30)

**7-8 September 2009**

7th International NCCR Symposium on New Trends In Structural Biology, Swiss Federal Institute of Technology (ETH), Zurich, Switzerland  
<http://www.structuralbiology.uzh.ch/symposium2009/>

**8 September 2009**

Annual Meeting of the SGK/SSCr, Fribourg, Switzerland  
<http://www.sgg-sscr.ch/>

**8-10 September 2009**

Synchrotron Radiation and Polymer Science 4, Rolduc, The Netherlands  
<http://srps4.chem.tue.nl/index1.html>

**13-18 September 2009**

Aperiodic09, University of Liverpool, UK  
<http://www.aperiodic09.org>

**13-18 September 2009**

XIV International Conference on Small-Angle Scattering (SAS-2009), Oxford, UK  
<http://www.sas2009.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](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>

**20-24 September 2009**

XXI Conference on Applied Crystallography, Zakopane, Poland  
<http://crystallography.us.edu.pl/>

**21-25 September 2009**

Clays, Clay Minerals and Layered Materials - 2009, Moscow, Russia  
<http://www.cmlm2009.ru/>

**27 September - 2 October 2009**

SRI2009: 10th International Conference on Synchrotron Radiation Instrumentation, Melbourne, Australia  
<http://www.sri09.org/>

**5-8 October 2009**

JCNS Workshop : Trends and Perspectives in Neutron Scattering on Soft Matter, Tutzing, Germany  
<http://www.jcns.info/Workshop/>

**5-7 October 2009**

Studying Kinetics with Neutrons by SANS and Reflectometry, SKIN2009, Grenoble, France  
<http://www.ill.eu/news-events/workshops-events/skin2009/>

**19-23 October 2009**

Basic and Advanced Rietveld Refinement & Indexing Workshops, Newtown Square, PA, USA  
<http://www.icdd.com/education/rietveld-workshop.htm>

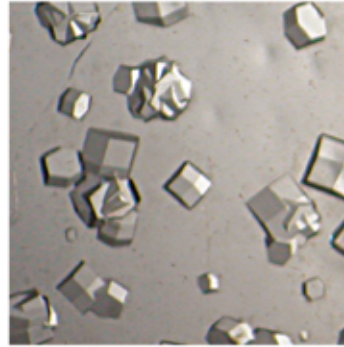
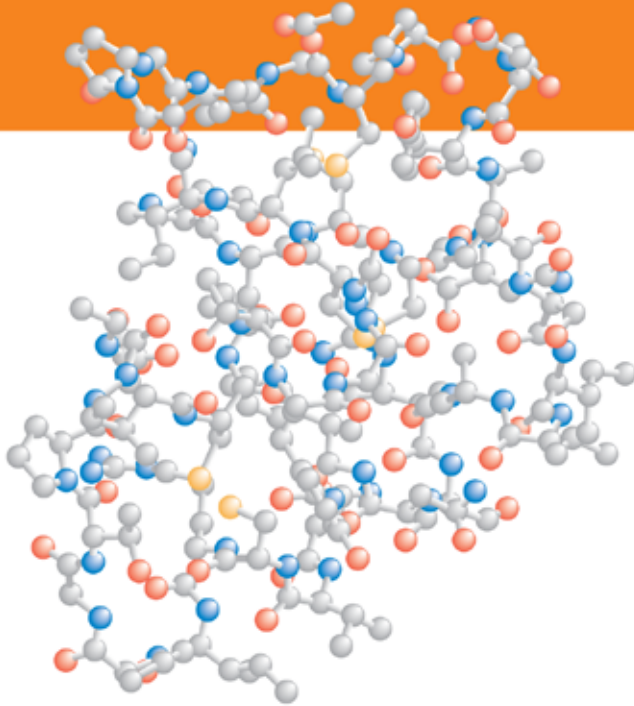
**28-30 October 2009**

International Workshop on the Analysis and Refinement of the Electron Density, Marrakech, Morocco  
<http://www.ucam.ac.ma/fssm/adr/>



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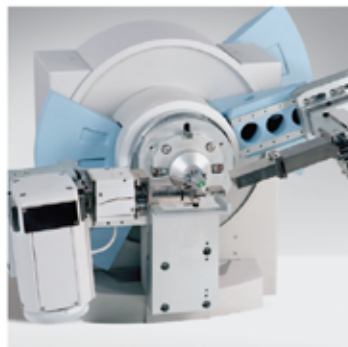
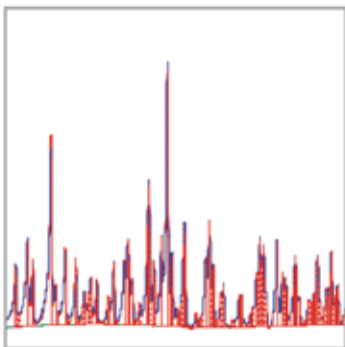
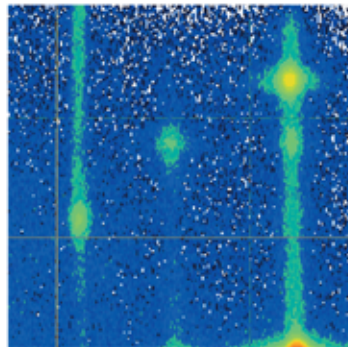
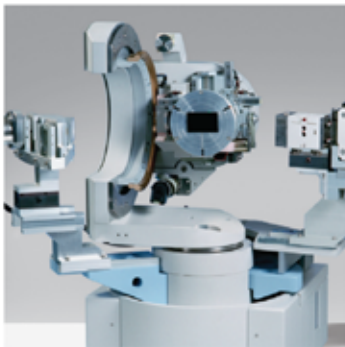
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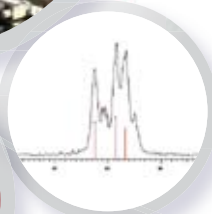
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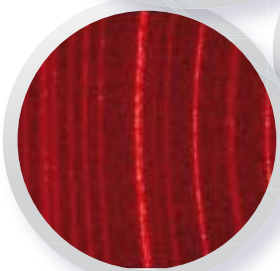
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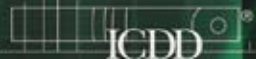
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