

Crystallography News

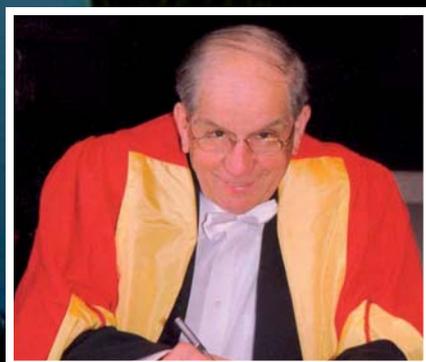
British Crystallographic Association



Issue No. 102 September 2007

ISSN 1467-2790

BCA Spring Meeting 2008 - York p7



Some Random Thoughts p6

Canterbury 2007 p12

Meetings p19

News from the Groups p24

Contents

From the President	2
Council Members	3
Puzzle Corner	4
Festival Pattern Group Ties	4
From the Editor	5
Some Random Thoughts	6
BCA Spring Meeting 2008 - York	7-11
International Tables Online	8
Visiting the ROM	9
BCA 2007 Meeting	12-17
News from CCP14	17
Sam Motherwell Symposium	18
ACA and other Meetings	19-23
News from the Groups	24-25
Meetings of Interest	26-27



**BCA
Administrative
Office,**
Elaine Fulton,
Northern Networking
Events Ltd.

1 Tennant Avenue,
College Milton South,
East Kilbride, Glasgow G74 5NA
Scotland, UK

Tel: + 44 1355 244966

Fax: + 44 1355 249959

e-mail: bca@glasconf.demon.co.uk

CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by William Anderson and Sons Ltd, Glasgow. Text should preferably be sent electronically as MSword documents (any version - .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (e.g. awards, honours, retirements etc.), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews. Please ensure that items for inclusion in the December 2007 issue are sent to the Editor to arrive before 25th October 2007.

Bob Gould

33 Charterhall Road
EDINBURGH EH9 3HS
Tel: 0131 667 7230
e-mail: gould@ed.ac.uk

The British Crystallographic Association is a Registered Charity (#284718) As required by the DATA PROTECTION ACT, the BCA is notifying members that we store your contact information on a computer database to simplify our administration. These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

Designed & printed by Wm. Anderson & Sons Ltd.
34 Loanbank Quadrant, Glasgow.
Tel: 0141 440 2881
e-mail: enquiry@andersonprinters.com

This month's cover:

Something to look forward to -
spring on the campus at the
University of York, and someone
to remember - a smiling
Durward Cruickshank.



From the President



LET me start this article with some news that is of considerable importance and will feature in articles throughout this issue.

Because of certain logistic issues with the Swansea site, it has been decided to move the venue of the BCA Spring Meeting next year to the University of York. The

dates of the meeting, however, remain unchanged, from 8 - 10 April, 2008. When we visited York a few years ago, we had a very successful meeting and I am sure that the same will be true next year.

Planning for the Spring Meeting is already well advanced, and I am most grateful to **John** and **Ivana Evans** and the Programme Committee for all the hard work that they have already put in assembling a very exciting programme that should appeal to a wide audience. The outline of the programme is mapped out in this issue of *Crystallography News* and the full details will be published in the December issue and on the conference website. Among the highlights is the *BCA Prize Lecture* which, I am very pleased to say, will be given by Dr **Tony Crowther**, FRS, from the MRC Laboratory in Cambridge. The Prize Lecture is given by one eminent scientist in recognition of another, and Tony will be honouring Professor **Michael Rossmann**, and relating some of the areas pioneered by Michael Rossmann to his own research on viruses.

I am writing this column in mid July, watching the rain fall, and wondering where the summer has gone. However, the summer conference season is upon us with the ACA Meeting in Salt Lake City in late July and the ECM-24 Conference in Marrakesh in late August. I know that

there will be a good representation from the UK at both meetings and, since you will read this in September, I hope that you had an enjoyable and productive time. Some of you will already be planning your visit to Japan next year to attend the XXI Congress of the IUCr in Osaka from 23 - 31 August. Again, the UK will be well represented, and BCA members have been involved in the preparation of the scientific programme. I am also pleased to say that the BCA Officers have submitted 20 nominations for officers and members of the various IUCr Commissions from the membership of the BCA so the Association should continue to be well represented on the international stage.

It is again the time of year when I have the very pleasurable duty to invite nominations for Honorary Members of the BCA, and I would also like to thank those of you who have already sent nominations into me. Honorary Membership is the highest membership accolade of the BCA, and is awarded to a small and select group of colleagues who have contributed significantly to crystallographic science and to the work of the BCA. In recent years we have elected **Paul Barnes**, **Chris Gilmore**, **Mike Glazer**, **Mike Hursthouse**, **Peter Main** and **George Sheldrick**. In the coming year we anticipate electing one or two new Honorary Members. Please send your nominations, together with a short supporting case to me at president@crystallography.org.uk by the 31st October, 2007.

Finally, it is with great sadness that I have to report the death of **Durward Cruickshank**, FRS, at the age of 83. **Durward** was one of the fathers of modern crystallography and has been an inspiration to many of us. He was an Honorary Member of the BCA and continued to contribute enthusiastically to the Association right up to his death. He will be sadly missed.

Paul Raithby



BCA Council 2006-07

COUNCIL MEMBERS



President (2009)
Prof. Paul R. Raithby
Department of Chemistry
University of Bath
Claverton Down
BATH BA2 7AY
Tel: 01225 383183
p.r.raithby@bath.ac.uk



Vice President (2010)
Prof. Alexander J. Blake
School of Chemistry,
University of Nottingham
University Park
NOTTINGHAM NG7 2RD
Tel. 0115 9513488
A.J.Blake@nottingham.ac.uk



Secretary (2010)
Dr Georgina Rosair
School of EPS - Chemistry
Perkin Building
Heriot-Watt University
EDINBURGH EH14 4AS
Tel: 0131 451 8036/4241
g.m.rosair@hw.ac.uk



Treasurer (2008)
Dr Sheila Gould
33 Charterhall Road,
EDINBURGH EH9 3HS
Tel: 0131 667 7230
treasurer@
crystallography.org.uk

ORDINARY MEMBERS



Dr Richard Cooper (2009)
oXray Ltd
Oxford Centre for Innovation
OXFORD OX2 0JX
Tel: 01865 811107
Richard.cooper@
oxray.com



Dr Elspeth F. Garman (2009)
Laboratory of Molecular
Biophysics
Rex Richards Building
University of Oxford
South Parks Road
OXFORD OX1 3QU
Tel: 01865 275398
elspeth@biop.ox.ac.uk



Prof. William Clegg (2009)
School of Natural Sciences
(Chemistry),
University of Newcastle,
NEWCASTLE UPON TYNE
NE1 7RU
Tel: 0191 222 6649
W.Clegg@newcastle.ac.uk

GROUP REPRESENTATIVES



Biological Structures
Dr Sheila Gover
131 Main Road
Middleton Cheney
BANBURY, OX17 2PW
Tel: 01295 711636
sheila.gover@tesco.net



Chemical Crystallography
Jonathan Charmant
School of Chemistry,
University of Bristol,
BRISTOL BS8 1TS
Tel. (0117) 928 8253
jon.charmant@bris.ac.uk



Industrial
Dr David Beveridge
Harman Technology -
ILFORD Photo
Town Lane, Mobberley,
KNUTSFORD WA16 7JL
Tel: 01565 650000
David.Beveridge@
harmantechnology.com



Physical Crystallography
Dr Matt Tucker
CCLRC Rutherford
Appleton Laboratory
DIDCOT OX11 0QX
Tel: 01235 445581
M.G.Tucker@rl.ac.uk



Young Crystallographers
Dr Simon Coles
Department of Chemistry
University of Southampton
SOUTHAMPTON SO17 1BJ
Tel: 023 8059 6722
s.j.coles@soton.ac.uk

CO-OPTED MEMBERS



Prof. Garry Taylor
Centre for Biomolecular
Sciences
North Haugh
University of St Andrews
ST ANDREWS KY16 9ST
Tel: 01334 4677301
glt@st-and.ac.uk



Prof. Paul Fewster
PANalytical Research
Centre
Sussex Innovation Centre
BRIGHTON BN1 9SB
Tel: 01273 704422
paul.fewsterpanalytical.
com

EX-OFFICIO MEMBERS



Education Coordinator
Prof. Chick Wilson,
Department of Chemistry,
University of Glasgow
GLASGOW G12 8QQ
Tel: 0141 330 8522
chick@chem.gla.ac.uk



Editor
"Crystallography News"
Dr Robert Gould
33 Charterhall Road
EDINBURGH EH9 3HS
Tel: 0131 667 7230
gould@ed.ac.uk



Webmaster
**Dr Jeremy Karl
Cockcroft**
Department of Chemistry
University College London
LONDON WC1H 0AJ
Tel: 020 7679 5802
cockcroft@
img.cryst.bbk.ac.uk

GROUP CHAIRMEN



**Biological
Structures Group**
Dr Andrea Hadfield
Department of
Biochemistry
University of Bristol
BRISTOL BS8 1TD
Tel: 0117 331 2151
a.t.hadfield@bristol.ac.uk



**Chemical
Crystallography Group**
Dr Richard Cooper
oXray Ltd
Oxford Centre for Innovation
OXFORD OX2 0JX
Tel: 01865 811107
Richard.cooper@oxray.com



Industrial Group
Dr Anne Kavanagh
AstraZeneca
MACCLESFIELD, SK10 2NA
Tel. 01625 517454
Anne.Kavanagh@
astrazeneca.com



**Physical
Crystallography Group**
Prof. Paolo Radaelli
Isis Facility Rutherford
Appleton Laboratory
Chilton
DIDCOT OX11 0QX
Tel: 01235 445685
p.g.radaelli@rl.ac.uk

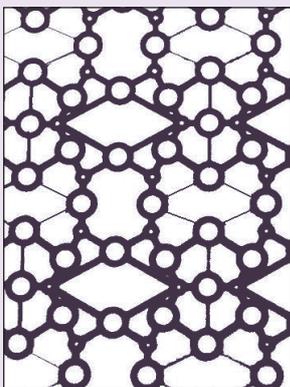
Full committee details on the BCA website www.crystallography.org.uk

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

Puzzle Corner

AFTER we've all had a hard summer working at the puzzle books as we hope the rain will go away, here's a nice easy one. In the following text, fill in the missing six- or seven-letter words indicated by the blanks. A little judicious rearranging of the first letters of the words will "reveal" what we are looking at. As most of you can probably guess that, I'd like all eight words in submitted answers.

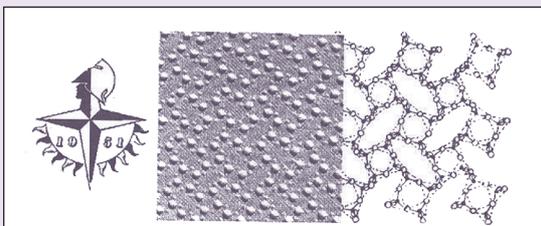
Whether in the monoclinic or _____ form, those of _____ (or, more traditionally, _____) are _____ in colour. Viewed through _____, one of them may appear to be two. They are _____ and hence not pyroelectric. If the molecules in them are treated as rigid, they may translate and screw, they may also _____, and this motion is represented by a symmetric _____.



LAST month's puzzle attracted one answer, from Lindsay Sawyer, who is thus the clear winner, even if his answer (apophyllite) is probably not right! It is admittedly difficult to say what a structure is supposed to represent without knowing what the symbols mean - for example, KI will mean the salt potassium

iodide to some crystallographers and the dipeptide lysylisoleucine to others! This picture is possibly a silicate of some kind, where the small circles are the Si (or other T) atoms, and the large circles O.

Lindsay points out, that we have previously had something similar in *Crystallography News*, in the article about Helen Megaw's 90th birthday in December 2001. The illustration there was of the apophyllite structure, with a commercial glass pattern based on it, and used at the Festival of Britain. The pattern is a section normal to the tetragonal axis of the structure exhibiting the plane group $p4g$.

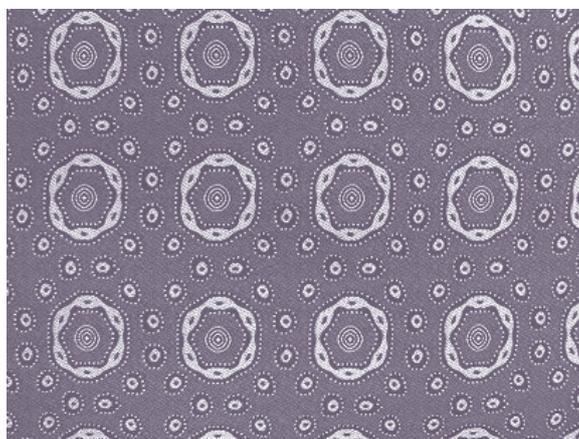


Pattern of figured rolled glass made by Chance Bros. for many years. The repeat is small, and the blobs are small enough so that the sunshine does not set fire to any nearby curtains! See also the article about ties on this page by Lesley Jackson.

Festival Pattern Group Ties

(The following relates directly to the Puzzle in the last issue. See this month's Puzzle Corner. Lesley hopes to write a longer article about this project in a future issue. Ed.)

DID you attend the International Congress of Crystallography Conference in Cambridge in 1960? Did you purchase a woven silk tie decorated with crystal structure patterns?



If so, I would like to hear from you. I am curating an exhibition about the Festival Pattern Group for the Wellcome Trust at the newly opened Wellcome Collection galleries in London next year. The Festival Pattern Group was a remarkable project spearheaded by pioneer crystallographer Dr Helen Megaw. The idea behind the scheme was for textile companies and other manufacturers to use X-ray crystallographic diagrams as the basis for patterns on fabrics and other domestic products. The resulting creations were showcased at the Festival of Britain in 1951. The Festival Pattern Group ties proved so popular with crystallographers that they were revived again for the 1960 Conference.

Other products created for the Festival Pattern Group included glass ashtrays, wallpapers, lace and various other printed and woven fabrics. If you think you might have a tie or indeed any of the other items, that might be borrowed, please contact me: lesley.jackson@3-c.coop; tel 01422 842026.

Lesley Jackson

From the Editor



AS the President says, the death of **Durward Cruickshank** has left a big gap in the BCA, for he was a lively and faithful attender of our meetings until his final illness.

He not only always had much that was useful to say on almost any topic, he did so with remarkable kindness and humour. He was frequently of great assistance to your Editor! Unfortunately his death

has occurred at a time when it is difficult to get an appropriate obituary into this issue of *Crystallography News*. We hope to have a fitting tribute in the December issue, and would welcome reminiscences from as many of you as possible.

The shift of next year's Spring Meeting from Swansea to York will come as a surprise to many, but York has proved itself in 1986 and 2003 to be an excellent location for us. The programme is well advanced, as you will see, and **John** and **Ivana Evans** have been wonderful in their appreciation of deadlines.

Most of the remaining sessions from the 2007 meeting in Canterbury are written up here, and I am particularly grateful to **Mark Farnworth** for organising these. There is also an account to the Motherwell Symposium from **Frank Allen**. Finally, **Lindsay Sawyer**, last year's programme chair occupier, has submitted some useful and amusing thoughts on that exalted location.

We are, as always, grateful for those rare unsolicited items of interest of which you will find a few here. **Kate Crennell** is a great finder of these - thank you Kate!

As usual in September, there are some announcements for various group autumn meetings. The full direct web address for these is fairly complex. Many of you may take our viewpoint that typing crystallography.org.uk and then following the links is really quicker!

While *Puzzle Corner* didn't get many entries - I could count them on the fingers of one finger - it has raised a little interest in those crystallographic patterns that give rise to art. **Lesley Jackson** of the Wellcome Trust is preparing an exhibition on these, and will write more for us later.

Finally, we have three accounts of international meetings, and a metaphorical bunch of roses for **Gary Nichol**, formerly of Newcastle and now of Arizona, who has kindly written up the ACA meeting for us - his many reports on BCA meetings have clearly got him in the habit, even when he didn't get a bursary from us!

Bob Gould

BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
- A 10% discount on exhibition stands on the annual BCA Spring Meeting, OR - A promotional poster at the annual BCA Spring Meeting.
- Free insert in the annual Spring Meeting delegate bag.
- Two free full registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly BCA Newsletter.
- Corporate Members will be listed in every BCA Newsletter and on the BCA Web Site with links to your corporate site.

The cost of this membership is **£750.00** per annum

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

Elaine Fulton | BCA Administrative Office

Northern Networking Events Ltd
1 Tennant Avenue, College Milton South
East Kilbride G74 5NA
Phone 01355 244966 Fax 01355 249959
e-mail bca@glasconf.demon.co.uk

Corporate Members

Astex Technology
Bruker AXS Ltd
Cambridge Crystallographic Data Centre
CCLRC
Chemical Computing Group
CrystalMaker Software Ltd
Hampton Research
International Centre for Diffraction Data
Malvern Instruments Ltd
Marresearch GmbH
Molecular Dimensions Ltd
Oxford Cryosystems
Oxford Diffraction
PANalytical
Rigaku MSC
Thermo Fisher Scientific

Some Random Thoughts

Some Random Thoughts from an Old Programme Chairman



PERHAPS the most difficult thing to come to terms with when approached to take on the task of Programme Chair, was whether to insist upon being referred to as a Chairman rather than as a piece of furniture, genderless though that might be (*la chaise, der Stuhl; Europe*

doesn't help much!). In fact my recruitment was a total surprise to me but had obviously been carefully planned by committees and officers and the sundry others. I sit on a research ethics committee and one of the guiding principles is that of informed consent and indeed that potential recruits be given at least a day to consider. Fat chance; the President, VP, Secretary, Group Chair(men) all thanked me for agreeing to do it; so what chance did I really have?

As it turned out of course, the whole process worked out remarkably well thanks to the huge amount of help from the previous committee, and more particularly from the group programme organizers. An early meeting decided deadlines, who was to do what, what still needed to be found out - this smacks a bit of **Donald Rumsfeld** - and, roughly speaking, what were the topics of the various sessions. One of the unknowns which was fortunately fairly quickly resolved, was whether we would have three or only two named lectureships. That decided, a little bit of juggling of which groups were responsible for which sessions, and the PC could relax.

Well, almost. The deadline for the September *Crystallography News* was close and it was necessary to put out the first notice with calls for abstracts for submitted oral presentations and as much of the programme outline as was extant. Cajoling, pleading, even just asking, all had their effect, different in each case: some produced outlines without asking, others didn't! Then it was off on a site visit to walk the course with Northern Networking and the helpful Canterbury folk. We had agreed to have the programme more or less complete by the December *Crystallography News* and, apart from a few gaps, we managed it with a bit of help from an accommodating editor.

Abstract deadlines approached almost before the New Year hangover had abated, and of course the modifications and

tweakings necessary as titles, winkled out of speakers long before they had really noticed, had to be modified. Poster abstracts had to be assigned to the various groups, which was relatively straightforward except in a few cases. The 'final' programme and house-keeping details for the meeting were assembled for the March BCA News and then a series of frantic communications about accommodation, session times, how to find Canterbury ('Is it lost?'), led up to the meeting itself, which, when all is said and done, went off extremely well!

Northern Networking carried out the essential logistics for the meeting with efficiency, skill and good humour and consequently played a huge part in its success. Use of the web clearly helped the organization, and with some careful repositioning of deadlines, some of the more fraught moments in March will be avoided in future. Group programmers also were extremely supportive and did a sterling job, and finally, having the Editor down the corridor was a help!

Full incorporation of the Young Crystallographers as a fifth group is excellent and it will be interesting to see if the general timetable for the York Meeting will be altered to reflect the change. Whatever, the programme is in better hands and so it will be an even more excellent meeting. See you there!

Lindsay Sawyer

Guinier: Small-Angle Scattering of X-Rays (*from the SAXS discussion list*)

ASTOLOGOS Books (<http://www.astrologos.org/>) can print-to-order copies of Christopher Walker's translation of André Guinier's 1955 classic textbook on SAXS.

Description: AS NEW - Print-to-order B&W REPRINT of original book published: New York Wiley 1955. 282 Pages Expertly printed on acid-free archival quality paper - Softcover perfect bound (or Hardcover Cloth Buckram binding for additional \$10.) Charts photographs & graphics may reproduce less than perfectly & may be reduced to fit pages. SPECIAL ORDER Allow 6 to 8 weeks for delivery. No Refund or Exchange. Price: \$106.00 (Soft Cover)

Wim Bras (ESRF) has recently acquired a copy that he describes as "pretty decent".

Steve King

BCA Spring Meeting 2008

“Structure, Property & Function” in York

FOLLOWING the success of the 2003 Spring Meeting we've decided to return to the **University of York for 2008**. As many of you will know York has a delightful self-contained campus. Accommodation is within easy walking distance of the conference facilities and the lectures, exhibition and (most importantly) tea/coffee facilities will be co-located at the same lakeside venue. York is also a wonderful city to visit - perfect for a pre/post-meeting break. Links to York, the University campus, travel information and the meeting website are given below:

York:

<http://www.york.gov.uk/visiting/>

York University:

<http://www.york.ac.uk/>;

<http://www.york.ac.uk/np/maps/hes.htm>

Travel to York:

<http://www.york.ac.uk/np/maps/>

Spring Meeting website:

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

As always, the BCA Spring Meeting will be **the place** to hear about the latest structural science, to network with colleagues and to meet with our exhibitors. We hope to see you there!

John and Ivana Evans

john.evans@durham.ac.uk; ivana.radosavljevic@durham.ac.uk

Main Meeting

THE main meeting will follow the successful format of recent years and run from **11:30 on Tuesday 8 April to 13:30 on Thursday 10 April (Easter Day 2008 is 23 March)**. The overall theme of the meeting is “Structure, Property & Function” and there are 20 exciting symposia (titles below) around this theme. Thanks to a committed organizing team we have a very strong scientific programme; all plenary lectures and many keynote session talks are already in place. There is, however, still time for **you to contribute** to the meeting. We've allocated slots in each symposium for contributed talks. Details on how to submit abstracts are given below.

Plenary Lectures

BSG Plenary: Tony Crowther (MRC LMB Cambridge)
From Molecular Replacement to the Structure of Viruses: a Tale of Two Careers

CCG Teaching Plenary - Controlling Difficult Refinements:
Peter Muller (MIT) *Dead End Highway 13 - the Carriage of No Return*

IG Plenary: Rob Delhez *X-ray Diffraction on Mars?*

PCG Plenary: Paul Attfield (Edinburgh)
Charge Order in Oxides - Putting the Fun into Functional Materials

Selected Speakers

A selection of the scientific highlights includes:

Jamshed Anwar (Bradford): *Phase Transition Phenomena from Molecular Simulation*

Alison Burke: *Application of XRD within the Pigments Industry*

G rard Coquerel: *The Different Roles of Water Molecules in Chiral Discrimination in the Solid State*

Edmund Cussen (Strathclyde): *Switching on Fast Lithium Ion Conductivity: Structure and Transport Properties of the Garnet Structure*

Judit Debreczeni: *Protein Structures in Drug Discovery*

Ashley Hulme: *Application of XRD and Other Analytical Techniques to Pharmaceuticals*

Stuart James (Belfast): *Solvent-Free Synthesis and Some 'Design' Aspects of Metal-Organic Frameworks*

Matthew Johnson (GSK): *Pharmaceutical Crystal Structures from Powder Diffraction Data*

John Mitchell (Cambridge): *Informed by Informatics?*

Thomas Proffen (Los Alamos Neutron Science Center): *Total Scattering: the Key to Understanding the Local- and Medium-Range Structure of Materials*

Jeremy Rawson (Cambridge): *Sulfur-Nitrogen Radicals: Systematic Design of Spin-Transition Materials*

Martin Schr der (Nottingham): *Metal-Organic Framework Materials: Porosity and Storage*

Peter Skabara (Strathclyde): *Controlling the Conformation of Conjugated Molecules through Non-Covalent Interactions*

Parallel Sessions

Symposium Title	Chairperson	Contact
<i>Local Structure and Disorder in Crystalline Materials</i>	Matt Tucker	m.g.tucker@rl.ac.uk
<i>Crystal Chemistry of Functional Extended Solids</i>	Ivana Evans	ivana.radosavljevic@dur.ac.uk
<i>Functional Molecular Materials I</i>	Andrew Bond	adb@ifk.sdu.dk
<i>Functional Molecular Materials II</i>	Serena Margadonna	serena.margadonna@ed.ac.uk
<i>Strongly Correlated Electron Systems I</i>	Paolo Radaelli	p.g.radaelli@rl.ac.uk
<i>Strongly Correlated Electron Systems II</i>	Peter Hatton	p.d.hatton@durham.ac.uk
<i>Calculating Properties from Structure</i>	Simon Coles	s.j.coles@soton.ac.uk
<i>Design of Functional Materials</i>	Neil Champness	neil.champness@nottingham.ac.uk
<i>Structures from Pharmaceutical Powders</i>	Kenneth Shankland	k.shankland@rl.ac.uk
<i>Jekyll and Hydrate</i>	Roy Copley	royston.c.copley@gsk.com
<i>Applied Crystallography Showcase</i>	Chris Staddon	chris.staddon@nottingham.ac.uk
<i>Small Is Smart</i>	Judith Shackleton	judith.shackleton@manchester.ac.uk
<i>Big Is Beautiful</i>	Judith Shackleton	judith.shackleton@manchester.ac.uk
<i>Membrane Proteins I</i>	Neil Isaacs	n.isaacs@chem.gla.ac.uk
<i>Membrane Proteins II</i>	Neil Isaacs	n.isaacs@chem.gla.ac.uk
<i>Neutrons in Biology</i>	Garry McIntyre	mcintyre@ill.fr
<i>Probing Fast Biological Reactions</i>	David Leys	david.leys@manchester.ac.uk
<i>Complementary Methods in Structural Biology</i>	Helen Saibil	h.saibil@mail.cryst.bbk.ac.uk
<i>Ligand Binding and Drug Design I</i>	Rod Hubbard	rod@ysbl.york.ac.uk
<i>Ligand Binding and Drug Design II</i>	Rod Hubbard	rod@ysbl.york.ac.uk

Abstract Submission

There are slots reserved in each symposium for contributed talks. Please submit abstracts for consideration using the word template (available from the conference website) by Friday, 28 September. Applicants will be informed by 25 October whether their talk has been accepted.

As always, the poster session will be one of the main fora for scientific discussion. We'll also be offering poster contributors the opportunity to display graphical abstracts on screens throughout the exhibition. More details on this to follow. The deadline for poster abstracts will be in early February.



International Tables Online

WE are pleased to announce that the first edition of International Tables Online is now available. Any feedback on the use of the Tables and the "guided tour" would be welcome.

To benefit from this exceptional reference work, please ask your librarian to order International Tables Online from Springer at <http://www.springer.com/978-1-4020-5259-0>. The price quoted represents a one-off cost (not an annual subscription) and provides perpetual access to the first online edition.

Once your librarian has registered, you and your colleagues will have access to the full set of all the Volumes A to G including A1 (6000 pages) as pdfs via SpringerLink. In addition, access to the full text of the series as both pdfs and richly interlinked html, along with many innovative features and additional resources, will be available via the interactive International Tables Online website at <http://it.iucr.org>. A guided tour of this website is available at <http://it.iucr.org/services/guidedtour>, which contains five sample chapters and numerous examples showing the functionality of the site, and the illustration is taken from this.

For more information, please visit <http://it.iucr.org>.

Michael Dacombe, IUCr

Workshops and Satellites

IN addition to the main meeting the Young Crystallographers are running a satellite symposium on Monday afternoon and Tuesday morning. There are also two hands-on computer workshops being arranged. Immediately prior to the meeting Matt Tucker (ISIS) and Thomas Proffen (Los Alamos National Laboratory) are running a PDF workshop; on Tuesday afternoon Kenneth Shankland will run a DASH workshop - come along and learn about the latest software developments from the experts.

Workshops

PDF WORKSHOP: *Shedding Light on the Local Structure and Disorder in Crystalline Materials*

Organisers: Matt Tucker (ISIS) & Ivana Evans (Durham)

Matt Tucker (ISIS) and **Thomas Proffen** (LANSCE) will run a full day hands-on PDF workshop. The importance of local structure and disorder in crystalline materials is increasingly being recognised as a key property of many functional materials. From negative thermal expansion to solid state amorphisation and the 'nanoscale' problem to improved fuel cell technology, a clear picture of the local atomic structure is essential to understanding these phenomena and solving the associated problems. A powerful technique for exploring the local structure of materials is total scattering, also known as the PDF method. Synchrotron X-ray and/or neutron powder diffraction data can be used to obtain information on the local, medium and long range atomic structure simultaneously. To gain the maximum information from the data, specialised refinement methods are required. Two of the most powerful methods currently available for refining this type of data are RMCPProfile and PDFFIT. The aim of this workshop is to provide an overview of the methods and the opportunity to gain some hands-on experience of applying them to total scattering data. No previous experience is required. For more information about the PDF workshop please email Matt Tucker (m.g.tucker@rl.ac.uk) or Ivana Evans (ivana.radosavljevic@durham.ac.uk).

DASH WORKSHOP

Organisers: Richard Cooper (oXray) & Kenneth Shankland (ISIS)

Kenneth Shankland will be running a hands-on workshop in the computing lab, using the DASH software. DASH is a program for crystal structure determination from powder diffraction data. This workshop is aimed at students and researchers who have no previous experience using DASH and who are interested in structured determination from powders. For more information please email Richard Cooper (richard.cooper@oxray.com) or contact Kenneth Shankland.

Visiting the ROM

LIKE many other natives of the wonderful city of Toronto, to me the letters ROM don't refer to a chip, they mean Royal Ontario Museum. It was a wonderful, exciting place I remember from earliest childhood, and has, among other things, a particularly wonderful mineral collection. It has been undergoing extensive rebuilding for some time, but has just reopened, with a much-celebrated extension called "The Cristal". So, as we had friends with us in Canada this summer, that was the place I took them on a short visit into the city.



The original building is good solid Edwardian, and the extension, as you will see in the picture, certainly breaks the mould. As the new building is mainly of glass, it is certainly suitable that at least the spelling of the word "crystal" had been changed. It is, indeed, a remarkable piece of work. I had, however, to agree with my friend, who works for a museum in Edinburgh, that people don't go to a museum to see *it*, they go to see *what's in it*, and it's hard to imagine a less efficient provision of display space!

However, the worst was yet to come. I had missed the small print, and the minerals are not to be back on display for more than a year! Fortunately, our friends are biologists, and the animals are there. As for the crystals, in or out of the Cristal, I'll have to remember to look back in 2009. And meantime, for anyone who wants to look *at* a museum rather than *in* it - this is the place, and the exterior is free!

Bob Gould

BCA 2008 Spring Meeting -

	Monday, 7th April		Tuesday, 8th April			
9:00			YC 4	PDF workshop		
9:15						
9:30						
9:45						
10:00						
10:15						
10:30			Registration/exhibition 10.30-11.30			
10:45						
11:00			BSG Plenary 11.30-12.30 From Molecular Replacement to the Structure of Viruses: a Tale of Two Careers			
11:15						
11:30						
11:45						
12:00						
12:15						
12:30						
12:45			Lunch/exhibition/registration 12.30-13.30			
13:00	YC 1	PDF workshop	Sessions 13.30-15.00			
13:15						
13:30				Local structure	Membrane proteins	Pharmaceutical powder diffraction
13:45						
14:00						
14:15						
14:30						
14:45						
15:00	Coffee 15.00-15.30		Coffee 15.00-15.30			
15:15			Sessions 15.30-17.00			
15:30	YC 2	PDF workshop	CCG Prize	Membrane proteins	Hydration of pharmaceutical materials	
15:45						
16:00				PCG Prize		
16:15						
16:30						
16:45						
17:00	Break	Break	Break 15 minutes			
17:15						
17:30	YC 3	PDF workshop	Exhibitors Forum 17.15-18.45		DASH workshop	
17:45						
18:00						
18:15						
18:30						
18:45	Break	Break				
19:00	YC dinner	Dinner	Dinner, exhibition and posters			
19:15						
19:30						
19:45						
20:00						
20:15						
20:30						
20:45						
21:00						

Timetable

Wednesday, 9th April			Thursday, 10th April		
PCG Plenary 9.00-9.45 Charge Order in Oxides: Putting the Fun into Functional Materials			Teaching Plenary 9.00-9.45 Controlling Difficult Refinements		
Coffee 9.45-10.15			Coffee 9.45-10.15		
Parallel sessions 10.15-11.45			Sessions 10.15-11.45		
Functional extended solids	Neutrons in biology	Applied crystallography	Strongly correlated systems	Ligand binding and drug design	Design of functional materials
PCG AGM 11.45-12.30	BSG AGM 11.45-12.30	IG AGM 11.45-12.30	Break 15 minutes		
Lunch, exhibition 11.45-13.30			Sessions 12.00-13.30		
		CCG AGM 12.45-13.30	Strongly correlated systems	Ligand binding and drug design	Calculating properties from structure
Sessions 13.30-15.00			Close 13.30		
Functional molecular materials	Probing fast biological reactions	Small is smart			
Coffee 15.00-15.30					
Sessions 15.30-17.00					
Functional molecular materials	Complementary methods in structural biology	Big is beautiful			
Break 15 minutes					
IG Plenary 17.15-18.00 IG: X-Ray Diffraction on Mars					
BCA AGM 18.00-19.00					
Comfort time					
Conference dinner 19.30 for 20.00					

Canterbury 2007

Diffraction from surfaces and Two Dimensional Crystallography - 18th April 2007



Left to right: Tom Hase, Judith Shackleton (Co-Chair), Donna Arnold, Richard Morris (Co-Chair), Peter Laggner.

DONNA ARNOLD (University of Cork), *Structural Studies of Ordered Mesoporous Silica in Channelled Substrates*. Mesoporous silicates are produced when a surfactant is used as a template to produce a silica backbone. The surfactant is added to a sol-gel mix.

Rod-like silica 'micelles' are produced. Mesoporous silica is used in areas such as electronics, catalysts, photonics and medical applications. Donna described research centred on establishing a relationship between etched silicon channels and their effect on mesoporous thin films. Using lithographically patterned (100) oriented substrates and a dip-coating method produced reproducible alignment of the pores across the substrate surface with the pores aligned parallel to the long side of channels. Etched silicon substrates or pillared silicon substrates are used and it was found that the latter produces poorer film qualities. Small angle X-ray diffraction (SAXS) and reflectivity (XRR) measurements showed strain effects when compared with simple films. A supercritical fluid inclusion technique is used to incorporate cobalt into the pores. High resolution Secondary Electron Microscopy was used for imaging. They discovered a high degree of pore order, large domain sizes, strong adherence to the channels, good thermal stability and that quality was dependant on the channel dimensions. The results indicate that the topographic structure can be used to engineer the placement and directionality of the pore structure.

Tom Hase (University of Durham) *X-ray Characterisation of Nanomagnetic materials*. Tom began by saying that it is now possible to produce patterned elements and nanostructures, with control of lateral dimensions. Patterning is achieved using Focussed Ion Beam (FIB) or lithography using photoresist. Arrays of nanoscale elements form the background for fundamental studies of magnetism which are important in realising both magnetic memory and high-density storage media. Several techniques are used to analyse small groups of nanostructures or small areas of nanostructured materials. The problem is that small volume / small area analysis may not give information that is representative of the sample as a whole. However, by imaging arrays of nanoscale material in reciprocal space this problem can be overcome. Averaged array parameters can be determined. Rocking curve analysis is a good technique because the presence of a repeat pattern in the plane results in satellites of coherently scattered intensity equi-spaced on either side of the 'specular ridge'. The spacing of these satellites gives the periodicity of the nanostructures; the width of satellites the coherence and the 'envelope' of the scattered intensity the shape of nanostructures. The use of resonant magnetic scattering to probe the element specific magnetisation processes in arrays was presented. With magnetism, there is a need to know the scaling behaviours, anisotropies and the structure of domains. One avenue of research is to link the magnetic peak envelope obtained from Rocking Curve analysis to the magnetic size and shape and to compare with the physical size and shape. Tom clearly showed how X-ray data is providing new insights into the magnetic properties of these important systems.

Peter Laggner (Institute of Biophysics and Nanosystems Research, Austria), *SAXS and GI applications using a novel modular laboratory system*. Peter's presentation covered the use of Grazing Incidence Small Angle X-ray Scattering (GISAXS) and SAXS for the nanostructure analysis of bulk materials, nanoparticle solutions and thin solid films. A high brilliance 50 W microfocus beam (Hecus X-ray Systems) is used with 1D and 2D detectors. Key issues are the micro-source size (point focussing), the small beam footprint at the detector and the detector sensitivity. GISAXS is used in reflection mode and a gas or liquid environment can be used. Peter concluded by saying that this 'low power' system offers a performance that compares with high power rotating anode systems and small synchrotron sources.

Mark Farnworth

XRF/XRD joint session on thin films 18th April 2007



Speakers - Left to Right: Chris Staddon (Co-Chair) Brian Tanner, Heiko Ress, Joachin Woitok, Tom Ryan, Dave Taylor (Co-Chair)

TOM RYAN (Nanometrics, Oregon, USA), *Thin Films and Coatings by XRF and XRD: an overview*, began by saying XRD, XRF and XRR are universally acknowledged to be more direct and less model-dependant than optical methods. However, practical difficulties have limited their application in a production environment. XRF can analyse all film types and can determine elemental composition and obtain quantitative analysis. XRD can analyse crystalline and polycrystalline material whilst XRR can analyse all thin film types. Thin film analysis with X-rays became firmly recognised as a result of the 1954 Paper by **I G Parratt** dealing with surface studies using X-ray Reflectivity. Reflectivity measurements from oxide layers on copper had been obtained and simulated reflectivity curves produced. [It was shown that the peak to peak separation of the measured 'oscillations' was proportional to the wavelength of the X-rays and inversely proportional to the thickness of the layer].

In the semi-conductor industry, X-ray metrology for thin films is driven by the use of ultra-thin layers for new gate dielectrics, the use of localized stress to enhance channel mobility and the use of novel low-k dielectric materials. All these present metrology problems that are poorly served by classical optical methods. Tom told everyone about the Gartner Hype Cycle, devised by 'marketeers' to describe the path to technological maturity for a product! To begin with there is a technology trigger, followed by a peak of inflated expectation, followed by a trough of disillusionment, a slope of enlightenment and a plateau of productivity!

Commercial GAXRD made an appearance in the 1980's - it gets rid of the 'high' backgrounds observed when thin films are analysed by traditional XRPD. HRXRD is an enabling technology in band-gap and strain engineering for III-V optoelectronics and is an industry standard metrology technique for III-V epitaxial structures. XRF from light elements is strongly absorbed so the detected intensity is independent of film thickness. Conversely, the intensity from heavy elements is dependant upon thickness. The substrate signal is attenuated by a thin film and is thus dependant upon film thickness. XRR metrology offers several

advantages. It is independent of the optical parameters n and k , it can measure opaque metal films and is sensitive to interfacial layers and interfacial roughnesses. The technique is very good for low k dielectrics. On the negative side it generally uses a large spot size and needs a flat surface for analysis. Layer thickness information can be determined very accurately by XRR and these can be used as calibration standards for XRF. It leads the way for micro-focussed XRF calibrated by XRR. Tom concluded by saying that the semi-conductor industry provides the technological 'push' to analyse smaller and smaller features. In 2003, 90 nm features were of interest. It is predicted that in 2011+ features as small as 10 nm will need to be analysed. In line with these increasing demands there have been exciting developments over the last 10 years. Improvements in the focussing of X-ray beams combined with advances in detector technologies has reduced XRD, XRF and XRR probe sizes to a few hundreds of, and in some cases less than 100, microns.

Joachim Woitok (PANalytical, The Netherlands), *Advanced Solid-state X-ray Detector for the analysis of Thin-layered Structures*, began by saying structural analysis of thin layered structures involves different X-ray scattering techniques like rocking curve, reciprocal space mapping or reflectivity measurements. These methods require high angular resolution and a high dynamical intensity range as compared with standard measurements on polycrystalline materials. X-ray reflectivity measurements usually require parallel beam geometry and high resolution with crystal monochromators. Reflected intensities can be very high, up to 100×10^6 cps and so there is a requirement to use beam attenuators or reduce the X-ray source intensity.

Historically, these measurements are time consuming to obtain and so what is now needed is an ultra-fast solution - 'one detector for all applications'. Joachim informed everyone about a recently introduced solid state detector for thin film analysis - based upon the very latest pixel detection technology. Development was through the Medipix 2 Project which was run by a large international consortium. The detector has 256×256 pixel resolution (65536 pixels with each pixel covering an area of 55×55 microns). It has 97% count linearity up to 100,000 cps per pixel or 25 million cps per strip. There is no need for a beam attenuator, and the detector can operate in 0 D or 1 D, and resolution can be further improved by reducing the active area from 6 to 1 mm^2 . XRR scans can be carried out in 0 D mode with an analysis time of typically 10 mins. Rocking curve scans typically take 10 to 15 minutes with traditional detectors. With this ultra-fast solution scans can be obtained in 10 or so seconds for the same measurement quality.

The detector can be combined with all diffracted beam optics and due to its superior resolution and unmatched dynamic range it can be used for all types of X-ray scattering techniques. More information about this detector and its applications can be found in a paper by **Paul Fewster** - *J. Appl. Cryst* 38(2005) 62.

Hugues Guerault (Bruker AXS, Germany), Up-To-Date XRD-Techniques for investigating ultra-thin films and ultra-small features. The rapid progress in nanotechnology and nanomaterials has resulted in an increasing demand to characterize ultra thin films, nanostructure and organic thin films with laboratory X-ray instrumentation. Hugues went on to say that this data can be used as preliminary sample screening before synchrotron / neutron measurements or to monitor and improve sample growth. Typically, X-ray probe sizes are 50 to 100 microns. A ω -2- θ goniometer is used with a Eulerian cradle, a ceramic X-ray tube and 50 micron mono-capillary. Hugues explained how stress can be measured for copper wire structures using the Cu(331) crystallographic reflection. For the semi-conductor industry SiGe thin films have been studied and the strain in silicon films determined. XRF with a 100 micron spot has been used to investigate Cr(5nm)/Al(200nm)/MoN_x(10nm)/CdTe(3 micron) structures. For very thin layers, the VANTEC-1 with a sealed gas filled tube and linear detector has been used.

Brian Tanner (Bede), *X-ray Probes of the layer and interface structure of nano-scale films for Opto-Electronics and Spintronics*. Brian began by saying that very high resolution XRD developed in the 1980's due to the need to measure composition and lattice strain in thin semi-conductor films. He showed examples of diffraction profiles taken from the early days and from recent times. A recent interest is the determination of the composition of Al_xGa_{1-x}As thin films on GaAs. Aluminium has been detected at the 1% level. Graded SiGe structures have also been investigated and Brian showed by use of reciprocal space maps, evidence for the asymmetric relaxation of test structures. He illustrated the application of laboratory-based grazing incidence in-plane diffraction to obtain independent twist and tilt data from GaN films grown on thin Al_xGa_{1-x}N buffers on sapphire. Brian went on to discuss grazing incidence X-ray reflectivity, This has now become a standard tool for the measurement of layer thickness and interface width in nanoscale thickness metal films for spintronic devices and data storage. Measurement of the off-specular scatter enables topological roughness to be distinguished from chemical intermixing across interfaces. He illustrated this by showing the measurements obtained for ultra-thin epitaxial layers of Co, Cu and Ni on silicon. Grazing incidence scattering becomes particularly powerful when combined with grazing incidence fluorescence measurements. This was illustrated in a study of the effect of Bi as a surfactant in the sputtering of smooth Fe₅₀Mn₅₀ exchange bias films. By a simple consideration of the Bi fluorescence signal or by more complex modelling, it has been shown that Bi does act as a surfactant under conditions of one or two monolayer coverage.

Mark Farnworth

XRF Applications - including cultural heritage - Wednesday 18 April, 2007



Speakers - Left to Right: Jean-Philippe Gagnon (inset), Margaret West, David Beveridge(chair), Luisa Carvalho, Rene van Grieken. Claire Collins, Charles Gowing, Malcolm Haigh (inset).

AS might be expected from its content, this session produced lots of nice pictures of fine buildings and other works of art. We got off to a good start, with **Luisa Carvalho** from Lisbon, who spoke on the use of XRF for characterising documents. XRF permits the characterisation of different papers and, by use of cluster analysis, the grouping of different samples into their types. This work is also of use in detecting forgeries. She was followed by **Claire Collins** (Oxford Instruments), who described the use of a hand-held XRF analyser for examining a range of objects which may broadly be grouped as "cultural heritage". Hand-held XRF analysers are becoming popular, with several different types on the market, and the sorts of things they can do are impressive.

Malcolm Haigh (Spectro) moved over to more general applications in his talk, which centred on the use of a polarised-beam EDXRF unit. This has sundry advantages over the more traditional types, in giving more intensity and lower backgrounds. This was applied to geological samples. **Charles Gowing** (British Geological Survey) continued the geological theme, with his talk on a compact benchtop EDXRF which can be taken on site in the BGS Mobile Environmental Laboratory. They hope to accredit the method under UKAS and for soils under the MCERTS scheme. Many geological samples are analysed as fused beads, and **Jean-Philippe Gagnon** (Claisse) showed in his talk how to get fast analytical results by fusion without knowing the Loss On Ignition. In fact, by using net intensities, it is now possible to calculate the concentration of the volatile compounds lost during the fusion. The last two talks contained most of the pretty pictures.

Margaret West (West X-Ray Solutions) described some work that had been done for English Heritage. Conservation

and restoration can be controversial, and much modern conservation work involves putting right the mistakes of the past. To take one example, the eleventh century carving at Kilpeck church, in Herefordshire - among the best of its era in England - is being attacked by sulphate-rich encrustation. Understanding what is happening requires XRF and XRD. In the final talk, **René van Grieken** (Antwerp) followed on with the theme from Kilpeck - damage to buildings caused by atmospheric aerosols. Examples came from all over Europe (and also New York) and showed what can happen, not just to stonework, but also to stained glass and paintings within a building. A range of techniques, not just XRF, were used to analyse the pollutants and their reaction products.

David Beveridge

Industrial Group Keynote Lecture -18th April 2007 Robert Snyder - Georgia Institute of Technology



Jeremy K Cockcroft(chair) with Robert Snyder.

ROBERT began by saying that one of the most important needs of industry is to produce computer models for the behaviour of products and processes. The modelling of materials is an important element of this. For 10,000 years, material properties have been obtained from studies of chemical composition and of how the materials are affected by temperature and pressure. It was only in 1976 when a new 'tool' came on the scene - surface free energy. The origins of catalysts are borne out of the knowledge of surface free energy. For 100 nm structures the surface free energy is 1 % of the Total Free Energy - a relatively small contribution. Nanomaterials can be zero dimensional (quantum dots) or 1 or 2 or 3 dimensional. 'Surface shell' reconstruction is used for the study of nanomaterials. For nanomaterials the 'surface' can be a very significant part of the sample volume. Computer models are used. However, there needs to be experimental constraints otherwise the models produced are nonsense.

X-ray Diffraction can be used to determine lattice parameters (peak positions), crystal structure (positions and intensities) and 'real' structure from the full XRD profile. 'Line' profiles can be used to separate size and strain broadening. They can also be used to determine defect density and dislocation density. Robert went on to say that there is a distortion of the lattice parameter as the sample reduces in size - towards 0.6x0.6x0.6 nm.

Nanostructures can be analysed with Transmission Electron Microscopy (TEM), Field Emission Gun - Secondary Electron Microscopy (FEG-SEM) and synchrotron focussed X-ray beams. XRD analysis of the core structure and microstructure gives information about stacking fault density / types, size / strain and preferred orientation. Analysis of the 'surface shell' give information about the Pair Distribution Function (PDF) and the 'shell' can also be analysed with X-ray Photoelectron Spectroscopy (XPS) and described using computer models.

Mark Farnworth

A Standardless future for Quantitative XRPD - 19th April 2007



Speakers - Left to Right: Steve Norval (Chair), Rob Hill, Chris Gilmore, Paul O'Meara.

GORDON CRESSEY (Natural History Museum) **Random Mounts and Reproducibility? The Key to Standardless Quantitative Phase Analysis (QPA).** Gordon began by saying flat-surface mounts of materials such as clays can be prepared that produce close-to-random diffraction patterns when recorded by a curved position sensitive detector (PSD) with a large solid angle. This means that QPA of materials prone to preferred orientation (such as clays) can become an easy routine. The 'standard' whole pattern need only be run once and placed in the databank. Only a flux correction needs to be applied to the data for the day of measurement. Gordon showed the results of QPA of peat obtained from Keri, Greece. For materials with well established structures,

calculated pattern intensities can be compared with whole pattern results from the PSD to verify the randomness. In the case of unknown or poorly-defined structures the XRD-PSD method can still be used by simply comparing with ('real' material) experimental whole patterns in the databank, unlike an approach that requires calculated intensities from known structures. Thus, accuracy is controlled by 'best-matching' to the standards available. In effect, standardless QPA by XRD-PSD is simply a pattern comparison procedure.

Christopher Gilmore (University of Glasgow) *Quantitative Analysis of Mixtures using High Throughput Instrumentation without the use of standards*. Chris described the PolySNAP computer program which uses the full powder diffraction pattern to carry out the quantitative analysis of mixtures from powder diffraction data. It does not, in general, use calibration standards and is capable of achieving an accuracy of 1% under favourable conditions. Experiments involving 2- and 3-phase mixtures of organic samples were carried out on a Bruker D8 GADDS system and on a Bruker D4 and the TOPAS software as a reference. Following data collection, the next step is 'visualisation'. Every pattern is compared with every other pattern. The correlation matrix is converted into a 'distance' matrix and similarities discerned by the use of dendrograms. The final step is data processing in which quantitative analysis is obtained for all the input data. It was found that for a typical 2-phase system e.g. paracetamol and lactose PolySNAP gave better results than TOPAS. However, TOPAS gave better results for 3-phase mixtures. Christopher concluded by saying that PolySNAP can give mixture compositions, in a high throughput environment, to within 10%, quickly and without user intervention.

Rob Hill (Bruker AXS) *Rietveld Analysis and its applications to the cement industry*. XRD with Rietveld analysis is the most powerful method for quantitative phase analysis. The Rietveld methodology has been known for some 40 years and it was the lack of computing power that prevented its breakthrough until relatively recent times. The method uses the full XRD pattern for analysis - all data points are used. The TOPAS software was used since there is then no need for standards. In the cement industry quality control of raw materials is required. Chemical and physical properties of the raw materials are determined by the phase composition rather than the elemental analysis. Rob showed how Rietveld analysis has been used to analyse Alite - caused by clinker dust in the pre-heating. Rietveld analysis has been used to determine the true clinker composition.

Paul O'Meara (PANalytical) *Applications of Rietveld in Aluminium production*. Paul explained that the production of aluminium starts with the mining of its principal ore Bauxite. To convert the Bauxite to aluminium, it is washed, ground and dissolved in caustic soda at high pressure and temperature - the Bayer process. The resulting liquor contains a solution of sodium aluminate and undissolved bauxite residues known as 'red mud'. This needs to be disposed of carefully, usually on the seabed

or as landfill. Bauxite contains three principal aluminium bearing constituents:- gibbsite (an aluminium hydroxide) and boehmite and diaspore which are aluminium oxide hydroxides. The temperature and pressure in the digester are determined by the relative abundance of each of these. The sodium aluminate solution is pumped into a 'precipitator' where the alumina particles are separated. These are then heated at 1100°C to produce the white, pure alumina powder. Single line methods of quantitative analysis involve the use of Relative Intensity Ratio's (RIR's), internal standard, straight line method and matrix flushing. Rietveld involves whole pattern fitting and has been found to give very accurate results. The method is good when preferred orientation is known to be present, when standards are unavailable, when 'occupancy' varies and when peaks overlap. Paul concluded by saying the Rietveld method is used to control the manufacturing process and reduce the environmental impact.

Mark Farnworth

XRF and Environmental Issues 19 April, 2007



Speakers - Left to Right: Margaret West (chair), Stan Piorek, Ros Schwarz, Nick Marsh, Chris Vanhoof, Rene Van Grieken.

Nick Marsh (University of Leicester) *Climate records - lurking in the small print? What's at the bottom of your lake?* Nick started the lecture with a reminder that it was much warmer during the Jurassic, a time when there was no ice and not much land, and many animals, such as plankton, lived fast and died young, thereby preserving the oxygen isotope signature of the atmosphere at that time. Much research into oxygen isotopes has benefited from the easy release of oxygen from carbonate phases by dilute mineral acids followed by analysis by ICP-MS. However, conditions in naturally acidic lakes do not allow for the preservation of carbonate fossil remains and processes such as dolomitisation can change the delta-oxygen ratios. Fortunately several planktonic and other aquatic creatures utilise silica to produce their skeletal matter. A series of fascinating SEM pictures showed the array of skeletal

remains that have been collected from lake sediments as well as some contaminant materials that can be found in the samples. It is difficult to remove completely silica contaminants from samples, so XRF was identified as a reliable technique capable of determining a wide range of chemical data to enable mass balance calculations on the various contaminants in the sample. A fused bead method using very small < 0.1 g sample sizes with 3 g of high purity flux had been developed for this purpose. An inverse correlation was observed between $\square^{18}\text{O}$ and Al_2O_3 due to the presence of silt in the samples.

Chris Vanhoof (MITO, Belgium) *Development and validation results of a new European Standard prEN 15309 for the determination of the elemental composition of waste and soil by XRF.* The growing interest of government and industry to implement XRF as an analytical tool for the characterisation of waste and soil has led to the development and validation of a new European Standard. This method was working to EU and landfill directives; the EU directive had previously been based upon aqua regia or HF digestion methods. Work instructions were developed in 2000-2001 and the Standard went through a series of improvements between 2003 and 2006 and was approved in 2007. This was achieved against the background of a wide range of matrix compositions and lack of suitable reference materials for inhomogeneous materials like waste. Chris explained that on-site verification of the method would follow the basic characterisation and control analysis. A range of methods were considered comparing qualitative or quantitative, field- or lab-based etc. The Standard incorporates two procedures, a screening / qualitative phase followed by energy or wavelength XRF in the laboratory. The method validation was based upon two soils, one fly ash and ink and an electronic sludge sample. The characterisation was carried out by an interlaboratory exercise, participated in by labs from seven countries. The relative reproducibility of the soils and fly ash materials was 10-20% (pellet analysis) or 2-10% (fused bead analysis) with trace elements > 20 ppm being 8-15% and < 20 ppm 25-30%. The waste material data had a relative reproducibility up to 50% and the ink sample data had high standard deviation and a large loss on ignition. All that now remains is for the on-site verification to be carried out.

Stan Piorek (Niton) *Screening of electronic products with a "small-spot" hand-held XRF analyser for compliance with Restriction of Hazardous Substances (RoHS) Directive.* Industry now has to fully comply with EU RoHS, Waste Electrical and Electronic Equipment (WEEE) and End of Life Vehicles (ELV) directives. Complying with these directives for testing all components and raw materials could prove very costly, e.g. £1300 per sample for a simple component such as a printer cable. Manufacturers have responded by producing compact spectrometers with robust calibrations that can perform non-destructive analysis in a shop floor situation. This spectrometer utilises a collimated beam to reduce the beam size to 1 mm² spot size that can be targeted using an integrated CCD camera. A number of images illustrated that analysis of individual solder points

is possible, and its use for screening for the presence of brominated flame retardants was also described. Stan concluded his presentation by coining a new term, HH-XRF, hand held XRF as distinct from field portable XRF.

Ros Schwarz (Oxford Instruments) *Micro-spot XRF in RoHS compliance testing : performance and pitfalls.* This presentation also covered the analysis of electrical components to meet EU RoHS directives. Ros described a micro-spot XRF that could use a video camera to target analysis with spot sizes of 0.15, 0.3 or 1 mm² for screening analysis. Difficulties encountered with analysis of materials such as Sn₆₃Pb₃₇ solder were discussed and illustrated, particularly spectral line overlap caused by elements in the matrix substrate. Another persistent difficulty is the scarcity of Reference Materials (RMs) and Ros urged caution against using inappropriate RMs if no suitable ones were available.

Charles Gowing

News from CCP14

I have created a wiki site for CCP14. The primary purpose is to provide tutorials, examples and installation instructions for crystallographic software. The secondary purpose is to include other help topics and discussions connected with crystallography, encompassing experimental techniques through to analysis.

It is very much in its infancy, so please feel free to add any contribution. I unfortunately can not spare the time to build it up, therefore I will be very grateful to you all for any contribution. I do hope it can become a worthwhile resource.

The link is <http://www.ccp14.ac.uk/ccp/wikiccp14/>

As it is in its early stages please let me know of any problems, issues or anything that needs to be amended.

William Bisson
CCP14



Sam Motherwell

Sam Motherwell Symposium, 19-20 April 2007



SAM MOTHERWELL'S formal crystallographic career has spanned the period from 1963-2006, but with a 13-year break (1978-1991) as Head of Automation at the University of Cambridge Library. In his 30 years in crystallography, Sam is best identified

with computational developments and structure interpretation. His best known contribution was the PLUTO structure visualiser, forerunner of many modern graphics packages. However, he also contributed to the early implementation of direct methods, to many original and current software tools that accompany the Cambridge Structural Database, to packing energy calculations, and, more recently to examining how CSD information could inform crystal structure prediction, and the possibilities for searching the CSD for H-bonded and other motifs in extended crystal structures. As Associate Director of the Pfizer Institute for Pharmaceutical Materials Science (PIPMS) from 2002, his work within the CCDC and with Prof. **Bill Jones** of the Department of Chemistry in Cambridge, Sam has used many of these tools in the interpretation of crystal structures from the CSD to devise improved systems of salts, solvates and co-crystals for drug delivery - crystal engineering in its truest sense.

The Symposium concentrated on the current state of the art, and the future, in many of the areas mentioned above, delving into history only when necessary. A set of excellent scientific talks were provided by a wide range of speakers and a celebratory dinner was held in the evening of 19 April. The event was chaired by **Frank Allen** (CCDC) and **Graeme Day** (PIPMS), who were pleased that an initial audience of 60+ was only minimally diminished for the morning session on 20 April. The list of speakers and titles is provided as an accurate flavour of the event:

Robin Taylor (CCDC): *Using small-molecule crystal-structure data to validate protein-ligand structures*

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

Carol Brock (University of Kentucky, Lexington, USA): *Phase Sequences in Some Crystals Containing $M(NO_3)_2$ water, and 15-Crown-5*

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

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

James Chisholm (CCDC): *Searching the CSD for extended motifs and other challenging queries*

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

Elna Pidcock (CCDC): *Symmetry, space groups, molecular packing and chirality*

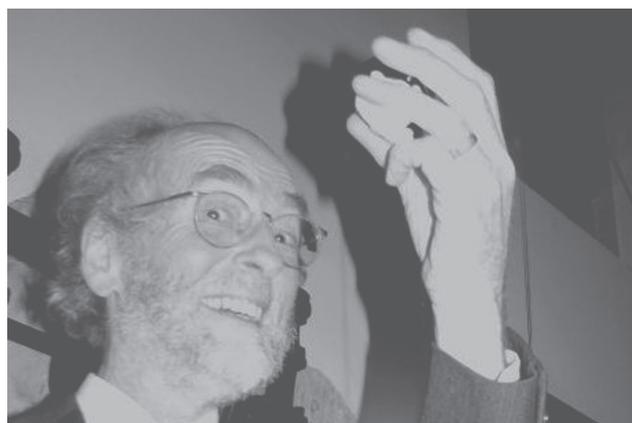
Peter Wood (University of Edinburgh): *Understanding High-Pressure Phase Transitions with Pixel Calculation*

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

Sam Motherwell (CCDC): *The CSD - 400,000 answers ... but what are the questions?*

In conclusion, **Frank Allen** noted the good news that Sam will continue his research interests as a part-time Emeritus Research Fellow at the CCDC. He also asked the question: "If this is what Sam has done for the CCDC, then what has the CCDC done for Sam?". The associated graphics on this page show that (a) Sam has matured under the CCDC's influence, and (b) the CCDC has not diminished his enthusiasm for crystals!

Frank Allen



Meetings



Some of the delegates who attended the meeting

Meeting Report - Small Angle Scattering SIG organised by the BCA Industrial Group - 2 - 3 July 2007 ILL, Grenoble

THIS meeting was organised by Richard Morris (Morris Analytical X-ray), Dave Taylor (ICDD) and Jeremy Cockcroft (UCL) and hosted by the ILL and ESRF on the joint site at Grenoble. Arriving in Grenoble, the first impression is of how stunningly beautiful the scenery is. Lying in a valley, surrounded by the Alps, this would certainly be a pleasant setting to live and work. On to the site itself and after the briefest of stops at security we settled into our en suite rooms at the guesthouse.

Day 1, 2 July Delegates were first treated to a tour of the ILL facility by **Charles Dewhurst** and **Isabelle Grillo** (both ILL). As the reactor was undergoing maintenance, and no experiments were currently running, this was an excellent opportunity to get a close look at the experimental stations. Entrance to the reactor shell is through an enormous airlock, as the interior of the reactor is held at less than atmospheric pressure. Once inside, one is struck by the sheer size of the equipment and engineering and in the very centre, safely shielded behind concrete and lots of heavy water, was the reactor core pumping out neutrons. We were also afforded a rare sight; some of the waveguides carrying neutrons to the experimental halls were exposed as the concrete shielding had been removed to install a new guide. Back out through the airlock, accompanied by the peculiar sensation of re-pressurisation. After a quick check, to see if any of us had become contaminated by a small speck of radioactive material (we were all ok), it was off to the experimental halls at the other end of those neutron

waveguides. Again the scale of the place is astounding. The scientists and engineers working around and about had an unhurried manner, for them this was just another day at work. As my first visit to such a facility, I thought it was all fascinating, and really quite exciting.

After coffee, we got down to the real business of the day. **Peter Laggner** (Institute of Biophysics and Nanosystems Research, Graz) gave a broad overview of the techniques of SAXS and SANS, starting with the basic theory of scattering. A brief history of the development of these techniques led into a discussion of systems suitable for SAXS/SANS analysis and the "4 limiting cases" for the treatment of data from such studies. Improvements in laboratory based SAXS equipment were presented and the point made that many studies could now be conducted, more conveniently, in the laboratory without having to travel to a central facility such as the ESRF.

This was followed by **Françoise Ehrburger-Dolle** (Laboratoire de Spectrométrie Physique, CNRS-UJF) who described smectic ordering in side-chain liquid crystal polymers (LCPs) and in LCP-silica nanocomposites. She described the types of polymers that can form liquid crystals and the phenomenon of inter-digitation. A series of SAXS experiments at different temperatures showed clear changes in the crystal layer spacings at specific temperatures. This was attributed to a change in the degree of inter-digitation within the system. Results from further studies, in which the LCP's were confined within a silica xerogel, suggested that this change was inhibited for LCP's residing in the smaller pores where they may not have the space to rearrange.

Richard Görgl (Materials Centre, Leoben) presented the NanoSTAR system from Bruker, a laboratory solution for SAXS studies. Recent improvements to this system were reported, including a new microfocus X-ray source and a

radiation-hard detector that requires no beam-stop. A study of crack propagation in polyvinylidene fluoride (PVDF) films, using this system, was presented and a comparison made with similar data collected using a synchrotron source.

An excellent lunch was followed by a presentation by **Charles Dewhurst** (ILL) on D33 - the third Small-Angle Neutron Scattering (SANS) instrument to be installed at ILL. The new instrument will be capable of experiments in high magnetic field strengths, something previously impossible at its predecessor D22 due to that instrument's proximity to extremely sensitive spin-echo experiments. Combined with a neutron polariser, D33 will be a superb instrument for the study of magnetic materials and superconductivity phenomena.

Adrian R. Rennie (Uppsala) presented results of *in-situ* studies of flowing samples with SAXS and SANS. The example given was surfactant templated synthesis of mesoporous silica. Contrast matching techniques were used to remove the effects of silica from the scattering data and reveal the structure of surfactant micelles present in the system. It was shown that, while the micelles have a strong influence, there is a densification step late in the crystallisation process that determines the final structure. Further experiments showed that the addition of salts to the synthesis could affect the structures obtained by modifying the surfactant micelles.

Alberto Saiani (Manchester) then talked about creating 3D-networks and hydrogels from self-assembling peptides. This study was based on synthetic octa-peptides, which were designed to self-assemble into rod-like structures solution. Changing the octa-peptide was shown to alter its self-assembly behaviour in solution; longer or shorter rods could be obtained. Hydrogels formed by these differing systems had markedly different morphologies. The longer rods gelled by simply entangling like spaghetti, while the shorter rods formed a true 3-dimensional network with branching points.

Alexis Deschamps (SIMAP, France) summarised some of the recent progress made in characterising precipitates in metallic alloys using small-angle scattering. The microstructure of these precipitates has a strong influence on the mechanical behaviour of the metal. This was illustrated with a study of Aluminium-Zirconium-Scandium alloys, in which precipitates of ZrSc are found, with a Scandium rich core surrounded by a shell that is relatively rich in Zirconium. SAXS was used to characterise these precipitates in terms of their size, composition and thickness of the shell.

This was followed by **Andrew Harrison** (ILL), who discussed applications of microwaves in materials science. The ability of microwaves to selectively heat one component of a system was presented. This effect could be utilised for

“quick-start” catalytic converters in which the catalytic metal particles are rapidly raised to their operating temperature, increasing the efficiency of the converter. The effects of microwaves on biological materials were also discussed. It was shown that microwaves, at the wavelength used by mobile phones, had a small heating effect on phospholipids (which form cell membranes within the body). Is this bad news for the telecommunications industry? Probably not; the size of the effect is too small and mobile phones simply don't emit enough microwaves.

Jennifer Hiller (Diamond Light Source Ltd) followed this with details of I22, the new beamline at Diamond. Specifically designed for work on non-crystalline systems, I22 is now ready to receive its first users and Jennifer extended an invitation to all for applications for beam-time. This came with the caveat that Diamond is still a very new facility and that early users should expect some teething problems.

Peter Laity (Cambridge) ended the day with details of recent work using SAXS to investigate the deformation of polymeric powders undergoing compaction. Understanding this process is of particular importance to the pharmaceutical industry for the manufacture of pills. The use of SAXS to study powder compaction has not previously been reported in the literature. After a discussion of possible mechanisms for the compaction of powders when loads are applied, Peter demonstrated that powder compaction can be understood in terms of the packing of the particles at low pressures, followed by so-called affine deformations in which the particles change shape to give greater interfacial contact and hence better bonding between neighbouring particles.

The evening provided an opportunity for socialising over the conference dinner. A short coach ride into town brought us to “La Panse” where we were able to enjoy some of the cuisine for which the region is justifiably famous. This was accompanied by plenty of good red wine, a most welcome and enjoyable end to the first day.

Day 2, 3 July The second day was kicked off by **Jean-Paul Simon** (SIMPAP) who spoke about ultra low k dielectrics for microelectronics. In order to reduce “cross-talk” between the copper tracks on integrated circuit boards, nanoporous materials have been developed to make use of the very low dielectric constant of air. Jean-Paul spoke about how the pores in these materials are produced and the use of grazing incidence SAXS (GISAXS) to characterise them.

Christian Riek (ESRF) followed this with an introduction to small- and wide-angle X-ray scattering (SAXS/WAXS) using micron- and submicron-sized synchrotron radiation beams. The small size of these beams allows scanning of a sample to build up a composite “image”. This was demonstrated with a study of starch grains showing the

internal morphologies. The high flux of synchrotron radiation allows for time resolved studies, once again demonstrated with starch, this time determining the kinetics of starch hydration. One of the stranger applications of this technique was a study of spider silk, drawn directly from the spider's spinnerets. We were assured the spider did not mind being strapped to a table, inches from a synchrotron x-ray beam. Next, **Tim Wess** (Cardiff) discussed structural hierarchies in biological molecules. The properties of biological materials depend strongly on the arrangement and interactions of the molecules that comprise them. Using the example of fibrillin, an elastic component of connective tissues, Tim showed how the arrangement of the molecules could be elucidated from SAXS data and how this related to the mechanical properties of the tissue.

Vladimir Kogan (DANNALAB & PANalytical BV, The Netherlands) presented the results of SAXS evaluation on nanoparticles, polymers and biological macromolecules conducted on the conventional X'Pert MRD diffractometer equipped with dedicated collimation system, optics and source.

Wim Bras (ESRF) then gave an entertaining talk titled "The Joy of SAXS and other toys". Using the example of crystallization in glass ceramics, Wim demonstrated the enormous benefit of combining SAXS data with that garnered from other techniques when elucidating structures and determining kinetics. Ideas that are suggested by one set of data can be confirmed or rejected based on other results.

Finally, **Richard Morris** (Morris Analytical X-ray) gave an overview of the history of Morris Analytical X-ray and shared some his knowledge of surfactant meso-phases.

To close the meeting, **Dave Taylor** thanked all speakers and delegates for making the BCA's first foray onto foreign soil such a success. Thanks were also given to the meeting's sponsors, without whom we would all have gone hungry on Monday night. After the meeting proper, there was an optional tour of the ESRF located just next door to the ILL. Having heard so many talks about synchrotron SAXS experiments, I was keen to see the sort of kit used to perform them. Inside the synchrotron building, there is the same sense of massive complexity as at the ILL but a much more enclosed feeling due to the curvature of the ring. Wim Bras once again demonstrated his enormous enthusiasm for his work whilst describing the features of his own beamline (DUBBLE).

Andy Smith

There is another bursary report from a French student and more photographs on the web pages at:

<http://crystallography.org.uk>

European Workshop on Bacterial Protein Toxins



AFTER a short but exciting journey with an extraordinarily skilled driver, who took us through those narrow and hilly roads from Ciampino airport to the conference location, we arrived at San Martino al Cimino, a beautiful medieval village nearby Viterbo, in central Italy. This was the ideal

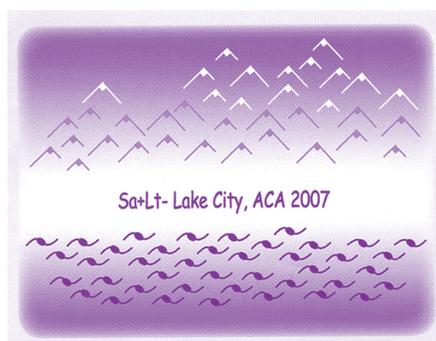
location for a scientific meeting: beautiful views with a relaxing swimming pool, full of taste of Italian culture, fantastic local food and drink, and most importantly: not a single night club to distract participants.

The ETOX meeting (European Workshop on Bacterial Protein Toxins) has a long tradition of bringing together some of the best experts around the World on bacterial toxins. The first meeting was held in Seillac, France in June 1983, and since then it has been successfully run every other year in Belgium, Germany, Italy, The Netherlands, United Kingdom, Denmark and Czech Republic. The scientific program started on the 23 June 2007 with an opening lecture given by **Rino Rappuoli**, a world-renowned scientist for his pioneer work on the development of reverse vaccinology, a genomic approach to identify new vaccine targets. He gave us an inspiring lecture on the advances of vaccine development based on current availability of whole-genome sequencing of bacteria and advances in bioinformatics. Also, he gave us a fantastic historical review of some of the vaccines he has helped to develop in the last 10-20 years, including vaccines against meningococcal-C and pertussis diseases. The meeting went on until the 27 June and was divided in 6 sessions: (i) Genomics, Toxins, Genes and Regulators, (ii) Receptors, Binding and Entry, (iii) Cell Biology and Signalling, (iv) Applications of Toxins, (v) Injected Toxins, Type III and IV systems, and (vi) Novel Bacterial Toxins and Targets. During the time of the conference we had the opportunity to hear about mechanism of action and pathogenesis of over 14 different bacteria, such as *Mycobacterium ulcerans*, *Escherichia coli*, *Pseudomonas aeruginosa*, *Bacillus anthracis*, *Clostridium botulinum*, *Clostridium tetani*, *Clostridium difficile*, *Staphylococcus aureus*, *Pasteurella multocida*, *Bordetella pertussis*, *Yersinia pestis*, *Shigella flexneri*, *Helicobacter pylori* and *Legionella pneumophila*.

This meeting was particularly beneficial for me as I had the opportunity to meet people working in the same area, and also present my current work on the structural characterization of *Clostridium difficile* toxins: TcdA and TcdB.

David Albesa-Jove

American Crystallographic Association Annual Meeting 2007, Salt Lake City



SOME forty minutes after take-off from Tucson I looked up from the newspaper and glanced out of the window. As the clouds below parted I saw what I later learned from the researcher's friend Wikipedia is around one mile in depth, 18 miles wide and 277 miles long. We were flying over the Grand Canyon.

Possibly the single most arresting natural sight in the United States, if not the world, the Grand Canyon lies around one-third of the way along a 558 mile straight line drawn between Tucson and Salt Lake City in Utah. This crow-flying line does not intersect with any other city or town of any significant size. Phoenix, the only real city to come close to the line, lies to the west. The US "out West" (as my friends from "back East" describe this part of the world) really is big and empty.

Salt Lake City - SLC to locals - was the location of the 2007 annual meeting of the American Crystallographic Association. There are probably more misconceptions about SLC than any other city in America, all of which result from the reasons behind the city's founding 160 years ago. Indeed at the 2006 ACA meeting in Honolulu serious, genuine concern was expressed at the potential lack of coffee during the daytime, and wine for the evening sessions. Happily I can report that SLC is refreshingly cosmopolitan. Naturally it's not a New York, a Sydney, a Paris or a London but when compared to the rest of Utah it does pretty well. They brew their own beer here too and it's pretty good stuff; with drink names like Polygamy Porter the locals also have a good sense of humour.

The city was founded on 24th July 1847 (this I know because the date is a state holiday and it coincided with the meeting - lots of celebrations and street parades) by Mormon pioneers led by their prophet Brigham Young who is said to have declared "this is the place!" when seeing the area. The pioneers were fleeing religious persecution from the Midwestern area of the US (which is actually in the eastern part of the country...) and the city is probably

best known for being the headquarters of The Church of Jesus Christ of Latter-day Saints - LDS or simply Mormons for short. This dominates both the city (all street addresses are on a grid referenced to Temple Square) and the state of Utah itself. Owing to this LDS heritage there are a number of misconceptions surrounding SLC and Utah, most commonly that alcohol and coffee are difficult to get hold of, and that polygamy is common. Whilst polygamy was made illegal over a century ago some of the state's alcohol laws remain somewhat archaic, especially when viewed from a European point of view. Alcohol with food is OK, but to drink without ordering a meal requires one to be a 'member' of the bar, with the fee ranging from \$4 to \$10. Supermarkets cannot sell any alcoholic drinks stronger than 3.2% and it's illegal to have more than one beer at any one time. This did make us wonder if holding someone's glass of wine along with your own made you a felon in the beady eyes of the law!



For those weaned on a diet of BCA Spring Meetings, attending the ACA meeting can be an arresting experience. Far more businesslike than the homely

BCA (the meetings are usually held in costly conference centres with attendees urged to stay at overpriced hotels) the meeting has more an air of the IUCr-type of congress, with many parallel sessions and certainly a lot more people in attendance. This was to be a pretty long meeting, from a Saturday morning to a Thursday afternoon. Biological crystallography has a much greater dominance at the ACA than is found with the BCA, and sadly this means that for those of us who still consider ourselves to be chemists the choice of interesting parallel sessions, posters and even exhibitors are sometimes limited. Even the Peter Müller-organised SHELX workshop on Saturday devoted half the time to protein crystallography, although everyone was encouraged to attend both parts of the workshop. Starting with an overview on constraints, restraints and esds by **George Sheldrick**, topics included refinement of twins (**Regine Herbst-Irmer**), disorder (**Peter Müller**), protein refinement at atomic resolution (**Thomas Schneider**) and the correct use of CIF (**Ilia Guezi** and **Ton Spek**). The evening session marked the formal opening of the meeting proper. A chance to catch up with some of the people whom I met in Hawaii last year, aided by food and drink was also a chance for **Judith Flippen-Andersen** and **Peter Müller**, both playing the **Bob Gould** role as Photographers-General, to take pictures galore. One wonders on which website they'll end up...

Sundays are quiet mornings in Utah and a surprisingly large number of people made it to the beginning of the scientific sessions. Attending the day-long Important Science from Small Molecule Structures session I particularly enjoyed

Marilyn Olmstead's talk on some recent forays into the world of photocrystallography and our very own **Chick Wilson** describing how improving neutron technology could pave the way for "high throughput" analysis. With the recent passing of **F. Albert Cotton**, this parallel symposium was in his memory and some of Cotton's contributions to chemical crystallography, both scientifically and in practical terms, were highlighted by **Larry Falvello** and **Lee Daniels**. Who would have thought that Cotton's agreement to three of his group using the lab diffractometer for outside work would have led to the formation of Molecular Structure Corporation and, quite possibly, to the development of Rigaku's US arm?!

Monday brought both the **Bruker** technical luncheon, at which their new dual-source diffractometer was unveiled, and the much-fêted **MarUSA** event. Rumours abounded of the scale and opulence of this evening party, although I'm sure the one involving the hire of a medieval castle was stretching the truth somewhat. Sadly I had no tickets for this, consoling myself with the Mentor/Mentee evening meal (my mentor proffered the advice "never sign up for anything that clashes with the Mar party") in a rather nice 'brewpub' with, get this, an open bar! Except it wasn't quite open since Utah's laws forbid a barmaid from actually handing a beer to a customer. Instead it had to be handed to an adjacent waiter who then handed it to the drinker, an exercise in full employment to make any trade unionist proud. Of the day's scientific diversions the most interesting was Tricks of the Trade: Interpretation of Structural Results. Organised by Arizona graduate **Paula Piccoli** the talk generating the most discussion was by **Phillip Fanwick** on Is Small Molecule Crystallography Still Science? He gave an example of a well-refined, well-behaved X-ray structure which he'd submitted to *Acta Cryst*. The authors were told that the work would not be accepted since all C-H hydrogen atoms (which were all on aromatic rings) had been freely refined while the hydrogen atom geometry should be constrained to typical values. Phillip went on to explain by way of Cambridge Structural Database analysis that the distortions from such typical values were actually the norm for this particular kind of organic compound and he asked the question of whether we can still call crystallography a "science" when we insist on applying pre-conceived ideas to certain apparently misbehaving atoms, rather than observing what they do and trying to draw conclusions from this. Naturally much discussion ensued, particularly involving the *Acta Cryst* co-editors who were present.

Tuesday was Awards Symposia day. Of the two running in parallel, I chose the symposium presented in memory of **Kenneth Trueblood**, hearing Trueblood award winner **Angelo Gavezzotti** talk about the development of crystallographic computing over the last forty years, and the subsequent impact on our understanding of intermolecular interactions as helped by solid-state calculations. Following this but on a similar theme **Graeme Day** discussed some very recent developments in the field of crystal

structure prediction whilst **Jack Dunitz** presented some new work on an old topic of the role played by fluorine in intermolecular interactions. During the afternoon session, **Gautam Desiraju's** analogy of "six blind men describing an elephant" when discussing how intermolecular forces are reported in the literature caused much mirth and is one to commit to memory methinks.

Having taken a slow morning on Wednesday to recover from the effects of more free beer (who would have believed it?!) at the Young Scientist mixer I attended the interesting and useful Teaching Gadgets and Educational Tools session. Topics ranged from the use of home-built gizmos for demonstrating the derivation of the Bragg equation, rotational symmetry, diffraction using laser pointers and net curtains and, most originally, the use of a hamster running ball ("hamster torture device" as described by the session chair) to build a very elegant model of the Ewald sphere construction. This was by far the most useful of all the sessions from an educational point of view and I left with plenty of ideas for developing teaching 'toys', although my limited DIY skills might mean some don't get off the ground. In addition, **Jenny Glusker** described how to teach crystallography in fifteen minutes, and in four hours, **Bruce Foxman** led us through how PowerPoint can actually be useful in the development of space group teaching methods and **Henk Schenk** showed how the phase problem can be (relatively) easily explained using good old-fashioned overheads. The evening Awards Banquet will also linger in the memory, with problems caused by technology (laptops not speaking to projectors), the IUPAC (virtually all winning posters had unpronounceable IUPAC nomenclature in the titles), and also much ethanol, as evidenced by the Hawaiian karaoke of former ACA president **Bob Bau**, and the impromptu baritone of former IUCr president **Bill Duax**.

By Thursday the conference crowd was starting to thin out, with the exhibitors gone and general fatigue setting in, but there was no thinning of the programme, which ran until 17:00. The Cool Structures session was particularly, er, cool, with **Christine Beavers'** talk on an unexpectedly complicated gold and barium polymer containing no less than seven metal centres being one of the more enjoyable ones. As the conference wound down I looked back on the week and am pleased I came. Some good science, an enjoyable meeting and Salt Lake City itself way exceeded my expectations. I encourage you to come and visit. Just make sure you visit the Grand Canyon first!

I thank The University of Arizona for funding my attendance at this meeting.

Gary S. Nichol
University of Arizona

(P.S. - Please note that the website for the ACA is now:
<http://www.AmerCrystalAssn.org> Ed.)

News from the Groups

Biological Structures Group

THE BSG sessions at the 25th Anniversary BCA Spring Meeting in Canterbury were well attended and very well received. Thanks go to Dr. **Katy Brown** (Imperial College) and Professor **Randy Read** (University of Cambridge) for putting together an excellent programme. Reports of the sessions were compiled by student attendees and published in the June issue of *Crystallography News*. The David Blow Prize was awarded to **Ivan Laponogov** and colleagues of King's College for their poster on the structure determination and conformation of a 55kDa N-terminal breakage reunion domain of *Streptococcus pneumoniae* topoisomerase IV. The number and high standard of posters led to a joint award of the runner-up prize to **Halina Mikolajek** of the University of Southampton for insights into the interaction between C1q and C-reactive protein in atherothrombotic disease, and **Birger Dittrich** and colleagues of the University of Western Australia for refinement of the structures of a new erythromycin solvate and amoxicillin trihydrate using invariom modelling of aspherical valence scattering. BSG Chairman **Andrea Hadfield** gave the keynote talk to the Young Crystallographers' satellite meeting and it was particularly encouraging to see so many stay on for the main meeting. Representatives of the newly-constituted Young Crystallographers Group were also welcomed as observers to a BSG committee meeting.

We are pleased that Professor **Simon Phillips** and Dr. **Arwen Pearson** of the Astbury Centre for Structural Molecular Biology, University of Leeds have agreed to organise BSG sessions on Structure, Function and Mechanism for the **2008 BCA Spring Meeting**.

Sheila Gover

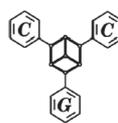
BSG Winter Meeting Structural Investigation of Gene Regulation

This year's BSG Winter Meeting will be held on **Tuesday 18 December** at the **School of Pharmacy, University of London**. The organisers are **Snezana Djordjevic** (ISMB/UCL) and **Gary Parkinson** (CRUK, School of Pharmacy) and the talks will concern the structural investigation of gene regulation. The programme is being finalised and details will be posted on the BSG website (www.crystallography.org.uk/bsg). As ever, we especially hope to encourage young and new crystallographers to attend and will offer BCA membership with the registration fee.

The Winter Meeting will incorporate the 2007 BSG AGM. Several members of the committee will have served their elected term and offers are invited from any BCA member who

would like to stand. Please e-mail the BSG Secretary (sheila.gover@tesco.net) if you are interested or wish to suggest someone else for nomination. The minutes of the 2006 BSG AGM and the Treasurer's 2006 report can be found on the BSG website. BCA members are reminded that funds are available at the Treasurer's discretion to support biological crystallographic activities and in particular, student participation.

Sheila Gover



CCG Autumn Meeting 2007 Chemical Crystallography at Diamond

Wednesday 14 November: Diamond Light Source, Chilton



Sponsored by Bruker AXS and Diamond Light Source

THIS meeting will be of interest to experienced chemical crystallographers, young researchers and students alike. The programme outlines some of the new opportunities available for research at Diamond, and highlights some results and techniques from existing synchrotron beamlines. In addition to a first-rate selection of speakers, there will be an extended lunch break during which there will be tours of Diamond.

10:30 Registration (with coffee & tea)

11:15 Prof. Peter Luger (Freie Universität Berlin)

"Experimental charge density studies on small and larger molecules: experiences with various synchrotron beamlines and an in-house diffractometer"

12:00 Dr Dave Allan (Diamond Light Source, Beamline I-19)

"Small-molecule single-crystal diffraction at Diamond"

12:30 Lunch / Tour of Facilities*

14:30 Prof. Paul Raithby (University of Bath)

"Photoactivated structural changes in molecular complexes"

15:00 Dr Stephen Moggach (University of Edinburgh)

"The effect of high-pressure on molecular compounds, from peptides to magnets"

15:30 Coffee & tea

15:50 Peter Byrne (University of St Andrews)

"Structural studies of ionic liquids and ionothermally prepared materials"

16.10 Prof. Bill Clegg (University of Newcastle)
"Structure determination from synchrotron sources: past, present and future"

16.40 Close

Online registration or printable registration forms are available at http://img.cryst.bbk.ac.uk/BCA/ccg/next_meeting.html

Programme Contact: Andrew Bond (adb@ifk.sdu.dk)
Local organiser: Harriott Nowell (harriott.nowell@diamond.ac.uk)

* Tours must be booked when registering. Places are limited and will be allocated as registrations are received.



Industrial Group Autumn Meetings

THE Pharmaceutical Special Interest Group and the IG Autumn meeting will be held "back-to-back" at AstraZeneca, Macclesfield, Cheshire on 7 and 8 November 2007.

Pharmaceutical SIG - 7th November 2007, Chaired by **Anne Kavanagh** and **Roy Copley**.

Speakers at this meeting will be:

Tal Austin: *Understanding relative polymorph stability through structure and thermodynamics*

Jonathan Burley: *Cocrystals and Other Complex Pharmaceutical Materials: Structure Solution from Powder Diffraction*

Roger Davey: TBC

Chris Gilmore: *Is PXRD the Gold Standard in High Throughput Experiments?*

Jerry Heng: *Crystal Engineering: The Importance of Surface Properties*

Bill Jones: *Screening for New Crystal Forms Based on Mechanical Activation of Mixtures*

Maryjane Tremayne: *Powders and 'Peer-Pressure': Pitfalls and Progress*

Jacco van de Streek: *Semi-automated Rietveld Refinement of Molecular Crystal Structures with DASH & TOPAS*

Fred Vogt: *X-ray Diffraction, Computational Chemistry and Solid-state NMR: A Multi-disciplinary Approach to Understanding the Pharmaceutical Solid-state*

Autumn Meeting - 8th November 2007

This is a call for papers for this meeting!

Morning session:

Rietveld applications.

Organisers: **Steve Norval & Jeremy Cockcroft**

Afternoon session:

Crystallography in Industry - a varied mix of short talks of interest to a wide audience.

Organiser: **Judith Shackleton**

To offer a talk at these meetings please contact a session organiser. Travel directions by air, public transport or road:

see: http://www.astrazeneca.co.uk/aboutus/findus/maps/macclesfield_map.pdf

Local organiser: **Dr Anne Kavanagh:** anne.kavanagh@astrazeneca.com

Full details can be found at <http://bca.cryst.bbk.ac.uk/bca/ig/meet07AM.htm>



XRD and Minerals - 15 May 2008

THIS meeting, at the British Geological Survey, Keyworth, Nottingham, will follow on from the previous day's XRF meeting at the same venue. This is a call for papers for the meeting.

Organiser: **Martin Gill** Email: m.gill@nhm.ac.uk

Speakers include: **Helen Maynard** (Edinburgh)

Caroline Kirk (Natural History Museum)

Eric Ferrage (Laboratoire Environnement et Mineralogie)

Jenny Huggett (Petroclays)

Full details can be found at

<http://bca.cryst.bbk.ac.uk/bca/ig/meet08MIN.htm>



PCG News

FOLLOWING the AGM at Canterbury, the committee of the Physical Crystallography Group (BCA) and the Structural Condensed Matter Physics Group (IoP) is as follows:

Prof. Paolo Radaelli Chair Rutherford Appleton Laboratory

Dr. Dave Allan Vice-chair Diamond Light Source

Dr. Matt Tucker Secretary/Treasurer Rutherford Appleton Laboratory

Dr. Ivana Evans Department of Chemistry, Durham University

Dr. Andrew Goodwin Department of Earth Sciences, University of Cambridge

Prof. Peter Hatton Department of Physics, Durham University

Dr. John Loveday CSEC, Edinburgh University

Dr. Serena Margadonna Department of Chemistry, Edinburgh University

Dr. Andrew Wills Department of Chemistry, University College London

The "autumn" meeting of the PCG is actively being planned, but it will be in January. Full details in the December issue of *Crystallography News*.

Meetings of interest

FURTHER information may be obtained from the website given. If you have news of any meetings to add to list please send them to the BCA Web Master cockcroft@img.cryst.bbk.ac.uk or to the Editor, gould@ed.ac.uk. The help of Dr Simon Parsons and the IUCr listing is gratefully acknowledged.

1-6 September 2007

4th International Workshop on Functional and Nanostructured Materials, Gdansk Poland
www.fnma07.gda.pl/?wh=home

2-5 September 2007

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

2-7 September 2007

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

3-4 September

British and Irish Society for Crystal Growth and Bernal Symposium, Structural Biology. Dublin
www.bacg.org.uk

3-6 September 2007

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

4-14 September 2007

10th Oxford School on Neutron Scattering Oxford
www.oxfordneutronschool.org

5-7 September 2007

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

5-8 September 2007

Structural Biology of Disease Mechanisms Murnau, Germany
www.murnauconference.de/

6-7 September 2007

SMARTER: Structure elucidation by combining Magnetic Resonance, computation modelling and diffractions. Portugal
www.primarius.pt/smarter/

10-13 September 2007

Euromat 2007: Advanced Materials and Processes. Nürnberg, Germany
<http://euromat2007.fems.org>

11-12 September 2007

User Meeting of the Swiss Light Source. Villigen, Switzerland
www.psi.ch/sls

12-13 September 2007

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

13-14 September 2007

Synchrotron Radiation User Meeting 2007. Chilton
www.diamond.ac.uk/ForUsers/SRUser07/default.htm

13-18 September 2007

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

16-21 September 2007

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

17-21 September 2007

Symposium on New Opportunities and Challenges in Material Research using Synchrotron and Free Electron Laser Sources. Warsaw, Poland
www.e-mrs.org/meetings/fall2007/1.html

17-21 September 2007

Application of Neutrons and Synchrotron Radiation in Engineering Materials Science. Hamburg Germany
www.hmi.de/events/PNAM_school/

24-26 September 2007

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

24-26 September 2007

Pharmaceutical Co-Crystals 2007. Amsterdam, Netherlands
www.iqpc.com/cgi-bin/templates/genevent.html?topic=237&event=13542&

25-30 September 2007

MSM07 - Magnetic and Superconducting Materials. Khiva, Uzbekistan
www.quantummatter.org/msm07

26-28 September 2007

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

1-2 October 2007

6th ANKA Users Meeting Karlsruhe Germany
<http://ankaweb.fzk.de/conferences/users-meeting-2007/first%20page.htm>

4-6 October 2007

2007 ALS Users Meeting Berkeley CA USA
www-als.lbl.gov/als/usermtg/index.html

7-9 October 2007

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

7-13 October 2007

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

8-11 October 2007

GTBIO Lille, France
www.ibl.fr/gtbio/Start.html

22-23 October 2007

Workshop on Total scattering Pair Distribution Function. ESRF, Grenoble, France
www.esrf.eu/events/conferences/PDFPowderDiffraction

23-26 October 2007

International School - Scattering for Biologists.
PSI, Villigen, Switzerland
<http://kur.web.psi.ch/ScatBiol/>

28-31 October 2007

CANSAS V: Collective Action for Nomadic Small Angle Scatterers. Gaithersburg, MD USA
www.smallangles.net/canSAS/

28 October - 1 November 2007

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

29-31 October 2007

Short course on amphiboles.
Rome, Italy
www_crystal.unipv.it/amphiboles/home.htm

3-4 November 2007

1st IUCr International School of Crystallography in Asia on Electron and X-ray Diffraction. Taipei, Taiwan
<http://ms.nsrc.org.tw/>

7 November 2007

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

8 November 2007

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

14 November 2007

CCG Autumn Meeting, Chemical Crystallography at Diamond. Chilton
www.crystallography.org.uk/ccg/

26-30 November

MRS 2007: Fall Meeting, Materials Research Society. Boston MA, USA
www.mrs.org/s_mrs/sec.asp?CID=4749&DID=164574

6-11 January 2008

6th NCCR Practical Course on Biomolecular Modelling. Kandersteg, Switzerland
www.structuralbiology.unizh.ch/course2008.asp

3-6 February 2008

ICDDD 2008 Dubai, UAE
www.icddd.com/

4 -8 February 2008

Australian X-ray Analytical Association (AXAA) 2008 Schools, Conference and Exhibition. Melbourne, Australia
www.pco.com.au/axaa2008

3-6 March 2008

16th Annual meeting of the German Society of Crystallography. Erlangen, Germany
www.conventus.de

9-13 March 2008

The Minerals, Metals and Materials Society (TMS) 2008 New Orleans LA USA
www.tms.org/Meetings/Annual-08/AnnMtg08Home.html

27 April - 3 May 2008

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

6-9 May 2008

ICCBM12 2008 International Conference on the Crystallisation of Biological Molecules.
Cancun, Mexico
www.iqumica.unam.mx/ICCBM12/

18-23 May 2008

7th Symposium on High Temperature Corrosion and Protection of Materials.
Les EMBIEZ, France
www.htcpm-2008.uhp-nancy.fr/

18-25 May 2008

IWCGT-4 Fourth International Workshop on Crystal Growth Technology.
Beatenberg, Switzerland
www.beatenberg.ch/IWCGT-4

21-23 May 2008

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

31 May - 5 June 2008

ACA Annual Meeting - Knoxville, TN, USA
www.hwi.buffalo.edu/ACA/

9-14 June 2008

ICQ10 - 10th International Conference on Quasicrystals, Zurich, Switzerland
<http://icq10.ethz.ch/>

7-11 July 2008

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

21-26 July 2008

XRM2008 9th International Conference on X-ray Microscopy. ETH Zurich, Switzerland
<http://xrm2008.web.psi.ch/>

23 - 31 August 2008

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

31 August - 4 September 2008

ECTP2008:18th European Conference on Thermophysical Properties. Pau, France
<http://ectp.univ-pau.fr>

1-11 September 2008

EPDIC-11 European Powder Diffraction Conference.
Warsaw Poland
www.epdic-11.eu/

9-14 September 2008

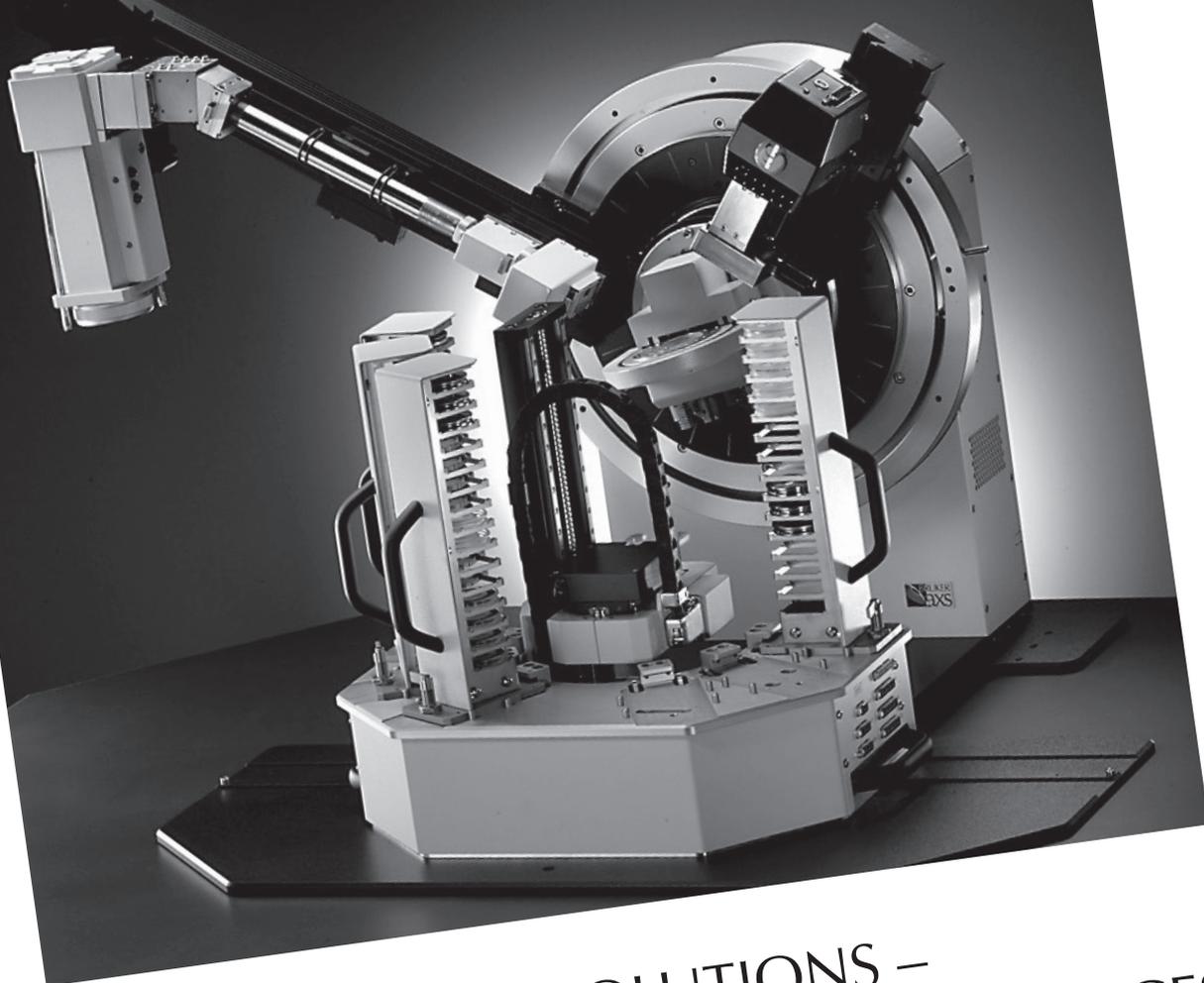
WATOC-08 World Association of Theoretical and Computation Chemists.
Sydney, Australia
www.ch.ic.ac.uk/watoc

17-20 November 2008

14th International Conference on Thin Films.
Ghent, Belgium
www.ICTF14.UGent.be

25-30 July 2009

Annual Meeting of the American Crystallographic Association 2009.
Toronto, ON, Canada
www.amerocrystalassn.org/meetingspg_list/futuremeetings.html



D8 DIFFRACTION SOLUTIONS – MANAGE YOUR ANALYTICAL CHALLENGES

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

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

BRUKER ADVANCED X-RAY SOLUTIONS

Banner Lane, Coventry, CV4 9GH. Tel: 024 7685 5200



www.bruker-axs.co.uk