Crystallography News

British Crystallographic Association

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Warwick April 2010 p6

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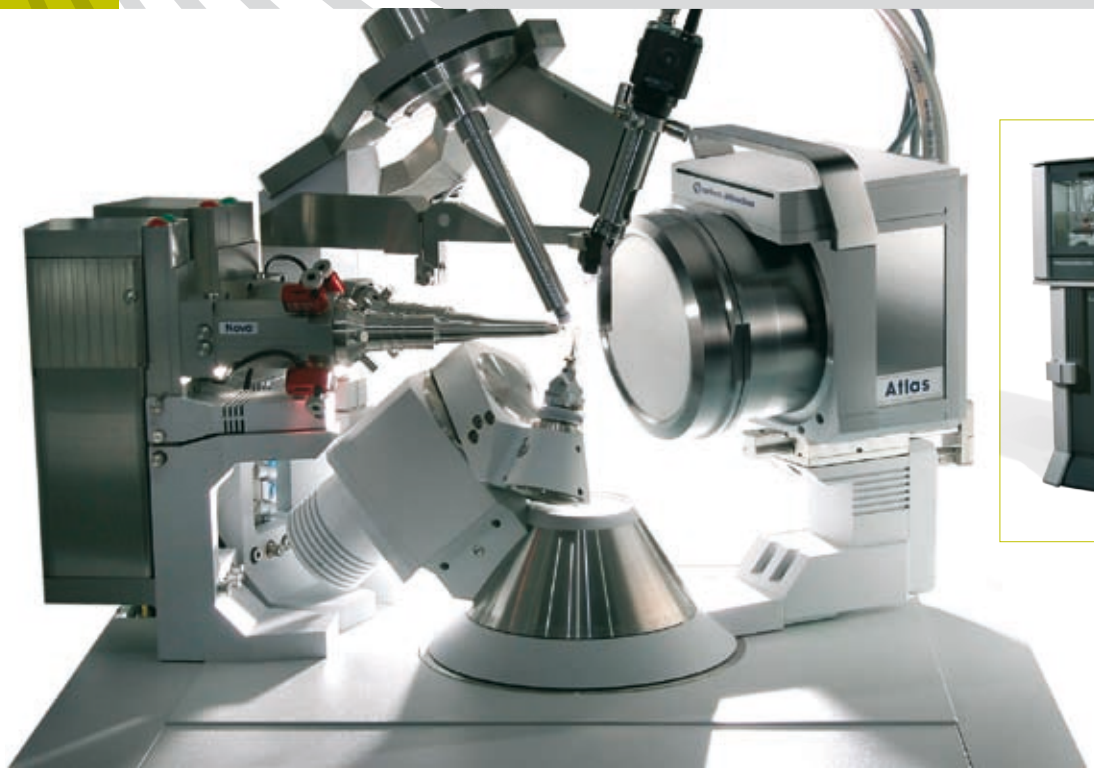

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think forward

XRD

Crystallography News March 2010

Contents

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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.

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This month's cover:

CCP4 photo-montage (Stuart Eyres and Laura Roe); artistic crystals (Keith Waters)

From the Editor

THIS issue highlights some important qualities of crystallographers and crystallography. Our main cover picture and the meeting report edited by Kate Brown celebrate the 30th anniversary of CCP4. By encouraging the dissemination of best practice and the free availability of software the cooperative spirit shared by almost all crystallographers and embodied in CCP4 has accelerated the progress of macromolecular crystallography. Our knowledge of molecular biology and our fight against disease have both benefited. Alert readers of our "Meetings of interest" column will notice another CCP4 activity: the next BCA/CCP4 Summer School, to be held in Oxford from 5th - 10th September 2010.

As we look forward to this spring, the title "Data Matters" of this year's BCA meeting reminds us of our reliance on data: diffraction data as the basis for structure determination, now being supported by computational data, and structural data held in the databases as the raw material for comparative studies. This meeting has relevance for every crystallographer.

Crystallography has its artistic side, too. I am grateful to **David Watkin** for sending our other cover picture (taken by **Keith Waters**) showing part of one of the entries for the 2009 Turner Prize, in which an entire flat was covered in $CuSO_4$ crystals. (Relying on the subscript-setting skills of our printers, I am using the formula, thereby avoiding the tricky decision whether to write "sulphate" or "sulfate".) Some years ago the Royal Society of Chemistry began to accept the latter spelling; but with feelings running high over the Kraft takeover of Cadbury, I would not want to impose an American spelling on *Crystallography News* unilaterally. Do readers know of any previous examples in *C.N.*?

Sometimes an experiment is carried out by accident. A famous incident occurred in 1992 when a container carrying a mixed load of plastic bath toys including ducks, turtles, beavers and frogs was washed overboard into the eastbound section of the North Pacific Subpolar Gyre. The toys proved to be excellent markers for ocean currents, some washing ashore on nearby beaches on every circuit of the Gyre. A few escaped the northernmost part of the Gyre, got frozen into Arctic ice, and traveled eastward with the slow rotation of the polar ice cap; a plastic frog even washed up on a Scottish beach in 2003. Dr. **Curtis Ebbesmeyer** devoted much of his scientific career to the tracking of ocean currents from the motion of flotsam and has written entertainingly on this subject. I thought I had inadvertently carried out a readership survey with my column in the December issue. Describing **Linus Pauling**'s Nobel Prize for Chemistry, I had originally written that it was for "work on structure and bonding in small molecules, from which he derived models for protein structure and preliminary attempts on DNA". To shorten the excessively long draft article, with one over-hasty swipe of the mouse I reduced it to "work on DNA". When, too late to change it, I saw the result in cold print, I expected a blizzard of e-mails asking if I had ever read *The Double Helix*. However, none came. I have derived three alternative possible conclusions. (1) Nobody reads this column. (2) Readers spotted the mistake but did not wish to hurt the Editor's feelings. (3) Most worryingly, people believe everything I write.

This issue also features a report by **John Helliwell** on Darmstadt, the venue for this year's European Crystallographic Meeting. While Darmstadt may lack the instant touristic appeal of Istanbul, Madrid or Warwick, John reports that Darmstadt is well worth a visit for its blend of high-tech modernity and antique charm. British crystallographers should not be put off by the literal translation of the German name, "Intestine City". In fact the origin of the name is unknown. Since 1997 the city has promoted itself as "Science City Darmstadt".

A major justification for this name is the presence of the Society for Heavy Ion Research, where element 110 was made and called darmstadtium. The conference centre where ECM-26 will take place also bears this name. Even better from our point of view, they also made element 111 and called it roentgenium. Finally, I have to declare a personal interest. My grandfather and near namesake **Carl Gustav Schwalbe** founded the Institute of Cellulose Chemistry at the Technical University there. More recently, when I was a post-doc in Germany in the early 1970's, the German Computing Centre in Darmstadt was the place that could rescue us by running calculations that were too hefty for our local facility.

One of the privileges of being the editor of Crystallography News is that I receive newsletters from our sister crystallographic societies. In the November 2009 issue from the German Society for Crystallography I found an article, "Customs Absurdistan: with Crystals to America" by **Peter Luger** which should dispel the idea that Germans lack a sense of humour (well, German crystallographers anyway; German customs officers are a different matter, but do customs officers anywhere have a sense of humour?). I am grateful to Peter and to Prof. **Dirk Meyer**, the editor, for permission to republish an English translation, which appears on page 34 in this issue.

Carl Schwalbe

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(The dates in parentheses indicate the end of the term of office).

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

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

From the President

DEAR MEMBER,

BY the time you get this, the spectacular winter snow of this year will (I hope) be a thing of the past, and the BCA Spring Meeting at Warwick will be fast approaching. Details of the exciting and wide ranging programme can be found in this issue, and I look forward to meeting many of you there.

November and December saw the annual one day BCA Group Meetings, and I very much enjoyed visiting (albeit briefly) the Physical, Chemical and Biological Groups, and thank the respective organisers for giving me the opportunity to draw the attention of attendees to various BCA issues and activities. Unfortunately I was unable to attend the Industrial Group meeting due to a clash with giving undergraduate lectures. Among these other activities was the continuing effort to update our e-mail database held by Northern Networking: only nine messages bounced back following the latest e-mail sent out. Despite this success, I suspect that some members are still not receiving any e-mails at all, and urge you to let me know if this is so for you - recent e-mails are on the BCA website at http://crystallography.org.uk/emails.

Our indefatigable Treasurer, **Harry Powell**, has masterminded the move from HSBC to CAF accounts for the BCA, and has arranged the facility to pay BCA subscriptions by Direct Debit. It is no longer possible to pay by Standing Order, and I regret that some of you feel that this is a retrograde step for the Association. However, the fact that almost 50% of Members who paid by Standing Order were underpaying what is already a very low fee meant that we had to make this change for the long term sustainability of the Association..

Thank you for all the nominations for Honorary Members of the BCA: we have a number of very strong candidates to consider.

We send our congratulations to Professor **Bill Clegg**, who was recently elected as an Individual Membership Representative to the Council of the European Crystallographic Association. Incidentally, registration for ECM26, to be held in Darmstadt from 29th August to 2nd September, is now open with deadlines of 15th March for student grant applications, 9th April for abstract submission, and 31st May for early bird registration.

At the BCA Spring Meeting in Warwick, we will be seeking a new Vice President of the Association, since **Sandy Blake** will come to the end of his three year term of office. I am particularly grateful to him for his rapid and wise e-mail response, giving advice on many issues, and for taking on the challenge of keeping me on the straight and narrow with unfailing good humour! I had the honour to attend Sandy's wide ranging, informative and very entertaining inaugural lecture for his Professorship last week in Nottingham, and we wish him well in this new role.

In September, on behalf of the BCA, I attended meetings of the Scientific Unions Committee and `Heads of Learned Societies' at the Royal Society. At the conclusion of the day, Professor **Deliang Chen**, the Executive Director of The International Council for Science (ICSU), addressed us and shared his vision for the future of the organisation. Since I was previously unaware of the existence of this body, I found it a very interesting afternoon. ICSU is a non-governmental organization representing a global membership that includes both national scientific bodies (117 members) and international scientific unions (30 members). The Royal Society (representing the UK) and the IUCr are members, and in fact as a result of this, the Royal Society contributes half of the BCA's IUCr Membership dues annually. For those interested in learning more about ICSU, information can be found at: http://www.icsu.org/5_abouticsu/INTRO.php

While on the subject of the Royal Society, the 12th May 2010 is the 100th Anniversary of **Dorothy Hodgkin**'s birth, and the Royal Society are marking this with a Dorothy Hodgkin Centenary Event to celebrate Women in Science and Dorothy Hodgkin in particular as part of their 350th Anniversary programme, so crystallography will be very much to the fore. Dorothy was the Founding Vive-President of the BCA.

On a less happy note, scientific fraud in crystallography is currently a big topic, and interesting information on this thorny issue can be found at:

http://journals.iucr.org/e/issues/2010/01/00/me0406/index.html

http://www.chinadaily.com.cn/cndy/2009-12/31/content_9249311.htm

http://journals.iucr.org/d/issues/2010/01/00/me0408/index.html

http://news.bbc.co.uk/1/hi/world/asia-pacific/8442147.stm

One of the `perks' of being BCA President is the range of e-mails I receive from all over the world. Two examples of this may be of interest to members: firstly **Robert B. Alcott** in the USA contacted me to point us to his wonderfully colourful crystalline art (http://crystallineartistry.net/), and secondly Professor **Grzegorz Jezierski**, of Opole University of Technology

in Poland, wrote to enquire about the possibility of obtaining donations of used (damaged) X-ray tubes. I quote: *`I have been doing industrial radiology for 30 years. I am an author of many scientific publications about radiology. I wrote a book "Radiography In Industry", Warsaw 1993. One of my hobbies is collecting Roentgen Tubes. I collect the vintage tubes (made of the glass) and the ceramic, modern ones (for industrial radiography, dental/medical, diffraction type, fluorescence type, microfocus X-ray tube, miniature X-ray tube, demountable X-ray source). Owing to the courtesy of many people and institutions I have a little collection of Roentgen Tubes. I would like to make a "Museum of Roentgen Tubes" in the future (photos enclosed). I was wondering if you could send me a couple of used or damaged X-ray tubes as an exhibit in the Museum.'*

As evidenced by the photos reproduced below, you can see that the collection is already significant. If any of you can augment it further, please send me an e-mail (elspeth.garman@bioch.ox.ac.uk), and I will put you in touch with Professor Jezierski.

See you in Warwick in April!!

Puzzle Corner

THERE are 100 light bulbs in a row operated by push button switches next to them: one push and the light comes on, another push and the light turns off again.

100 frogs are lined up ready to jump.

The first frog jumps on every switch and turns all the lights on.

The second frog jumps on every second switch and turns the even numbered lights off again. The third frog jumps on every 3rd switch etc, the 50th frog on switch numbers 50 and 100, etc and the 100th frog only on switch 100.

After all the frogs have jumped, how many lights are on?

(Contributed by **Elspeth Garman**)

BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
- A 10% discount on exhibition stands on the annual BCA Spring Meeting, OR - A promotional poster at the annual BCA Spring Meeting.
- Free insert in the annual Spring Meeting delegate bag.
- Two free full registrations to the annual Spring Meeting.
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BCA AGM 2010

2010 Annual General Meeting of the BCA

THE Annual General Meeting of the British Crystallographic Association will be held on Wednesday 14th April 2010 at 6.00 p.m. at the University of Warwick.

At this meeting we will elect a new Vice-president and one new Ordinary member of Council and possibly a new Secretary.

Draft Agenda

1. Approval of Agenda.
2. Apologies for absence.
3. Minutes of the last AGM (published in Crystallography News).
4. President's Report.
5. Secretary's Annual Report.
6. Northern Networking Events Report.
7. Report of the Treasurer to include Presentation of the Accounts for 2009 and the Examining Accountant's Report.
8. Acceptance of the Accounts.
9. Elections to Council.
10. Appointment of Examining Accountant for 2010.
11. Amendments to the Statutes and By-laws of the BCA.
12. Any other business.

Georgina Rosair
(Secretary to Council)

Scientific Programme: Data Matters

PLENARY LECTURES

Hodgkin Lecture (BSG): **Prof Dame Louise Johnson FRS** (University of Oxford) *'Forty years of structural biology: where have we come from and where might we be going?'*

Bragg Lecture (CCG): **Prof Sir John Meurig Thomas FRS** (University of Cambridge) *'The essence and promise of 4D electron microscopy'*

Teaching Plenary (IG): **Prof Simon Billinge** (Columbia University) *'Structure at the nanoscale: atomic pair distribution function analysis of nanostructured materials'*

Physical Crystallography Group: **Dr Lynne McCusker** (ETH Zürich) *'Polycrystalline materials, powder diffraction, electron microscopy and charge flipping - a remarkable brew'*

Parkin Lecture (YCG): **Prof Simon Parsons** (University of Edinburgh) *'Phase transformations in simple molecular solids'*

Alun Bowen Lecture (IG): **Dr David Taylor** *'Phase identification data - how it's changed over the years'*

Additionally the PCG Thesis Prize, the CCG CCDC Young Scientist Prize and the Young Crystallographers Industrial Group Prize Lecture will all be announced and presented at the meeting.

SESSION LECTURES

Data; what goes in (IG)
Chair: **Matthew Johnson**
Ross Harrington (University of Newcastle) *'Getting the best possible data from your crystals'*
Sarah Barnett (Diamond Light Source) *'Rough guide to synchrotron diffraction'*
Alastair Florence (University of Strathclyde) *'XRPD data in physical form identification and structure determination'*

Data; what comes out (IG)
Chairs: **Brett Cooper** & **Cheryl Doherty**
Trevor Rayment (Diamond Light Source) '*Food, formulation, foams, and fabrication - modern applications of synchrotron radiation for industry'*
Robert Hammond (University of Leeds) *'A molecular-scale*

perspective: new insights into the assembly of crystalline particles'
Young Crystallographer Prize Presentation: To be announced at the meeting

Complementary non ambient techniques (IG)

Chair: **David Beveridge**
Tim Hyde (Johnson Matthey) *'Catalyst studies using complementary and non-ambient techniques at Johnson Matthey'*
Axel Zeitler (Cambridge University) *'Terahertz spectroscopy of structure and dynamics in organic molecular crystals'*
Simon Watson (GSK) *'Running hot and cold: understanding crystal structure phenomena with variable temperature solid-state NMR'*

Unpublished Data and Almighty Blunders (CCG / IG)

Chairs: **Luca Russo** & **Richard Morris**
William Clegg (University of Newcastle) *'To publish or not to publish'*
Simon Coles (University of Southampton) *'eCrystals: Management and publication of small molecule data'*
Colin Groom (CCDC) *'Towards knowledge-based design and control of pharmaceutical crystal forms'*

Electron diffraction (PCG)

Chair: **Kirsten Christensen**
Ute Kolb (Johannes Gutenberg-Universität, Mainz) *'Enhanced electron diffraction data for "ab initio" structure solution using automated diffraction tomography'*
Sven Hovmöller (Stockholm University) *'Single crystal diffraction from powders using electrons'*
Wuzong Zhou (University of St. Andrews) *'Electron diffraction of some beam sensitive materials'*

Resonant X-ray diffraction (PCG)

Chair: **Peter Hatton**
Dr. Manuel Angst (Julich Forschungszentrum) *'Title: to be confirmed'*
Prof. Paolo Radaelli (University of Oxford) *'Title: to be confirmed'*
Prof. Sean Langridge (ISIS) *'Title: to be confirmed'*

New approaches to structure solution (PCG)

Chair: **David Keen**
Sarah Lister (Durham University) *'The use of complementary techniques in structure solution from powders'*
Maryjane Tremayne (University of Birmingham) *'Structure solution of multicomponent systems from powder diffraction data'*
Paul Midgley (Department of Materials Science and Metallurgy, University of Cambridge) *'Towards routine structure solution using precession electron diffraction'*

PDF: Local Structure (PCG)

Chair: **Matt Tucker**
Joseph Hriljac (University of Birmingham) *'PDF studies of the pressure-induced amorphisation of zeolites'*
Daniel P. Shoemaker (University of California) *'Local structure and the search for polar ordering in geometrically frustrated oxides'*
Samantha Chong (University of Liverpool) *'Investigating disorder in a pure bismuth A site perovskite using total scattering and RMC modeling'*

Structure and Property Prediction (CCG)

Chair: **Stephen Moggach**
Graeme Day (University of Cambridge) *'Lattice energy landscapes for predicting crystal structures and anticipating solvate formation'*
Caroline Mellot-Draznieks (UCL) *'From structure prediction to synthesis in hybrid framework materials'*
Peter Galek (CCDC) *'Truly prospective H-bond predictions: linking free energy and structural stability'*

Databases & Data Mining (CCG)

Chair: **Hazel Sparkes**
Peter Wood (CCDC) *'Hydrogen bonds: energy matters too'*
Anna Stevenson (University of Bath) *'Knowledge mining studies on gas storage materials using the CSD.'*
Gordon Barr (University of Glasgow) *'Data mining & data visualisation using cluster analysis and related technique'*

Data & Structure Validation (CCG)

Chair: **Ross Harrington**
Tony Linden (University of Zurich) *'Structure validation: automation versus vigilance'*
Ian Bruno (CCDC) *'From deposition to application: use of the CSD for crystal structure validation'*
Roy Copley (GSK) *'Structure validation: an industrial perspective'*

Dealing with Difficult Data (CCG)

Chair: **David Watkin**
Matthias Meyer (Oxford Diffraction) *'Optimal data collection strategies for area detector diffractometers'*
Aire Van der Lee (Université de Montpellier II) *'Charge flipping versus direct methods: tips and tricks'*
Christopher Serpell (Oxford University) *'Refinement of large supramolecular structures'*

High Throughput Membrane Proteins (BSG)

Chair: **Steve Prince**
Liz Carpenter (SGC) *'Progress in high throughput production of human membrane proteins at the SGC'*
Jon Hadden (Heptares Therapeutics) *'Crystallising membrane proteins: tips and techniques'*
Dr. Bernadette Byrne (Imperial College London) *'Stabilising your membrane protein the high and low-thoughput way'*

High Throughput & Screening (BSG)

Chair: **Bill Hunter**
Graeme Winter (Diamond Light Source) *'Automated MX at Diamond'*
Robbie Joosten (Netherlands Cancer Institute) *'PDB_REDO: an automated re-refinement method to keep the PDB up-to-date'*
Gerard Kleywegt (EBI, Hinxton) *'Model validation'*

<table>
<tr><th></th><th>Mon April 12th</th><th colspan="4">Tuesday April 13th</th></tr>
<tr><td>9:00</td><td rowspan="15"></td><td>LT3</td><td colspan="3" rowspan="2"></td></tr>
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Parkin Lecture:
Simon Parsons</td></tr>
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Chair: Elspeth Garman</td></tr>
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<tr><td>12:30</td></tr>
<tr><td>12:45</td><td colspan="3" rowspan="2">Lunch/Registratio/Exhibition 12.30-13.30
on/Exhibition 12.30-13.30</td></tr>
<tr><td>13:00</td><td>PLT</td><td rowspan="3">Alun Bowen
Lecture
David Taylor</td></tr>
<tr><td>13:15</td><td rowspan="8">YC 1</td><td colspan="3" rowspan="2"></td></tr>
<tr><td>13:30</td></tr>
<tr><td>13:45</td><td colspan="3">Sessions 13.30-15.00</td><td>B207</td></tr>
<tr><td>14:00</td><td>LT4</td><td>LT5</td><td>PLT</td><td rowspan="4">ICDD
Workshop
IG</td></tr>
<tr><td>14:15</td><td rowspan="3">Resonant X-ray
Diffraction
PCG</td><td rowspan="3">Structure &
Property
Prediction
CCG</td><td rowspan="3">New Techniques
BSG/YCG</td></tr>
<tr><td>14:30</td></tr>
<tr><td>14:45</td></tr>
<tr><td>15:00</td><td rowspan="2">Coffee
15.00-15.30</td><td colspan="4" rowspan="2">Coffee 15.00-15.30</td></tr>
<tr><td>15:15</td></tr>
<tr><td>15:30</td><td>PLT</td><td colspan="3">Sessions 15.30-17.00</td><td rowspan="2">B207</td></tr>
<tr><td>15:45</td><td rowspan="5">YC 2</td><td>LT 1</td><td>LT2</td><td>LT3</td></tr>
<tr><td>16:00</td><td rowspan="3">New Approaches
to Structure
Solution
PCG</td><td rowspan="3">High Throughput
Membrane
Proteins
BSG</td><td rowspan="3"></td><td rowspan="3">ICDD
Workshop
IG</td></tr>
<tr><td>16:15</td></tr>
<tr><td>16:30</td></tr>
<tr><td>16:45</td><td>Break</td><td colspan="4">Break</td></tr>
<tr><td>17:00</td><td>PLT</td><td colspan="4">LT3</td></tr>
<tr><td>17:15</td><td rowspan="5">YC 3</td><td colspan="4" rowspan="5">Exhibitors Forum 17.15-18.45
Chair: Elspeth Garman</td></tr>
<tr><td>17:30</td></tr>
<tr><td>17:45</td></tr>
<tr><td>18:00</td></tr>
<tr><td>18:15</td></tr>
<tr><td>18:30</td><td rowspan="10">YC Dinner</td><td colspan="4" rowspan="10">Dinner, Exhibition and Posters</td></tr>
<tr><td>18:45</td></tr>
<tr><td>19:00</td></tr>
<tr><td>19:15</td></tr>
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<tr><td>20:45</td></tr>
<tr><td>21:00</td></tr>
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<table>
<tr><th colspan="3">Wednesday April 14th</th><th colspan="3">Thursday April 15th</th><th>Friday April 16th</th></tr>
<tr><td colspan="3">LT3
PCG Plenary: Dr Lynne McCusker
Chair: David Keen</td><td colspan="3">LT3
IG Teaching Plenary: Prof. Simon Billinge
Chair: Matt Johnson</td><td rowspan="4">PDF Workshop
Location TBA</td></tr>
<tr><td colspan="3">Coffee 9.45-10.15</td><td colspan="3">Coffee 9.45-10.15</td></tr>
<tr><td colspan="3">Sessions 10.15-11.45</td><td colspan="3">Sessions 10.15-11.45</td></tr>
<tr><td>LT4</td><td>LT5</td><td>PLT</td><td>LT4</td><td>LT5</td><td>PLT</td></tr>
<tr><td>Dealing with Difficult Data
CCG</td><td>Dynamics
BSG</td><td>Electron Diffraction
PCG</td><td>Complementary & non-ambient techniques
IG</td><td>High Throughput 2
BSG</td><td>Data & Structure validation
CCG</td></tr>
<tr><td>IG AGM
11.45-12:30</td><td>BSG AGM
11.45-12.30</td><td>PCG AGM
11.45-12.30</td><td colspan="3">Break</td></tr>
<tr><td colspan="3" rowspan="2"></td><td colspan="3">Sessions 12.00-13.30</td></tr>
<tr><td>LT4</td><td>LT5</td><td>PLT</td></tr>
<tr><td colspan="2">Lunch, Exhibition 12.30-13.30
12.30-13.30</td><td>CCG AGM
12.30-13.15
LT1</td><td>PDF: Local Structure
PCG</td><td>Hot Structures
BSG</td><td>Unpublished Data & Almighty Blunders
CCG/IG</td></tr>
<tr><td colspan="3">Sessions 13.30-15.00</td><td colspan="3">Close 13.30</td></tr>
<tr><td>LT4</td><td>LT5</td><td>PLT</td><td></td><td>LT5</td><td></td></tr>
<tr><td>PCG Prize
Chair D. Keen</td><td rowspan="2">Data;
What Goes In
IG</td><td rowspan="2">Membrane Structures
BSG</td><td rowspan="6">PDF Workshop
Location TBA</td><td rowspan="3">CSD User Discussion Forum</td><td></td></tr>
<tr><td>CCDC Prize
Chair A. Bond</td></tr>
<tr><td colspan="3">Coffee 15.00-15.30</td></tr>
<tr><td colspan="3">Sessions 15.30-17.00</td></tr>
<tr><td>LT4</td><td>LT5</td><td>PLT</td></tr>
<tr><td rowspan="2">Databases & Data Mining
CCG</td><td rowspan="2">Data Management
BSG</td><td>Data;
What Comes Out</td></tr>
<tr><td>YC Prize
IG Sponsored</td></tr>
<tr><td colspan="3">Break</td></tr>
<tr><td colspan="3">LT3
Bragg Lecture: Prof. Sir John Meurig Thomas FRS
Chair: Elspeth Garman</td></tr>
<tr><td colspan="3">LT3</td></tr>
<tr><td colspan="3">BCA AGM 18.00-19.00</td></tr>
<tr><td colspan="3">Comfort Time</td></tr>
<tr><td colspan="3">Conference Dinner 19.30 for 20.00</td></tr>
</table>

Data Management (BSG)
Chair: **Keith Wilson**
Rob Esnouf (University of Oxford) *'The PiMS service - LIMS for all, no geek required'*
Geoff Barton (University of Dundee) *'The Taro protein target optimisation system and related tools'*
Vincent Postis (University of Leeds) *'LIMS for MPSI: PIMS usage in the University of Leeds'*

Dynamics (BSG)
Chair: **Mark Sansom**
Adrian Mulholland (University of Bristol) *'Title: to be confirmed'*
Phil Fowler (University of Oxford) *'Extracting more information from the structure: computer simulations of membrane proteins'*
Lucy Forrest (MPI Frankfurt) *'Title: to be confirmed'*

Hot Structures (BSG)
Chair: **Steve Smerdon**
Chris Oubridge (LMB, Cambridge) *'Structure determination of human spliceosomal U1snRNP'*
Dale Wigley (CRUK) *'Title: to be confirmed'*
Leo Sazanov (MRC-MBU) *'The architecture of bacterial respiratory complex I'*

Membrane Structures (BSG)
Chair: **Liz Carpenter**
Simon Newstead (Imperial College) *'Recent progress on the crystal structure of a new family of membrane transport proteins'*
Bonnie Wallace (Birkbeck College London) *'Structure and function of voltage-gated sodium channels'*
Gebhard F. X. Schertler (Paul Scherrer Institute Switzerland) *'Structural insights into G protein coupled receptor activation'*

New Techniques (BSG)
Chair: **Robin Owen**
Richard Neutze (University of Gothenburg) *'Time resolved structural studies of membrane proteins'*
Per Bullough (University of Sheffield) *'Visualising protein assemblies in a two dimensional world'*
Gwyndaf Evans (Diamond Light Source): *'Future directions for microfocus crystallography at Diamond'*

Tues 13th 13:30 - 17:00: ICDD Workshop (*Chairs:* **Cyrus Crowder** & **Timothy Fawcett**) during the conference.

Thurs 15th (14:30 - 18:30) and Fri 16th (09:00 - 12:30): Workshop on data correction for PDF (Pair Distribution Function) and total scattering analysis. Organizer, **Matt Tucker** (matt.tucker@stfc.ac.uk).

Thurs 15th 13:30 - 15:30: Cambridge Structural Database Discussion Forum

From the Secretary

Announcement of elections to Council

AT the 2010 Annual Meeting in Canterbury we will elect a new Vice-president and one Ordinary member of Council. The term of Office for the Secretary also expires this year although the present post holder is eligible for another term in office. Nominations for these posts are invited. Each nomination requires a proposer and a seconder and should you wish to nominate someone, please obtain their consent first.

Properly seconded nominations will be received up to two days before the date of the AGM which will be held on 14th April 2010. They may be sent by email to secretary@crystallography.org.uk

Georgina Rosair
Secretary to Council

Young Crystallographers Meeting 12th -13th April

Monday 12th April

12:00 - 13:00: *Registration*

13:00: *Welcome:* **Susanne Coles** (née Huth) (University of Southampton)

SESSION YC1: 13:00 - 15:30 *Chair:* **John Kaniuka**

13:00 - 13:30: *Plenary:* **Stephen Moggach** (University of Edinburgh) *Putting the squeeze on porous materials*

13:30 - 13:45: **Eloisa Angeles Tactay** (University of Cambridge) *Prediction of hydrate formation through computational methods*

13:45 - 14:00: **Jonathan Foster** (University of Durham) *Supramolecular gels: a new medium for crystal growth*

14:00 - 14:15: **Brian Boyle** (University of Glasgow) *Investigations of base-pairing in nuleic acid co-crystal complexes*

14:15 - 14:30: **Helen Maynard-Casely** (University of Edinburgh) *The structure of methane phase A - a new form of EX4 packing*

14:30 - 14:45: **Mark Warren** (University of Bath) *Photocrystallographic and raman spectroscopic investigation of metastable species*

14:45 - 15:00: **Duncan Sneddon** (Diamond Light Source Ltd) *Closely coupled crystallographic software developments and data acquisition at Diamond Light Source*

15:00 - 15:30: *Coffee & Tea*

SESSION YC2: 15:30 - 17:15 *Chair*: **William Lewis**

15:30 - 16:00: *Plenary:* **Andrew Goodwin** (University of Cambridge) *The atom's perspective: crystallography in real-space*

16:00 - 16:15: **Nicholas Funnell** (University of Edinburgh) *Krogmann's salt at extreme conditions*

16:15 - 16:30: **Areej Abuhammad** (University of Oxford) *Probing the architecture of the Mycobacterium marinum arylamine N-Acetyltransferase active site*

16:30 - 16:45: **Emily Mutambi** (University of Bristol) *Solid state interconversion of palladium (II) complexes*

16:45 - 17:00: **David Brown** (University of Oxford) *matchbOx: automatic structure matching to facilitate crystallographic refinement*

17:00 - 17:15: *Break*

17:15 - 17:45: *Annual General Meeting*

SESSION YC3: 18:00 - 19:00 Chairs: **Anna Stevenson** & **Duncan Sneddon**

18:00 - 19:00: *Flash presentations for poster contributors: sell your poster in no more than 3 sentences!*

19:00 - 21:00 *Poster session with dinner and wine*

Tuesday 13th April

SESSION YC4: 09:00 - 11:05 *Chair:* **Susanne Coles** (née Huth)

09:00 - 09:30: Plenary: **Elspeth Garman** (University of Oxford) *From hot to cool and more for less: new developments for structural biology*

09:30 - 09:45: **Craig Wales** (University of Glasgow) *Paracetamol form II: an elusive polymorph prepared through facile new crystallisation routes*

09:45 - 10:00: **Mark Eddleston** (University of Cambridge) *Analysing pharmaceutical materials by transmission electron microscopy*

10:00 - 10:15: **Christopher Woodall** (University of Bath) *Photochromism of dithienylethenes in the single crystalline state*

10:15 - 10:30: **Vicky Fawcett** (University of Manchester) *Polymorphism from a solution perspective: rationalisation at the molecular level*

10:35 - 11:05: Inaugural Parkin Lecture: **Simon Parsons** (University of Edinburgh) *Phase Transformations in Simple molecular solids*

11:05 - 11:30 *Registration for main meeting*

10th Biennial Conference on High Resolution X-Ray Diffraction and Imaging

XTOP 2010, the 10th Biennial Conference on High Resolution X-Ray Diffraction and Imaging, will take place from Monday September 20th to Thursday September 23rd 2010 at the University of Warwick, UK. The conference runs from Monday afternoon and finishes with lunch on Thursday 23rd.

En-suite accommodation on the University of Warwick's award-winning central Campus has been reserved for the nights of 20th-22nd September (further nights can be arranged on request) together with breakfast, buffet lunch and dinner on each day. There will be a conference banquet on the evening of Wednesday 22nd September.

Lectures and poster exhibitions will be held in the Physics Lecture Theatre and on the Physics concourse just 5-10 minutes walk from the accommodation. Details of the pricing structure and the first circular will follow shortly together with abstract submission and registration information. Please register the dates in your diary and reserve the time to come and join us in Warwick for XTOP 2010.

XTOP will bring together scientists from the fields of X-ray diffractometry, coherent and conventional X-ray diffraction imaging and topography, as well as X-ray phase contrast imaging (radiography and micro-tomography). XTOP is thus one of the central scientific platforms concerning methods and instrumentation in synchrotron-based high-resolution X-ray diffraction methods, phase contrast imaging, and microtomography.

For more information see:

http://www2.warwick.ac.uk/go/XTOP2010

BCA AGM 2009 Minutes

Minutes of the Annual General Meeting of the British Crystallographic Association held at Loughborough University on 22 April 2009 . The President, Paul Raithby, was in the Chair.

1. Approval of Agenda.

The President requested one alteration: namely that the Elections to Council will be held after the Treasurer's Report.

The revised agenda was approved (proposed by John Helliwell and seconded by Mike Glazer).

2. Apologies for absence: apologies were received from Chick Wilson and Paul Fewster.

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

These were accepted as a true and accurate record (proposed by Simon Parsons and seconded by Alex Griffin).

4. President's Report.

The President reported that we were halfway through a successful Spring Meeting with over 350 registrants and 80 Young Crystallographers delegates. He thanked the Chair of the Programme Committee, Simon Parsons, the Programme Committee and the session chairs. He also thanked the Industrial sponsors and exhibitors for their time and financial support. He is very grateful to Gill Moore and David Massey of Northern Networking Events for their organisation, together with Loughborough University conference office, the Elsegood family and local organisers. Next year Simon Coles will chair the Programme Committee; it has already held the first planning meeting for next year's meeting which will be at Warwick on 12-15 April 2010. The BCA was not free from the effects of the credit crunch and unfortunately the Spring Meeting in York in 2008 made a loss and investments are down in value. The Treasurer's report will explain the steps the BCA is taking to avoid further deficits. The President announced that David Watkin and Frank Allen have been awarded Honorary Membership of the BCA. Three ordinary members of Council had come to the end of their terms of office and he thanked Richard Cooper, Elspeth Garman and Bill Clegg for their hard work on Council. He looked forward to their continued participation. However, the President will be retiring at the end of his term. He thanked Jeremy Cockcroft for his services to Council as the retiring webmaster and welcomed Richard Cooper as the new webmaster. The President was saddened to report the passing of Andrew Lang, a founding member of the BCA and preeminent in the field of diffraction physics, and Andy Parkin, who was taken from us tragically last summer. There will be a Parkin Lecture organised by the Young Crystallographers which was arranged after discussion with Andy's family. A minute's silence was held.

At the IUCr congress in Osaka the BCA was well represented in the symposia and on Commissions. The next European Crystallographic meeting will be held in Istanbul where the BCA will be making a bid for ECM2013 to be held in Warwick, coordinated by the Vice President. The President finished by thanking the current and past members of Council and said that it was an honour to serve the BCA. There were no questions on the President's report.

5. Secretary's Report.

The Secretary, Georgina Rosair, was one of the UK representatives in Osaka and also expressed sadness of the passing of Andy Parkin. She reminded those present to update their entries in the World Directory of Crystallographers (WDC) and asked for any feedback as to ways in which this could be done, as she was the BCA contact for the IUCr who manage the WDC. Chris Gilmore commented that WDC members get discounts which are very worthwhile.

6. Northern Networking Events Report.

David Massey reported that the current BCA membership was 721 members, only 2 fewer than last year and consisted of 420 ordinary, 110 student/retired/unemployed, 129 corporate, 43 term (usually overseas) and 19 honorary members. He reported that the changeover of editorship of Crystallography news from Bob Gould to Carl Schwalbe went very smoothly. Due to the current economic conditions five Corporate Members had not renewed their membership, but these still want to remain in contact with the BCA. There are now 13 Corporate Members of the BCA, with Oxray being the latest member. A total of 200 delegates used the on-line credit card payment option when registering for the Spring Meeting. He thanked Simon Parsons and the Programme Committee for their assistance in producing the Programme book and to John Evans for the mini-programme guide. He listed the 24 exhibitors who play a vital role in supporting the Spring Meeting. Roger Tulley and Philip Taylor were thanked for their work on the Spring Meeting website and finally he thanked Paul Raithby for his work as President of the BCA.

7. Report of the Treasurer to include Presentation of the Accounts for 2008 and the Examining Accountant's Report.

The Treasurer, Harry Powell, reminded members that standing orders will be phased out and that the BCA will not receive money from any standing orders still in place next year. 350 people currently pay by standing order and 47% of these were for the incorrect amount. He encouraged members to pay by direct debit which will be available in 2010. He thanked his predecessor Sheila Gould who was always very helpful when he needed assistance with the accounts. This year has been a difficult year for the BCA financially, being £43,000 down from 2008. He said that the BCA reserves were used to cover this and such eventualities show the need for reserves. However, a retrospective gift aid claim will increase income by £1,500. General expenditure was down by £13,000, because the Durham School did not run that year. The effects of the credit crunch will make more impact in next year's accounts. Investment income is down by 25% but the change to CAF Bank has increased income from bank account interest because of CAF Bank's superior interest rates. He encouraged Interest Groups to move their accounts to CAF if they have not already done so. A major cause of this year's deficit was the late change in Spring meeting venue from Swansea to York. Looking more closely at the York Spring Meeting accounts, sponsorship income was down by £6,000 and registration income by £2,000 whilst expenditure on facilities was up by £12,000. However, catering costs were £5,000 less and notably speakers' expenses were down by £6,000. Advertising income from Crystallography News is up by £4,000 and membership income remains the same. 18 bursaries were given with a total value of £4,500. The NNE fee of £18,000

is less than last year, one reason being that there was no profit from the Spring Meeting and NNE are entitled to a percentage of the profits of a Spring Meeting. Council expenses were less than last year. The IUCr fund will be offered to Madrid for the IUCr in 2011. The Arnold Beevers Bursary Fund was given £926 by the Biological Structures Group. All Interest Group funds were at reasonable levels.

John Helliwell asked where CAF Bank was based: Georgina Rosair replied that it is based in the UK.

8. Acceptance of the Accounts.

The accounts were accepted, nominated by Andreas Goeta and seconded by Chris Gilmore.

9. Elections to Council.

(i) Election of President

Bill Clegg was nominated by Mike Glazer and seconded by Roy Copley.

Elspeth Garman was nominated by Dave Stuart and seconded by Judith Howard.

Both candidates gave strong presentations on their view of the future of the BCA. The election was held by secret ballot with Simon Coles and Jeremy Cockcroft acting as tellers.

At the end of the meeting Elspeth Garman was declared elected as President of the BCA and was congratulated on her election. In her speech she described how she started as a nuclear physicist but is now in the macromolecular crystallography field and works on techniques which enable big biological problems to be solved. She is highly involved in teaching and organizing International macromolecular crystallography schools and would like to develop the BCA website and its educational remit. She would also like to make CN available electronically to members who wish to receive it that way, which should be of benefit to the environment.

(ii) Election of Ordinary Members.

There were three vacancies and three nominations:

Dr Andrés Goeta was nominated by Judith Howard and seconded by Richard Cooper.

Dr Alex Griffin was nominated by Guy Orpen and seconded by David Watkin.

Dr David Beveridge was nominated by Anne Kavanagh and seconded by David Taylor.

There being three candidates for three posts, the candidates were declared elected as Ordinary Members and were congratulated on their election.

10. Appointment of Examining Accountant for 2009.

Appointment of examining accountants RA Young and company was recommended by the Treasurer. Re-appointment of the examining accountants was approved (proposed by Richard Cooper and seconded by John Helliwell).

11. Updating the BCA Statutes and By-Laws.

Sandy Blake gave an account of the updating of the BCA Statutes and By-Laws and advised that he will propose some changes to these. He thanked Paul Fewster and Georgina Rosair for helpful comments. Further discussion on the updating of Statutes and By-Laws will take place on the website.

12. AOB

Mike Glazer raised the issue of EPSRC's proposal to blacklist applicants who have three consecutive failed grant applications and the presence of e-petitions against this move. He urged the BCA Council to make a stand on this. Paul Raithby asked if anyone was opposed to Council writing a letter protesting against these proposals. Peter Moody asked that all the details should be made available to Council before any move were made. The President outlined EPSRC's proposals. This will be taken to Council for further discussion.

There being no further business, the AGM was closed at 7pm.

Georgina Rosair, Secretary to Council.

Puzzle Corner...

...DECEMBER ANSWER

THE December puzzle was set by Didem Rodoplu based on her studies of centuries-old Seljuk Turkish stone ornamentations, and the winning entry was submitted by Jim Trotter. Of course, these patterns were created not by computers but by human beings, albeit highly skilled artists. Thus the beholder has some freedom to decide how much to idealise the patterns.

Pattern 1 underwent some distortion during file conversion; an original JPEG is reproduced below. Assuming that the black shapes were intended to be squares, Didem assigned plane group p4mm, while Jim came up with p2mm on the basis of rectangles. For problem 2 one has to judge whether the horizontal and vertical figure-of-eight shapes are meant to be identical; the assignments were p2gg by Didem and p4gm by Jim. In pattern 3, depending on the degree of ideality assumed, Didem's p3 stands beside Jim's p31m. This analysis of man-made and somewhat time-worn materials shows that symmetry, like beauty, is in the eye of the beholder.

Biological Structures Group Winter Meeting 2009 - Pathological Proteins

THE Biological Structures Group 2009 winter meeting entitled '<u>Pathological Proteins</u>' was held at the Royal Free Hospital in north London on December 18th. Snow and ice across most of the country did not deter around 70 intrepid participants from all parts of the UK and beyond. The meeting was generously supported by several sponsors and exhibitors (Anachem, Bio-Rad, Bruker, Douglas Instruments, GSK, Molecular Dimensions Ltd, Oxford Diffraction and Rigaku).

The conference began with an opening address by BCA President **Elspeth Garman** (Oxford) who reminded everyone of the BCA's essential role and the importance of continued membership. The first speaker was **Leo James** (LMB, Cambridge) who gave an intriguing lecture on the structure and function of cyclophilin A, a proline isomerase which becomes incorporated into HIV virus particles and is essential for processing of the capsid protein. This lecture was followed by **Ian Taylor** (NIMR, Mill Hill) who showed some impressive EM pictures of the retroviral capsid and described a hexameric 18-helix bundle capsid protein (a domain of gag) from murine leukaemia virus. The final speaker in the morning session was **Salam Al-Karadaghi** (Lund, Sweden) who described the structure and function of the protein frataxin - a complex 24-meric assembly, which was illustrated impressively by EM reconstructions. The protein has an important role in iron storage and delivery within mitochondria - hereditary deficiencies give rise to the neurodegenerative disease Friedreich's ataxia.

The morning session was followed by the annual general meeting at which **Darren Thompson** (Sussex, BSG secretary) read a statement from **Andrea Hadfield** (Bristol) who, sadly, is standing down as BSG chairman. Andrea was thanked for her service to the BSG over more years than the committee could remember. **Vilmos Fulop** (Warwick) was appointed as successor and **Katy Brown** (Imperial) elected as the new vice chairman. **Pierre Rizkallah** (Cardiff, BSG treasurer) then presented the group accounts. Lunch followed during which the attendees perused the conference exhibition and posters.

The afternoon session on bacterial pathogens began with an impressive presentation by **Gabriel Waksman** (Birkbeck ISMB) who described the structure of a type-IV secretion system involved in bacterial infection and conjugation. The structure of this megadalton outer-membrane complex consisting of 14 copies of the proteins virB7, B9 and B10 was solved by a combination of molecular replacement and electron microscopy, and was presented as a series of impressive movies. Next, **Arefeh Seyedarabi** (Queen Mary, London) described the structure of the protein IpaH9.8 from the type-III secretion system of shigella which is involved in colonization of the host cell by down-regulation of the pro-inflammatory response. **Katy Brown** (Imperial) then described the crystal structures and solution scattering studies of two surface layer proteins from *C. difficile*, a notorious hospital pathogen. One of these multi-functional proteins (toxin B) possesses glycosyl transferase, cysteine proteinase, pore-forming and receptor-binding domains. This fascinating session was followed by afternoon tea and coffee with another chance to look at the exhibits and posters.

The final session (which was probably the closest to the stated theme of the meeting) began with an elegant presentation by **Carien Dekker** (Institute of Cancer Research, London) who described the structure of the chaperone protein CCT that is involved in poly-glutamine misfolding diseases. The next speaker was **Simon Kolstoe** (UCL Medicine) whose powerful message was one of the most memorable of the meeting - as the lecture was about to begin, the room was filled with a deafening and unremitting roar. The speaker, session chair and meeting organizer then spent several frantic minutes randomly pulling out cables and sporadically pressing buttons on the podium to try and quell the awesome sound, all to no avail. Only when the speaker's laptop was finally disconnected did the noise abate. Nevertheless, a quick change to the settings on the speaker's MAC resolved the matter and he resumed unperturbed, while the audience recovered. Simon then described how X-ray structural studies were assisting the discovery and design of drugs for treatment of transthyretin amyloidosis. Last, but not least, **Paul McEwan** (Nottingham) described the structure of a complex between the platelet glycoprotein GPIb and a peptide OS1 which inhibits the interaction with von-Willebrand factor and therefore has novel implications for the design of anti-coagulants.

The meeting concluded with a visit to a local hostelry which was followed by the speaker's dinner at a nearby pizzeria. The participants, speakers and exhibitors are thanked for attending this meeting in spite of the very unfavourable weather which struck the night before.

Jon Cooper
(UCL Dept. Medicine, meeting organizer)

BCA Autumn Meeting Report The World of Glass, St. Helens, 5th November 2009

WELCOME - **Anne Kavanagh**, *Chair*, BCA Industrial Group

Anne provided the welcome for the day from the Industrial Group of the BCA for this first meeting incorporating a session of talks from the Young Crystallographer Group. This was also a break from tradition by holding an Autumn meeting at a commercial meeting venue in a switch from the original plan of a meeting at Pilkington.

Morning Session - Young Crystallographers

Speakers, From left to right: John Kaniuka, David Berry Ludovic Renou, Suzanne Buttar, Min Zhao, Moataz Attallah

INTRODUCTION TO NSG/PILKINGTON

John Kaniuka, Pilkington Group Limited

John gave an overview of the company from its origins as a bottle maker on this site in St Helens in 1826 through the invention of the float process and the resultant expansion of the company leading to the privatisation of the original family firm and the takeover and assimilation into the NSG group in 2006. The group is divided by product lines into three groups, building products, automotive and speciality products with product lines ranging from window glass enhanced with coatings to keep it clean, retain internal heat, solar control, or decorative, noise insulation, structural and fire protection properties. Questions revolved around some keen interest in a glass concept car.

GROWTH OF FUNCTIONAL PHARMACEUTICAL CO-CRYSTALS VIA PHASE SPACE MANIPULATION

David Berry, AstraZeneca

David began, with the aid of Zaworotko's definition, by explaining what a co-crystal actually is and three reasons why they are important to the pharmaceutical industry; offer a route to novel pharmaceutical materials, altered physical properties (solubility, stability and bioavailability), can be designed because of hydrogen bonding and synthon engineering. Various screening methods are now employed for co-crystals, including robot solution screening, solvent drop grinding/dry grinding, thermal screen differential scanning calorimetry (DSC), hot stage microscopy (HSM) and nuclear magnetic resonance (NMR). He used four active pharmaceutical ingredients (API's) for study; Carbamazepine, ibuprofen, piracetam, paracetamol and divided the co-crystal formers into 5 fundamental groups; Mono-carboxylated acids, Di-carboxylated acids, Benzoic acid derivatives, Sugars and Nitrogenous heterocycles. He presented a table of screening results for the 4 API's and over 20 different formers, with only 5 showing positive results. The ibuprofen, nicotinamide, water co-crystal system phase diagram was presented and the advantages of this system explored.

FORMULATION AND CHARACTERIZATION OF A FULLY AMORPHOUS SOLID DISPERSION FOR A LOW TG (GLASS TRANSITION TEMPERATURE) DRUG

Min Zhao, School of Pharmacy, University of East Anglia.

Min explained that more than 40% of drugs had little or no water solubility and 95% of drugs approved since 1995 have poor solubility, poor permeability or both and that making amorphous forms would improve efficacy but with the possible disadvantage of low stability. Paracetamol with a Tg (glass transition temperature) of ~25°C was chosen in this trial with a spray drying technique. It was necessary to use a polymer stabiliser. Polymers HPMC Methocel K4M, HPMC Methocel E4M, HPMC Methocel 5cp, HPMC Methocel15cp and HPMC Methocel 50cp, PVP Kollidort 17PF, and PVP Kollidon 90F and co-polymer Plasdone S-630 and Kollidon VA 64 were tested with drug loadings of 10 to 100%. They were prepared with an inlet temperature of 110°C and 5ml/min pump rate. The resulting samples were characterised with a number of techniques including calorimetry, XRPD and SEM and results were presented. It was found that Plasdone S-630 is the best polymer for inhibiting the crystallization of paracetamol and that fully amorphous paracetamol was produced in solid dispersion with Plasdone S-630 and a 30% drug loading. Tests at various temperatures and humidity showed that this material possessed excellent long term stability.

USE OF COCRYSTALS IN THE PHARMACEUTICAL AND AGROCHEMICAL INDUSTRY

Suzanne Buttar, Pharmorphix® Solid State Services.

Suzanne introduced her talk with a definition of a cocrystal ("a crystal containing two or more components together" - Dunitz) and the proton transfer relationship between the cocrystal and salt. She went on to describe the modification in functional properties that cocrystallisation can impart, such as; morphology, structure "apparent" solubility, dissolution rate and colour with improvements in chemical stability, mechanical stability, bulk density and hygroscopicity. Identifying a suitable set of conformers is an important part of design and preparation. Preparation techniques generally fall into three categories, thermal

methods (DSC, Kofler), solvent interaction (slurrying, slow evaporation) and energy input (sonication, grinding, microwaves). Initial high throughput reaction screening analysis techniques are XRPD, ^{1}HNMR or ion chromatography and DSC.

With scaled up preparation if all three indicate co-crystal formation, a full spectrum of analytical techniques is used, including single crystal XRD. The following examples of cocrystal formers were discussed: caffeine, carbamazepine, gabapentin lactam, succinic acid, oxalic acid and benzoic acid.

CHIRAL RESOLUTION AT THE SOLID STATE, PHARMOPHIX'S APPROACH

Ludovic Renou, Pharmorphix® Solid State Services

Ludovic gave a definition of chirality as when two objects form a pair of enantiomers that are symmetrical about a mirror plane. He used Modafinil a psychostimulant used in the treatment of narcolepsy (and as a performance enhancing drug by athletes) as an example. The patented synthesis leads to a racemate containing 50% of each enantiomer and the object of the study was to produce a single enantiomer by crystallisation. He went on to explain the strategies for chiral resolution from the most common state of a racemic compound with no discrimination of the enatiomers in the solid state. The less common racemic conglomerate is the most suitable strategy for chiral resolution with preferential crystallisation or salt formation produced by AS3PC (Auto Seeded Programmed Polythermic Preferential Crystallization). XRPD, single crystal XRD and Raman spectroscopy were used to test the experimental products.

COMPARATIVE QUANTITATIVE CHARACTERISATION OF ALLOY MICROSTRUCTURES USING X-RAY DIFFRACTION AND ELECTRON MICROSCOPY TECHNIQUES

Moataz Attallah, Materials Science Centre, University of Manchester.

Moataz talk on the characterisation of alloy microstructures was aimed at highlighting the shortcomings of certain quantitative characterisation techniques when used without prior knowledge of the microstructure. The overall objective of quantitative characterisation is to establish the structure - property relations in metallic materials, by correlating the size/density of the microstructural features to the macro properties. In this work, electron microscopy (FE-SEM, TEM and EBSD) was compared with XRD (lab and high energy synchrotron) in performing quantitative phase analysis (QPA) of the alpha+beta titanium alloys. The work clarified that some techniques are incapable of performing QPA confidently, as they are limited by their resolution, sampling volume/area, surface or transmission, or quantitative errors (e.g. Rietveld refinement). It was found that the knowledge of the alloy microstructure using electron microscopy can be essential for a successful QPA using XRD as it can provide physically and chemically sensible fitting parameters for Rietveld refinement.

LUNCH BREAK- An excellent buffet lunch was rounded off with a conducted tour of the cone building - part of the World of Glass heritage site. Delegates are pictured inside the Victorian building in the photograph below.

Afternoon Session: Crystallography in Industry

Speakers, From left to right: Helen Blade, Graham Smith, Chris Staddon, David Beveridge, Mark Farnworth, Judith Shackleton

APPLICATIONS OF CRYSTALLOGRAPHY IN THE GLASS INDUSTRY

Mark Farnworth, Pilkington Group Limited

Mark ran through some examples of the XRPD work on refractories, thin films, reflectivity and the new micro XRD facility. The amount of glassy phase in refractory bricks used to build glass furnaces and float baths can affect service life. XRPD is used with a simple straight line calibration based on known mixtures of crystalline and amorphous quartz and the countrate obtained at a fixed goniometer angle. Coatings on the glass surface are important in enhancing glass performance and glancing angle XRD can provide useful insight into the character of the coating deposition. Columnar growth is often present and pole figures provide a useful tool to quantify the degree of crystal orientation. X-ray reflectivity (XRR) in a theta/ 2 theta scan at low angle (typically 0.2 to 5 degrees) provides information on coating thickness, density and both surface and interface roughness by refining a model of the coating structure. The new micro XRD capability is being used to identify tiny particles found from screening raw materials to see if they will be detrimental to glass making. Other applications are tiny faults in glass and coatings and typing the form of NiS inclusions.

CHARACTERISATION AND PREDICTION OF PHYSICAL STABILITY OF AMORPHOUS MATERIALS DURING PHARMACEUTICAL DEVELOPMENT: PAIR-WISE DISTRIBUTION FUNCTION

Helen Blade, AstraZeneca.

Amorphous drug formulations are becoming more common in addressing issues of bioavailability and stability. A comparative Pair Wise Distribution Function (PDF) is being used as a rapid screening method as a test for an amorphous product. A PDF can answer the questions: is the amorphous material stable, is it amorphous or nanocrystalline, is the formulation a true solid dispersion or is it phase separated? Conventional reflection XRPD scans are used to provide data for PDFgetX2 software. It is important to reduce background scatter in the scan and low background substrates and vacuum or light gas paths to reduce air scatter are recommended. Helen went on to explain how AZ are using PDF in the drug development process with the help of some case studies showing that amorphous drugs were stable, that amorphous and nanocrystalline could be differentiated, and a Felodipine - Copovidone example to show that solid dispersion and phase separation could be discriminated. PDF can provide a ranking of physical stability at the point of preparation, negating the need for stability studies, and helps to speed up the overall drug development process.

APPLICATIONS OF CRYSTALLOGRAPHY IN THE AEROSPACE INDUSTRY

Judith Shackleton, Materials Science Centre, University of Manchester

Judith highlighted the uses of XRD at Manchester but concentrated on their specialty, the measurement of residual stress in aerospace components for this talk with precise and accurate measurements being essential for quality control and necessary to certification. Typical applications are routine quality control, validating changes to manufacturing processes, manufacturing problems and, very rarely failures! The well documented $\sin^2\psi$ method is used to calculate the residual stress from small shifts in the position of high angle diffraction peaks. The great advantage of this method is that a stress free d-spacing is not required. Problems are encountered with large samples which usually have irregular geometries, with few flat surfaces. These can be overcome by careful positioning and limiting the irradiated area. Laboratory based systems are typically restricted to 10 to 20 micron beam penetration. For increased penetration, especially for large components, synchrotron or neutron radiation is employed. In this case a stress free d-spacing is required and their measurement using Hauk's method was discussed.

XRD N' CHIPS - WHAT MAKES GOOD SEMICONDUCTOR DEVICES

Chris Staddon, University of Nottingham

Advanced electronic devices based on semiconductors are a focus of research work at Nottingham. Molecular beam epitaxy and metal organic chemical vapor deposition are used to produce high quality semiconductor films based on GaAs or GaN for LED and solid state lasers etc. The structure and growth of these films are studied using XRD, TEM and photoluminescence. Chris highlighted three examples of the measurements; determining doping concentration, the cubic content of a hexagonal film and in plane orientation and size. Doping concentration of Mn in GaMnAs films was measured through the expansion of the lattice constant and simulation. For cubic / hexagonal ratio in GaN on sapphire a pole plot was used. The example for in plane orientation and size was GaN nano-rods.

POWDER X-RAY DIFFRACTION FOR PROCESS AND PRODUCT SUPPORT IN SHELL GLOBAL SOLUTIONS

Graham C. Smith, Shell Global Solutions UK

Graham started his presentation with an overview of the organisation and the migration from film and first generation automated systems to the modern equipment in use today. XRPD supports customer groups from within Shell (Fuels, Lubricant, Engine/Vehicle Testing, Refineries, Failure Diagnosis) and some work for external customers and went on to discuss some examples of their work. SEM-EDX was used to provide elemental composition (including the important light elements) for a boiler deposit which was a complex mix of iron sulphates and Haggite (Vanadium oxide hydroxide). A Plant deposit turned up a mix of FeF_2, $Fe_2F_{5.7}H_2O$ and $FeF_{2.4}H_2O$. Some contamination from a fuel filter contained Cu, Fe_3O_4, graphite and CuO. A new area of work is on engine valve deposits using capillary optics directly on the valve. Asphaltenes in crude oils cause pipe blockage and XRD work on liquid crude oils and asphaltene extracts is helping further the understanding of this problem.

XRD IN THE IMAGING INDUSTRY

David Beveridge, Harman Technology

Historically the silver halides were the cornerstone of the imaging industry with AgCl (Fm3m), AgBr (Fm3m), AgI (beta P63mc and gamma F43m) playing the major roles. For films AgBr is used at typically 5 - 10 mole % and size around 0.75µm, often core-shell structured with the core about 30 mole % and the shell about 5 mole %. For papers Ag(Cl, Br) is used typically near 50 mole % of each and around 0.3 µm size. The effect of the Iodide concentration on emulsion growth was shown in a series of images and diffraction scans.

Three examples of materials recovered from a photochemicals building were then shown with the presence of hydroquinone a possibility. Some brown material with white lumps turned out to be dust and oxidised sodium sulphite from XRF and XRD evaluation and the white lumps partly oxidised sodium sulphite. The brown material didn't show the presence of hydroquinone by UV-Vis on a solution, but material from a laminar flow booth did. A second sample from the laminar flow booth showed

Hydroquinone + KBr + various grots by XRD and XRF.

Anne Kavanagh closed the meeting by thanking all the speakers for the work that went into their presentations. She also thanked the staff at the venue for helping to make the meeting a success and an excellent lunch. She closed the meeting by thanking the delegates for sparing valuable time to attend and gave a reminder of the next meeting at Warwick in April 2010.

Dave Taylor, ICDD

Please note that the report on the web has links to the presentations (in PDF form) for nine of the meeting talks.

Bill Clegg Symposium

A one-day symposium is to be held to mark the retirement of Bill Clegg (though not from research!) and focusing on major aspects of his research career to date: synchrotron crystallography and structural alkali-metal chemistry, including both historical and current perspectives.

Speakers and topics

Professor Paul Raithby (University of Bath): *Bigger, brighter, faster: the development of single-crystal X-ray crystallography in the UK*

Dr Steve Liddle (University of Nottingham): *A journey from lithium to uranium: a structural tale*

Dr Gary Nichol (University of Arizona, USA): *Just trust me: synchrotron crystallography from a service perspective*

Dr Simon Teat (Advanced Light Source, Berkeley, USA): *Lord of the Rings*

Professor Rab Mulvey (University of Strathclyde): *Social and structural synergy: Clegg, Snaith, and Mulvey meet the alkali metals*

Professor Dietmar Stalke (University of Göttingen, Germany): *What a lithium chemist can learn from charge density*

The symposium will be held at Newcastle University on Thursday 18 March 2010 from 11 am till 5pm.

Coffee will available from 10am. Lunch will be provided. There is no fee for attendance.

To assist with catering plans, please register if you plan to come, preferably by 12 March: contact Isobel Lamb on **0191 222 7102** or isobel.lamb@ncl.ac.uk

British Society for Strain Measurement / Industrial Group Meeting University of Manchester, 10th March 2010

The Measurement of Residual Stress by Diffraction Methods Workshop at the University of Manchester

RESIDUAL stress is one of the most common causes of catastrophic and unexpected failures in engineering components. Today, engineers are developing tools and strategies for managing detrimental residual stresses and for introducing beneficial ones across component scales ranging from microelectronics through to aero-engine assemblies.

This workshop is aimed at anyone who would like to know more about measuring residual stress using diffraction techniques. It is suitable for beginners, as well as more experienced practitioners. The workshop aims to cover all diffraction methods, neutron, synchrotron and laboratory X-ray. Consequently it will also be of interest to those who already have experience in one field and would like to extend their knowledge into others.

We will also cover sample preparation techniques as well as layer removal by electro polishing. There will be an opportunity to make a measurement using two of Manchester's 'state of the art' stress diffractometers. You can bring a sample if you wish; please let the organiser know in advance.

To register for the event go to:
http://www.bssm.org Diary of Events / Events and Seminars

Contact: **Judith Shackleton**

Two Day Xrf/Xrd May Meeting

DAY 1: XRF Meeting - "Blanket cover"
12th May 2010, British Geological Survey (BGS), Keyworth, Nottingham

Meeting sponsors will have table top displays, see the web page for sponsorship details.

Speakers include:
Mark Ingham et al; British Geological Survey
Topic: *Wide range fused beads with difficult elements e.g. F, Cl & S*

Owen Butler; Health and Safety Laboratory
Topic: *New work on filters*
Richard Morris; Morris Analytical X-ray
Topic: *Platinum Group Metals in road dust*

CALL FOR PAPERS: To offer a talk at this meeting please contact the programme organiser **Ros Schwarz** (Use the contacts link on the XRF web pages)

DAY 2: XRD Meeting - Minerals: "Between the Sheets"
13th May 2010, British Geological Survey (BGS), Keyworth, Nottingham

Talks include:
Illite-Smectite in Basin Analysis (K-Ar dating and estimation of the maximum paleotemperatures)
Prof Jan Srodon; The Laboratory of Geology and Stratigraphy, Polish Academy of Science, Cracow

The Geology of Beer (includes tasting!)
Jenny Huggett; Petroclays

Experimental and numerical investigation of interlayer water organization in expandable clays
Eric Ferrage; Laboratoire HydrASA, University of Poitiers

Title to be advised
Joe Jackson, Loughborough University

The Analysis of Nano-clay Dispersions and Composites Using Small Angle X-ray Scattering and Polarised Light Microscopy
Richard Morris, Morris Analytical X-ray.

To offer a talk at this meeting please contact the programme organisor **Martin Gill**.

Please visit out web site for the latest programme information and to register for one or both of the days.

PANalytical Tube Factory Visit

NETHERLANDS, 14th to 16th Sept 2010
To summarise a proposal to host an Autumn 2010 Industrial Group Meeting in the PANalytical facilities in Almelo, the Netherlands.

PANalytical would like to offer a subsidised trip for up to 25 delegates for the Autumn meeting to visit the facilities in Acht (Tube Factory) and Almelo (Main Competence Centre). The BCA will have the meeting room facilities to hold the lectures by its appointed speakers. PANalytical would also provide a Keynote scientific talk to the delegates.

Aside from the meeting content, PANalytical would also arrange a view of the Technology involved in making X-ray tubes and other components in the Acht tube factory as well as a viewing of the Application Laboratories in the Almelo Competence Centre.

We would envisage the following logistics:

DAY 1:
- Delegates would fly into Schipol on the early morning flights.
- PANalytical would arrange an assembly point in Schipol
- PANalytical would bus delegates to Acht for the Tube Factory visit
- Lunch in Tube Factory
- Tour of Tube factory and insight into our technologies
- Insight into tube longevity and care
- Bus to Hotel in Almelo
- Evening meal in Almelo

DAY 2:
- Visit to Almelo Competency Centre
- Welcome and Keynote talk by PANalytical
- Normal technical presentations
- Lunch
- Tour of the Application Laboratory
- Complete technical programme
- Bus back to a hotel in Amsterdam
- Evening meal

DAY 3:
"Educational" event in Amsterdam in Morning
Delegates take mid day flights back to UK.
The Industrial Group would be keen to arrange similar visits to other suppliers in future years.

Industrial Group Autumn Meeting

Diamond Light Source, Harwell Science and Innovation Campus 3rd to 4th November 2010

Draft itinerary:

DAY 1:
Start 12pm: lectures for Diamond beamline scientists and science officer finish around 6pm.

DAY 2:
9.30am: Diamond Tour inside the ring and selected beamlines.
1.30 (after lunch): lectures by application scientists (academic and industrial).
Finish: at 5pm.

Visit the Industrial Group web-site for detailed information about accommodation options and costs. The maximum number of attendees for this meeting is 60 so you will need to book early to secure your place.

Meeting Organiser: **Matthew Johnson**

CCP4 at Nottingham

THE annual Collaborative Computational Project in Macromolecular Crystallography (CCP4) Study Weekend returned to the East Midlands Conference Centre at the University of Nottingham for another successful meeting. Held on January 6-8, 2010, the meeting entitled "From Crystal to Structure with CCP4", provided a showcase to highlight key software in the package and accompanying new developments. The scientific programme was organised by Keith Wilson (University of York, UK), Kevin Cowtan (University of York, UK) and Paul Emsley (University of Oxford, UK). Registered participants numbered 381, the majority of whom did show up in spite of the snowbound weather conditions which affected the UK this year. The meeting drew scientists from a range of academic and industrial institutions in the UK and from 11 other European countries as well as the United States, China, India, Japan and Singapore.

The outgoing chairman of CCP4 Working Group 1 (WG1), **Jim Naismith** (St Andrew's University, UK) opened the meeting and reminded us of the importance of the open and collaborative nature of CCP4 and its long and well respected international reputation. He emphasised the important role of CCP4 study weekends in training and encouraged everyone to use and contribute to the package. On the second day of the meeting **Keith Wilson** thanked Jim for his outstanding work on WG1 and dedication to the carrying out the aims of the CCP4 package. **Martin Noble** (University of Oxford, UK) stepped in as the new WG1 Chairman and **Frank von Delft** (Structural Genomic Consortium, Oxford, UK) became the newest member of the executive. All UK-based PIs are eligible to become members of WG1 and can do so by contacting ccp4@ccp4.ac.uk.

Session 1, "Overview of CCP4. The Start Point: Crystallisation" opened with **Eleanor Dodson** (University of York, UK) who embarked on the historical overview of "30 years of CCP4" from its humble beginnings. A roll-call of past chairmen and secretaries was presented, reading a little like Who's Who in Macromolecular Crystallography. The initial mutual support group that handled common software issues embedded the basis for the current success. Common data structures and formats were established, and routines to handle them were bundled into a library to avoid duplications. The distinct 'feel' of 'design by a committee' is clear to see from the modular units in the package, arising from individual software contributions that are assimilated into the communal package. Arguably, this feature of CCP4 has to some extent eased updates in later years, as one routine became obsolete only to be superseded by a new algorithm. The successive versions of CCP4 did not require a complete revamp! But the real success story is in the popular bulletin board. None of the founders, nor even the second wave of contributors, could foresee the range of expert advice routinely offered by e-mail. No enquiry is so large or so small as to be devoid of receiving attention, and help for novice users is doled out with care and respect. Funding had been vital at various stages of the evolution of the package. CCP4 has evolved from a small discretionary budget from the previous UK Science Research Council. Now the current programme-type grant awarded from the UK Biotechnology and Biological Research Council is based upon an application which is overseen by the WG1 chairman. In addition, commercial income is now a critically important means of supporting the package with industrial users forming a vital part of the CCP4 community. Eleanor graciously concluded her talk by acknowledging the many contributors, past and present, to the package. However, for many of us Eleanor herself is "CCP4" and she continues to play an active and key role in its ongoing development and support.

Martyn Winn (STFC Daresbury Laboratory, UK) the outgoing CCP4 Secretary, reviewed the current status of the package in a talk entitled "Overview of CCP4 Suite and Current Developments" He noted the presence of parallel versions of software which is mainly due to the use of different algorithms for carrying out the same task such as molecular replacement or density modification. In 2000, the graphical user interface (GUI) was introduced to help users organise their work. Now, many of the steps of structure solution and analysis are benefiting from automation, via background pipelines, in order to free time for scientists to think. Tasks are grouped together according to the stage of the structure analysis: Data reduction, experimental phasing, molecular replacement, model preparation, phase improvement, refinement, validation and others. The current drive for automation in every step has also led to the need for database indexation of outputs, particularly where multiple trials are run in parallel. Interfaces to external databases are part of this effort, as well as incorporating other facilities like PRODRG, RAPPER, SLOOP and JLigand. Perhaps most important for users will be the new GUI to cover data management and the impending incremental updates via 'rsync'. Further down the line looms the integration of SAXS and EM methodologies into the package.

Zygmunt Derewenda (University of Virginia, USA) presented a talk "Protein Crystallisation - Overview and Current Trends", which started with a historical review. Crystals of proteins were known as long ago as the 19th century. Crystallisation was deliberately used for purification in the 1920s, and by the 1930s protein crystals were being used for diffraction studies. Later decades saw the screening of different species for a crystallisable protein, but more recently molecular biology allowed the manipulation of the protein of interest until it became crystallisable. The same framework was still in use in the late 20th century, where an experiment would see the protein screened against buffers, precipitants and additives. However the conditions scanned were minimal, representing a sparsely populated matrix, due to limitations of cost and protein availability. Robotics were then introduced to speed up every step in the process, and make much more efficient

use of the sample. Matrix coverage now is much higher, but still not continuous. Attention was directed at optimisation of hits that initially produced poor crystals. Crystallisation, Zygmunt discussed, is a process driven by many factors including the stability of the fold, surface contacts, structured water patches, along with some unfavourable features (loops, sugars, termini). Evaluation of the crystallisability of a protein sequence was described using the XtalPred server at http://ffas.burnham.org/XtalPred-cgi/xtal.pl. The talk concluded with an interesting overview of strategies for modification of protein sequences that have proved useful in a number of cases.

Chris Morris (STFC Daresbury Laboratory, UK) was gracious enough to step in at the last minute to present Rob Esnouf's (University of Oxford, UK) presentation, "PiMS, xtalPiMS and Beyond: Proteins, Crystals and Data". Chris explained how the new software was aimed at replacing the lab notebook for record keeping and information propagation, highlighting this point with recently withdrawn publications due to the loss of notebooks! Other benefits of PiMS include a standard vocabulary and metrics, easy data retrieval for comparison of experiments, and easy preparation for deposition. But there are problems, mostly in IT overheads. Data loss and data integrity are also areas in need of specific attention for long term data storage which needs to be addressed globally. Given how important it is to maintain records of the "pipeline" of studies that lead to crystals, one might predict that PiMS and PiMS-like systems will find increased usage in the not too distant future.

The second session "A Step You Must Get Right: Data Acquisition and Processing" is based upon the premise that the quality of the final structure determined by X-ray crystallography is highly dependent on the quality of the original data collection and processing. In this session, the speakers discussed these initial stages of a crystallographic experiment, highlighting both best practices and potential pitfalls and opened with **Gwyndaf Evans** (Diamond Light Source, UK). In his talk, "Designing an X-ray Experiment", he discussed the diffraction data collection experiment itself in the context of a macromolecular synchrotron beamline. The first message was that all beamlines are not the same and it is important to select the right beamline for the experiment you want to do. For example, using a microfocus beamline for very small crystals can help in obtaining good data by matching the beamsize to the crystal, reducing background scatter from the loop and mother liquor. Gwyndaf also discussed sources of noise/error in the diffraction experiment. One key tip from this part of the talk was that if the crystal is vibrating in the beam (for example when a large plate-like crystal is face on to the cryostream and is mounted on a long loop) a dab of grease where the pin joins the loop can stiffen the system and help reduce the crystal vibration, improving the data. He also discussed how optimisation of the beamline setup (tweaking of slits, beam focus and beamsize) as well as data collection strategy (i.e. at multiple points along the crystal to help mitigate radiation damage) can improve the data.

Andrew Leslie (MRC Laboratory of Molecular Biology, Cambridge, UK) then presented a detailed overview of IMOSFLM for indexing and integration of data in "Spots Before Your Eyes: Diffraction Data Integration with IMOSFLM". The new IMOSFLM graphical user interface (GUI) has been designed to provide visual feedback on data integration, as well as encourage users to actually have a look at the images during processing. This can help in spotting problems such as poor spot shape, anisotropy, multiple lattices, high mosaicity, direct beam position, shadows on the detector and ice spots/rings. Andrew gave lots of hints about how best to use the programme and the meaning of the wealth of information given by the GUI. For example, the local background determination works well for weak data, but can produce artefacts near shadows. These artefacts can be reduced by decreasing the size of the background box. When identifying the most likely indexing solution, the positional errors should be small (0.1-0.3mm), although for split data you can get position errors up to 1mm and still have a correct indexing solution. Very mosaic data can cause problems in indexing, Andrew suggested setting the threshold very high (100) to select strong spots in the middle of a lune. Ice rings should be less of a problem as, by default, the indexing step rejects all spots on known water ice rings. The intensity v. mosaicity curve sometimes shows a decrease in intensity at high mosaicity values. This is because overlapping reflections are not included in the calculation. During the integration step everything should remain stable. Values to keep an eye on include the direct beam (which should not shift by more than 0.2 mm) and the tilt (no more than 0.3). In addition, the rms error for the spots should not change unless the spot shapes vary across the dataset. Not excluding ice spots/rings can cause problems in the spot profiling and Andrew showed an example of integration with and without the ice rings removed to highlight this.

Phil Evans (MRC Laboratory of Molecular Biology, Cambridge, UK) followed with "Data Reduction: Space Group Determination, Scaling and Intensity Statistics" - a discussion of the scaling step of the data reduction process. He made two important points. The first is that until the structure has been solved, the space group assignment remains a hypothesis. For example, while higher symmetry space groups *must* have a β angle of 90°, there is no reason why a monoclinic cell cannot have a β angle of 90°. The second is that the job of scaling is to model the experiment in order to apply correction factors that make the data internally consistent. Phil presented case studies that illustrated the usefulness of the various plots and tables produced by SCALA to diagnose problems in the dataset, as well as the use of POINTLESS to examine the space group assignment from indexing.

The final talk in this session was from **Clemens Vonrhein** (Global Phasing Ltd., Cambridge, UK) who took a humorous approach in "Data Problems: How to Spot Them and What to Do" to present the methods he uses to diagnose problems with, and often solve, apparently intractable datasets that cannot be phased. He noted that many of

these “bad” datasets have problems in both the collection strategy and processing. Clemens advocated the use of HKLVIEW to generate pseudo precession images that aid in rapidly identifying possible problems. One striking example featured very strong high resolution reflections that had derived from ice rings in the original images. Removing these reflections allowed the structure to be solved. Several other examples helped hammer home the message that a problem in a single resolution shell can affect the whole dataset. Clemens also highlighted the utility of looking at the unindexed spots; these can often reveal ice scattering that is not immediately apparent when eyeballing the diffraction pattern. For example, even in cases where there is no distinct ice ring, there can be distinct reflections coming from the ice.

In final session of the first day, “Starting from a Known Structure: Molecular Replacement” **Gabor Bunkoczi** (Cambridge Institute for Medical Research, Cambridge, UK) presented his talk “Phaser: Molecular Replacement”. He provided an overview of the principles and steps involved in using Phaser, a state-of-the-art molecular replacement program. He described novel developments in experimental phasing and model editing to prepare an ensemble of search models.

Ronan Keegan (STFC Daresbury Laboratory, UK) followed with “Evaluating the Solution from MrBUMP and Balbes”, two recently developed programs from CCP4 to automate and speed-up the process of molecular replacement. MrBUMP takes a brute force approach, taking a large selection of the best homologues and preparing them in many possible ways before feeding them to Phaser and Molrep to carry out the molecular replacement. Balbes, based on Molrep and Refmac, takes a different approach concentrating on isolating the best template model from its own in-built database of all possible unique folds in the Protein Data Bank.

Bert Janssen (Utrecht University, The Netherlands) gave an account on the C3 and the pro-convertase complex in “Challenging Molecular Replacement: Complement Components and Convertase Complexes”. These proteins are key components of the mammalian immune defence, which is critical for resistance to infection. This highly complex structure was solved by the combination of multi-crystal averaging to combine MAD and SIRAS data. Molecular replacement has been crucial in solving these multi-domain structures to reveal conformational changes as a result of proteolysis and complex formation.

Gerard Kleywegt (Protein Data Bank in Europe, PDBe, Hinxton, Cambridge, UK) in his “Ghosts of PDBe Past, Present and Yet to Come”, briefly sketched the history of PDBe. He gave an overview of some of the issues involved in deposition and annotation. Then he discussed some of the key issues facing the PDB and PDBe in the future. A top priority for PDBe will be the development of new tools and interfaces to make it easier to access and use structural information, especially for non-expert users. Other directions include ligand validation and dictionary generation in the collaboration with CCDC, to obtain structures from industry and to develop new tools to serve new user communities.

The first session on Friday morning “Experimental Phasing: Using Phase Markers” began with a talk by **Raj Pannu** (Leiden University, The Netherlands) entitled “Automated Experimental Phasing in CRANK”. CRANK is a pipeline that brings together substructure determination (CRUNCH2 or SHELXD) with phasing (BP3), density modification (Solomon, DM, Pirate) and model building/refinement (Arp/Warp and Refmac). It uses a maximum likelihood description of the data using F+ and F- rather than the Bijvoet difference as the observations and successfully solves a large number of test data sets automatically, while allowing a large degree of customisation for difficult cases.

Randy Read (Cambridge Institute for Medical Research, Cambridge, UK) followed on with his talk “PHASER: Experimental Phasing”. He described how PHASER can carry out both SAD phasing and SAD combined with Molecular Replacement where the molecular replacement phases find the initial anomalous sites rather than substructure solution. This is due to the SAD equation in PHASER including the non-anomalous scatterers.

Finally **Pavol Skubak** (Leiden University, The Netherlands) spoke “On Bias Reduction in Density Modification”. The false assumption until recently was that the initial map was not correlated with the density modified map when they were recombined. An initial equation to remove this assumption was successful in allowing more complete models to be built but tests showed that bias still remained. Adding in an empirical estimate of the bias improved the bias suppression and the estimate of the figure of merit, although it only gave minor further improvements in model building. This was an interesting introduction to what goes on under the bonnet of the current phasing programmes and the presenters did an excellent job of making it comprehensible on the morning after the conference dinner.

The next session “Refinement, Automated & Manual Model Building” began with a clear and visually well illustrated talk by **Dale Tronrud** (Oregon State University, Oregon, USA) called “The Wonderful World of Maps”. The utility of a range of different calculated maps was presented demonstrating how one uses each in resolving features for model building. He also included examples of interpretation of odd map features such as ripples arising from series termination errors or peaks associated with poorly modeled occupancies or B-factors. He emphasised the importance of understanding the “true meaning” of map contouring levels at different stages of the model building and refinement process. The overall message was that maps can be truly powerful tools in the structural solution process as long as care is taken in using them correctly.

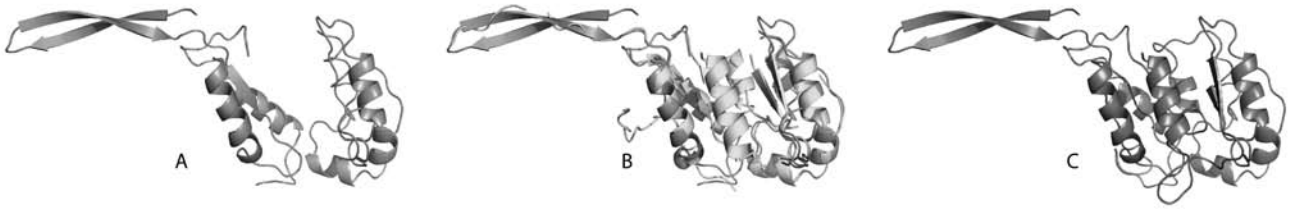
Garib Murshudov (University of York, York, UK) presented an interesting talk “Towards Low Resolution Refinement

Using the Program REFMAC" where he described new and "emerging" features of this highly respected refinement package which forms part of the CCP4 suite. A considerable amount of time was devoted to discussing twinning including detection of twinned data but also how maximum likelihood refinement procedures can be successfully used to refine datasets which contain a twin operator. He followed up with a nice discussion of the implementation of developments associated with improved methodologies in achieving refinement at low resolution including flexible NCS restraints and the utilisation of structural patterns from related high resolution structures for certain cases. The use of the less familiar "jelly body" in refinement was also presented. This is a "soft-body" representation of a low resolution structure which is locally rigid but globally moves, which Garib pointed out worked surprisingly well.

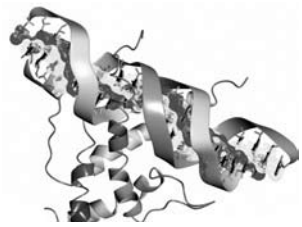
Henry van den Bedem (SLAC, Stanford University, California, USA) gave a very informative and technically detailed talk entitled "Comparison of Model Building Programs: JCSG". JCSG is the Joint Center for Structural Genomics which is funded by the US Protein Structure Initiative. Over the last six years the JCSG's automated structure solution pipeline *Xsolve* solved, traced, and partially refined over 800 MAD/SAD structures without human intervention. *Xsolve* samples a large number of different solution strategies by executing many publicly available crystallography software programmes in parallel on a commodity Linux cluster, resulting in multiple traces for a given target. Additional software programmes were developed and integrated into *Xsolve* to further minimize human effort in structure refinement. *Consensus Modeler* (unpublished) automatically combines all traces to increase completeness and correct errors. Henry also described *Xpleo* [Bedem et al. (2005). Acta Cryst. D61, 2], a powerful, robotics-inspired algorithm to build missing fragments; and *qFit* (Bedem et al., (2009). Acta Cryst. D65, 1107] automatically identifies and fits alternate conformations in high resolution data.

Jane Richardson (Duke University, North Carolina, USA), famed for her development of the ribbon diagram representation of protein structures, closed the session with an interesting presentation called "Structure Validation: Early & Often Smooths the Way". She spoke about the implementation of structure validation methods in the early stages of model building rather than just as a means of assessing the quality of a protein structure at the end of the refinement process. A key tool which has been developed within her laboratory is the MolProbity model-validation webservice which is available at http://molprobity.biochem.duke.edu. The ethos of this tool is to correct local and often systematic errors in protein structures affecting the geometries and orientations of individual residues in a polypeptide chain by using a multi-criteria validation strategy. Assessing the fit to electron density of favoured rotamers or scanning for the presence of genuine hydrogen bonding partners are some of the examples she showed. Some of these corrections are also amenable to automated correction such as flipping over branched side-chains. She indicated that a goal of this work was "to put ourselves out of business" when it comes to validation, reducing some of the subjectivity involved at early stages of model building which could indeed "smooth the way" to better quality structures in the end.

The final session of the meeting "Visualising & Analysing the Results" was opened by **Eugene Krissnel** (European Bioinformatics Institute, Hinxton, Cambridge, UK) who presented a talk entitled "Macromolecular Complexes in Crystals and Solutions". He described how the PISA programme works to automatically identify protein complexes and interactions in the crystalliine state. He first discussed how PISA identifies and defines stable assemblies by using crystal packing to define the possible interactions which are then evaluated by their chemical stability using the free energy of dissociation. The possible oligomers are then classified and ranked on the basis of a reference set. Eugene also discussed several examples when PISA appeared to get it wrong which gave some interesting insights into both PISA and the biology of the example system, as well as how crystallization buffer components can sometimes result in the formation of non-physiological complexes. He made the interesting point, when discussing whether the packing contacts in a crystal are representative of those made *in vivo*, that a crystal optimises the energy of the whole system and may sacrifice biologically relevant (and weak) interactions to favour non-specific contacts. For example, when trying to reproduce crystal packing interactions with docking simulations, 40% of simulations failed. He made it clear that crystallographic



Shown here are the results for a putative serine hydrolase (pdb id 3KSR) solved at 2.8Å resolution. Xsolve calculated a Buccaneer [Cowtan (2006) Acta Cryst. D62, 1002] trace (A) with 57% of residues traced and docked, and a Resolve [Terwilliger (2003) Acta Cryst. D59, 38] trace with 39% of residues traced and docked (B, cyan). The resulting consensus/Xpleo model (C) has 78% of residues traced and docked. (Figure supplied by H. van den Bedem, SLAC, Stanford University, USA)



Interface between the two nucleic acid strands of 1an4, as calculated by PISA, rendered in CCP4MG. (Figure supplied by S. McNicholas, University of York, UK)

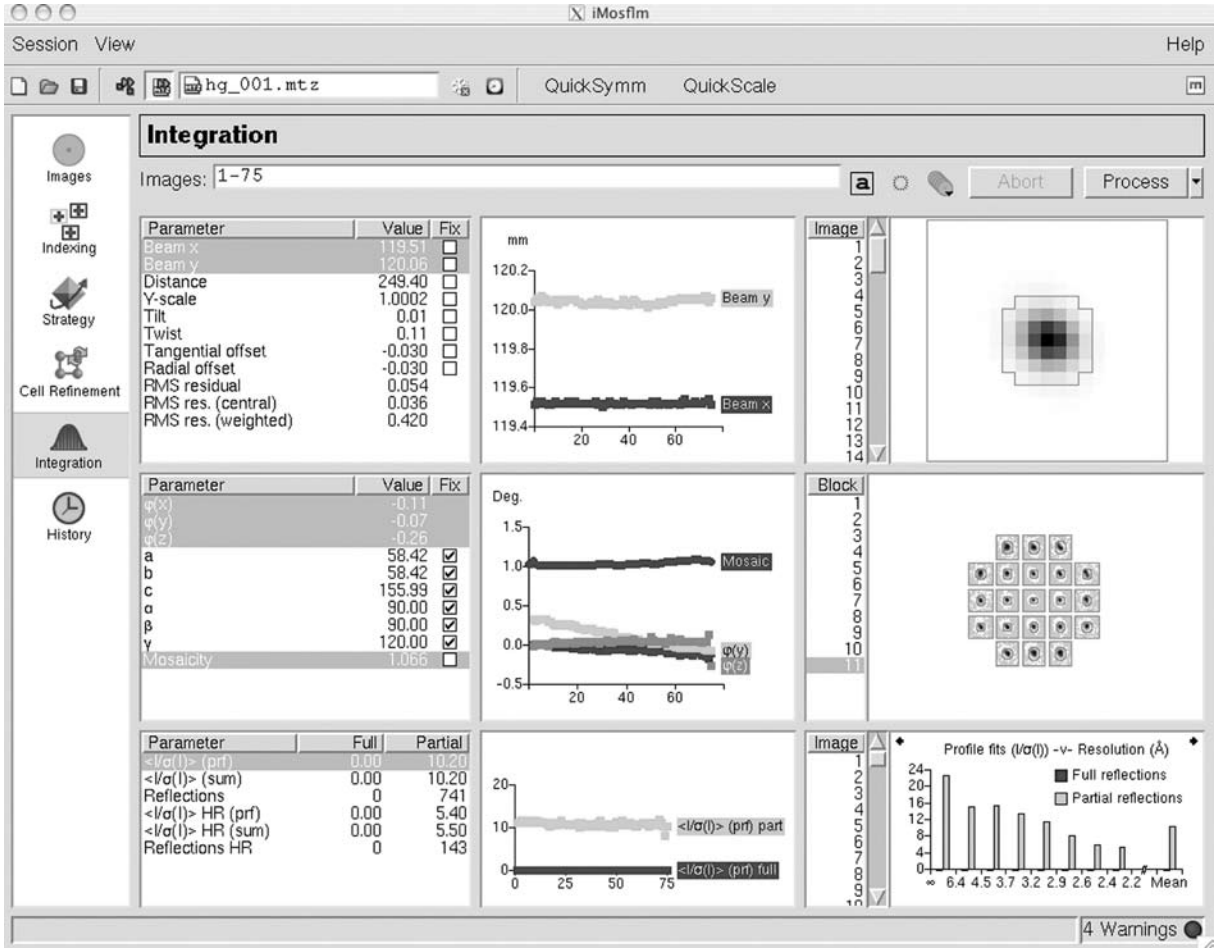
studies should be combined with complementary methods such as SAXS and EM to really probe biologically relevant oligomerisation and assembly.

The next talk "Recent Developments in CCP4MG" was given by **Stuart McNicholas** (University of York, York, UK) who gave us a whistle-stop tour of this molecular graphics package. After giving a quick overview of the software, he bravely continued with a live demonstration illustrating the different features and tools in CCP4MG that can be used to produce publication quality images. A very exciting development in the package is the ability to simply draw vectors, lines and planes and Stuart informed us that more geometrical shapes would be coming soon. Version 2 of CCP4MG is now available for download.

The final talk of the meeting was by **Paul Emsley** (University of Oxford, UK) who took us through the latest new tools available in COOT in "COOT: Hints and Tips". Like Stuart, Paul used a live demonstration to show exactly how the various applications in COOT work. A highlight was the new *sphere refinement* tool which enables the user to refine a set of neighbouring atoms that are not necessarily covalently linked, particularly useful when model building at protein-protein, protein-ligand or ligand-ligand interfaces. He has also implemented a *backrub rotamer* function to avoid distortions of the backbone when trying to fit side-chain rotamers at low resolution. Paul also demonstrated the utility of key-bindings in COOT that enabled rapid single keystroke navigation of the model and triggering of commonly used tools.

The longevity of the CCP4 workshops is not just due to the "star status" of the package itself but also to the dedicated professionals who ensure that all the CCP4 participants, from novices to groupies, are well catered for throughout the meeting. This year's excellent support team includes **Shirley Miller**, **Damian Jones, Laura Johnston**, **Tracey Kelly** and **Stuart Eyres** (photography). Thanks are especially due to **Stuart Eyre**s (a 20-year CCP4 veteran) and **Laura Roe**, both from Media Services at STFC Daresbury Laboratory, who prepared the montage of images which appear on the cover of this issue of Crystallography News - a genuine collector's item for all CCP4 fans!

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



The integration window of the new iMosflm graphical user interface.(Figure supplied by A. Leslie, MRC Cambridge, UK)

ECM26

ECM26 Scientific Programme

Keynote Lectures (*confirmed)

K1 *Very large complexes*
Nenad Ban (CH)

K2 *Flu virus*
Steven Cusack (FR)

K3 *How to do your MX experiment**
Elspeth Garman (GB)

K4 *Hydrogen bonding in proteins*
Mariusz Jaskolski (PL)

K5 *Membrane transport systems**
Poul Nissen (DK)

K6 *Structural aspects of errors in cell biology and cancer*
Titia Sixma (NL)

K7 *Can Nature do what Man can do? The Search for Natural Quasicrystals**
Luca Bindi (IT)

K8 *Single Crystal Diffraction Studies at Multimegabar Pressures**
Malcom McMahon (GB)

K9 *New phase transitions**
Bertrand Toudic (FR)

K10 *Charge Density for Understanding of Physical and Chemical Properties**
Wolfgang Scherer (DE)

K11 *Correlation between theoretical and computational methods with structural studies**
Carlo Mealli (IT)

K12 *Relevance of X ray Structure Data to Kinetic Studies**
Andreas Roodt (ZA)

K13 *Symmetry breaking in complex molecular assemblies**
Jürg Hulliger (CH)

K14 *Powder Diffraction at the Japanese Spallation Source*
Takashi Kamiyama (JP)

K15 *Resonant and coherent scattering on nanostructures**
Vincent Favre-Nicolin (FR)

Microsymposia

Focus Area 1: Biological and Macromolecular Crystallography (SIG 1)

MS1 *Micro-crystals and Synchrotron in Life Sciences*
MS2 *Twinning, Non-crystallographic Symmetry and Space Group Determination*
MS3 *Practical Solutions to Membrane Protein Crystallography*
MS4 *Experimental Phasing in Structural Biology, Phase Improvement and Refinement*
MS5 *Crystallography, SAXS and Electron Microscopy*
MS6 *Molecular Recognition*
MS7 *Regulatory RNA*
MS8 *Macromolecular Assemblies (Viruses and Phages)*
MS9 *Cytoskeleton, Protein Trafficking and Sorting*
MS10 *Challenges in Redox-Reactions*
MS11 *Exciting new structures*
MS12 *Infection and Disease*

Focus Area 2: Materials and Minerals (SIG 5, SIG 11, SIG 12)

MS13 *Complex metallic alloys*
MS14 *New inorganic materials for technological applications*
MS15 *Phase transitions in minerals and their planetary effects*
MS16 *Mineral and inorganic crystallography*
MS17 *High-pressure crystallography at elevated temperatures*
MS18 *Open structures and aperiodic crystals under in situ/non-ambient conditions*
MS19 *Structure and properties of functional materials at extreme conditions*

Focus Area 3: Physical including Fundamental Crystallography (SIG 2, SIG 3, SIG 4)

MS20 *Charge, spin and momentum densities for the prediction of physical properties*
MS21 *Aperiodic order: experiment and simulation*
MS22 *Diffuse scattering and disorder*
MS23 *Aperiodic composite structures*

Focus Area 4: Chemical Crystallography (SIG 7, SIG 13)

MS24 *Quantitative electron crystallography*
MS25 *Modern electron diffraction - exploring structures and properties*
MS 26 *Molecular interactions in crystal packing and molecular assemblies*
MS 27 *Molecular interactions in nanocrystalline, disordered and amorphous compounds*
MS 28 *Applications of molecular crystals simulations*
MS 29 *Inclusion compounds and porous materials*
MS 30 *From hydrogen to halogen bonding: proton-against charge-transfer interactions*

MS31 *Supramolecular assemblies and crystal engineering*
MS32 *Self-assembled functional materials: biomineralization, biomimetics and beyond*
MS33 *Structure-properties relationship in molecular crystals*
MS34 *Structural studies on coordination chemistry*
MS35 *Transformation in crystals: from polymorphism to solid-state reactivity*
MS36 *Interactions and reactivity in small and large molecules*
MS37 *Charge density for understanding of chemical properties*

Focus Area 5: Experimental and Computational Techniques (SIG 6, SIG 8, SIG 9, SIG 10)

MS38 *Current trends in protein and small molecules crystallization and monitoring*
MS39 *Surfaces, interfaces and nanostructures*
MS40 *Micro- and sub-micro-diffraction*
MS41 *Magnetism by neutrons and X-rays*
MS42 *Time-resolved X-ray diffraction and spectroscopy in biology and chemistry*
MS43 *Charge Flipping*
MS44 *Software development, automation and validation*
MS45 *Recent developments in software for chemical crystallography*

Miscellaneous

MS46 *Crystallographic Teaching*
MS47 *Crystallography in Art and Archaeology*

Workshops

Pair-distribution Function, PDF-workshop
Date: 24. -27. August 2010
Chair: **Reinhard Neder** and **Wolfgang Donner**
FEE: 20 EUR

Mathematical and Theoretical Crystallography Satellite Conference
Minimal Surfaces, Aperiodic Structures, Geometric Algebra
Date: 27- 2 August 2010
Chair: **Massimo Nespolo**
FEE: 50 EUR

For further information, please refer to the MaThCryst website.

Workshop on High Pressure crystallography
Date: 02-04 September 2010
Chair: **Ronald Miletich**
FEE: 20 EUR

First impressions of Darmstadt re ECM26, by John R Helliwell

THE ECM26 Planning Committee met in Darmstadt on October 17th and 18th 2009 and comprised the Conference Chair, Prof Dr Hartmut Fuess and the Conference Secretary Dr Helmut Ehrenberg as Hosts along with the ECA President, Prof Santiago Garcia-Granda, the Immediate Past President, Prof John R Helliwell, and the Conference Organisation represented by Herr Felix Angermüller, Conventus.

Santiago and I stayed at the Welcome Hotel, where the Planning Meeting was held in the Newton Room, and is across the road from the Congress Centre, named Darmstadtium, after element 110, discovered by the GSI in Darmstadt (Figure 1).

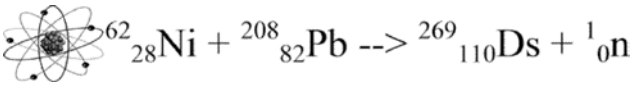


Figure 1. Darmstadtium (Ds = #110): On 9 November 1994 at 4:39 PM the first atom of the heavy chemical element with atomic number 110 was detected at GSI in Darmstadt, Germany.

During the Saturday afternoon we visited the Darmstadtium Congress Centre; some photos of the outside and inside are shown below in the Figures 2 and 3.

Figure 2. The Darmstadtium 'front-side'

Figure 3. The main entrance foyer of the Darmstadtium. Photographs courtesy of the Wissenschafts- und Kongresszentrum Darmstadt GmbH & Co. KG.

The Darmstadtium examples of lecture room names below again illustrate the strong way in which science is permeating the scene here.

2.01 carbonium
2.02 chromium
2.03 vanadium
2.04 titanium
2.05 palladium
2.06 argentum
2.07 aurum
2.08 platinum
3.01 oxygenium
3.02 hassium
3.03 germanium
3.04 europium
3.05 radon
3.06 xenon
3.07 argon
3.08 neon
3.09 helium
3.10 hydrogenium

There are large open plan spaces in the Darmstadtium and plenty of window-light for the Exhibition areas, the poster sessions and meal times.

The Welcome Hotel is the Conference Centre Hotel and has over 200 rooms (http://www.welcome-hotels.com/go/welcomehotel_darmstadt). The past-guest comments I saw on the internet were all giving very high scores across all categories and I concur completely. There is also a

Figure 4. The Darmstadt Rathaus and Beer Garden. Photograph courtesy of John Helliwell.

fitness/wellness suite on the 4th floor. Outside there is a pleasant garden and lawn, and it is opposite the now rebuilt theatre of Darmstadt.

A short walk into the Darmstadt city centre and one enters the olde worlde atmosphere of cobbled streets and traditional city hall, hotels and bars as well as a modern shopping centre.

The internet provides various photos of Darmstadt which feature a lot of cycling and bicycles. They are obviously enthusiastic about this in Darmstadt! There are various beautiful buildings in Mathildenhoehe, a Russian church also, “The Kiss” - mosaic in the Wedding Tower, etc etc:-

A few practical details. From Frankfurt Airport take the Airliner bus to Darsmstadt, and which takes 25 minutes:- Don’t do what Santiago and I did first and end up on the local i.e. ‘stopping bus’ to Darmstadt, which took 90 minutes, although at 3.70 Euros it’s cheap.

Where is Darmstadt? Obviously near to Frankfurt but also within easy striking distance of Heidelberg. Pre and Post Congress Tours will be available; details to be made available from ECM26’s managing agency, Conventus.

Control and Prediction of the Organic Solid State

CHARACTERISATION AND COMPUTATIONAL MODELLING OF COMPLEX BEHAVIOUR

ALL academic groups interested in characterisation of organic molecules in the solid state are invited to a one-day meeting on Monday 19th April 2010, at UCL. Guest speakers include Simon Billinge (Columbia University), Menno Deij (Avantium Technologies BV) and Paul Raithby (University of Bath). There will be ample time for networking, and contributions of posters from all interested academic groups will be welcome. Registration, via our website (www.cposs.org.uk), and lunch is free, thanks to sponsorship by members of the CPOSS Industrial Alliance.

cposs

Books

Diffuse Scattering and Defect Structure Simulations

A Cook Book Using the Program DISCUS
By **Reinhard Neder** and **Thomas Proffen**

SUPERFICIALLY at least, people come to cookery books for a variety of reasons: some simply feast on the glossy pictures; others enjoy the style of the writer whilst others might identify with the lifestyle that the book evokes. Ultimately, however, the long-term value of a 'cook book' depends on the quality of the recipes and the clarity of the instructions. It is therefore a somewhat bold move by Neder and Proffen to offer such a book in the field of diffuse scattering; will they succeed in drawing in readers, tempt them to experiment and give them something of lasting value? In this regard the style of the book clearly works. The layout - favoured by a number of OUP series - aids clarity, with pieces of coding script and figures largely confined to the generous page margins and the main text simply but effectively presented. Furthermore the authors have worked hard to integrate underlying principles with worked examples whilst, in the main, avoiding the book reading like a manual for a computer program. They also offer exercises, complete with solutions, at the end of each chapter and a CD containing the DISCUS program on which the book is based inside the back cover. They should be congratulated in producing a genuine cookery book dedicated to diffuse scattering.

Before reading this book, I was particularly interested in one thing. I wasn't expecting to take the practical route and get my teeth stuck into the program and work through all the examples, even though I knew that this was probably the way to get the most from the book. I wanted to see how well the authors explained structural diffuse scattering and whether this was a useful book as well as a good DISCUS manual. Diffuse scattering and defect structure are tricky areas of crystallography, often left to the aficionados (among whom I count the two authors), and entered into by others with some trepidation or only when their science leaves them with really no other option. Does this book treat its readers gently and give them the confidence to step into the world of diffuse scattering? The answer is a clear, 'Yes'; the authors consider most areas of defect structure (local defects, domain formation, stacking faults, structural modulations, nanocrystals etc.) in a manner that really works. The link between real and reciprocal space is maintained throughout the book, more often than not also aided by figures, and by using DISCUS examples at each step the book remains grounded and practical. The authors manage to explain why diffuse scattering is as it is and provide tools for taking the principles introduced in the book and applying them to real problems.

Inevitably there are a couple of areas where I would have liked to see more detail or the authors have omitted things that I would have liked to see included. For example, a greater coverage of the work using pair distribution function-based methods (such as PDFFIT and RMC) and a consideration of magnetic neutron diffuse scattering would undoubtedly have widened the readership. But perhaps this is unrealistic, after all perhaps the seminal text book on diffuse scattering, 'X-ray and Neutron Diffraction in Nonideal Crystals' by **M A Krivoglaz** was published over 20 years ago and ran (at least in the original Russian) to two volumes! It would therefore be somewhat churlish to criticise the authors for what they have omitted when what they have achieved is indeed a success. I would recommend this book to anyone who is studying interesting systems which display diffuse scattering and who wants to take their structural analysis beyond the Bragg peaks. This book is for you.

David Keen, ISIS Facility
January 2010

Dr Andrew Booth (1918-2009)

Dr Andrew Booth (1918-2009)

Booth: an Initiator of Crystallographic Computing

Andrew Booth, who died recently in Canada, was a confident inventor and pioneer in crystallographic computing. Photograph courtesy of Lakehead University.

BOOTH'S wartime crystallography PhD in EG Cox's Department at Birmingham (despite an unexploded bomb in the X-ray lab one morning) was supported by the British Rubber Producers Research Association (BRPRA, later Malaysian RPRA and Tun Abdul Razak Research Institute) where he was on the Physics staff. He worked there on an automatic analogue structure factor summation machine and other computing devices and devised the three-dimensional section Fourier synthesis. After the War, BRPRA sponsored research on digital computation, directed by **JD Bernal** (returning to a battered Birkbeck), who encouraged Booth to survey computer developments at Harvard and elsewhere in the US; he met **Von Neumann**, for example. Bernal wanted this 'very bright Fourier merchant' as much for physics and engineering (Booth had been a graduate apprentice in Birmingham) as for his crystallography as part of the aim to establish a Biological Centre. During 1946-7 at Princeton, Booth completed the compact comprehensive Fourier Technique in X-ray Organic Structure Analysis (Cambridge, 1948) (acknowledging **J Wilson**, Director of BRPRA until 1947, and Cox). This monograph assumed prior crystallographic knowledge but encompassed isomorphous series, Pattersons, differential syntheses, series termination corrections, and mechanical and electro-mechanical calculators, several of which Booth had invented. **George Jeffrey**, who wrote that Booth 'knew it all but not unpleasantly', failed to complete an intended experimental chapter, having left BRPRA for Leeds in 1945.

Using space at BRPRA and the Royal Institution as well as bomb-damaged Birkbeck, and assisted by the mathematician **Kathleen Britten** (later Professor Mrs Booth), Booth developed the first 2 in cylindrical magnetic storage drum (now at the Science Museum). In 1949, the computer group moved into an empty former static water tank and there followed ARC, SEC and, in 1951, the All-Purpose X-ray Computer for crystallographic calculations. At the X-ray Analysis Group (precursor of the BCA) Conference in London, 16/17 November, 1956, Booth assessed the computing needs for large-molecule crystallography (report B J Appl Phys 9, Jan, 1958). Conviction about the value of X-ray molecular structure determination and rapid computing led the energetic and largely unsung Wilson (1890-1976), later director of the Rayon and Synthetic Fibres RA, to support early computer construction, overseen by Booth, at both rubber and rayon institutes. Booth set up the Electronic Computing Research Lab in 1957, but left Birkbeck in 1962 for the University of Saskatchewan in Canada. He was later President of Lakehead University in Ontario, before retirement to British Columbia in 1978.

Derry W Jones
University of Bradford

Cambridge Crystallographic Data Centre archives 500,000th crystal structure

ON 10th December 2009 the Cambridge Crystallographic Data Centre (CCDC) proudly announced an important milestone in the history of crystallography - the archiving of the 500,000th small molecule crystal structure to the Cambridge Structural Database (CSD).

Professor Sir **David King**, former Chief Scientific Adviser to the UK Government, and Chairman of the CCDC Board of Governors 1998-2000, notes that *"The timely development of CCDC and the Cambridge Structural Database from very humble beginnings 45 years ago to become the key global source for crystal structures makes a remarkable story. The user-friendliness and versatility of the database has become the major resource for the chemical and pharmaceutical industries, and in the process has transformed their capability".*

Information derived from small-molecule crystal structures is vital to structural chemistry research in its broadest sense, and in particular to pharmaceutical drug discovery, materials design, drug development and formulation. The database is also a rich resource for teachers and has application across the entire span of the chemistry curriculum. There are clear indications that this knowledge will be equally vital in the development of future materials, such as gas-storage systems, and will play a key role in the development of nano- and green-technologies.

Dr **Colin Groom**, Executive Director of the CCDC says that *"the determination of 500,000 crystal structures is a remarkable achievement. However, the scientific community is hungry for the next 500,000 and the knowledge these will undoubtedly bring. As the CSD grows both in size and in the complexity of structures it contains, the database not only helps us to answer our questions about molecular structure and interactions, but tells us what those questions should be".*

The CSD's 500,000th structure is the anti-convulsant drug Lamotrigine, published in Acta Crystallographica, C65, o460-o464, 2009, by **Balasubramanian Sridhar** and **Krishnan Ravikumar** of the Indian Institute of Chemical Technology in Hyderabad. The CSD reference code for the structure is EFEMUX01. Lamotrigine (Lamictal®) was discovered by GlaxoSmithKline and approved by the US FDA for the treatment of epilepsy in 1994 and additionally for the treatment of bipolar I disorder in 2003. Lamotrigine is chemically unrelated to other anticonvulsant or mood regulating medications, and is distinguished by its relatively benign side effects.It is frequently effective in patients who have not responded to antidepressants or other mood stabilisers.

The CSD contains chemical structure information on several close variants of the compound, all of which, when used together, provide invaluable information to the life sciences community in their quest to optimise the efficacy of such medicines.

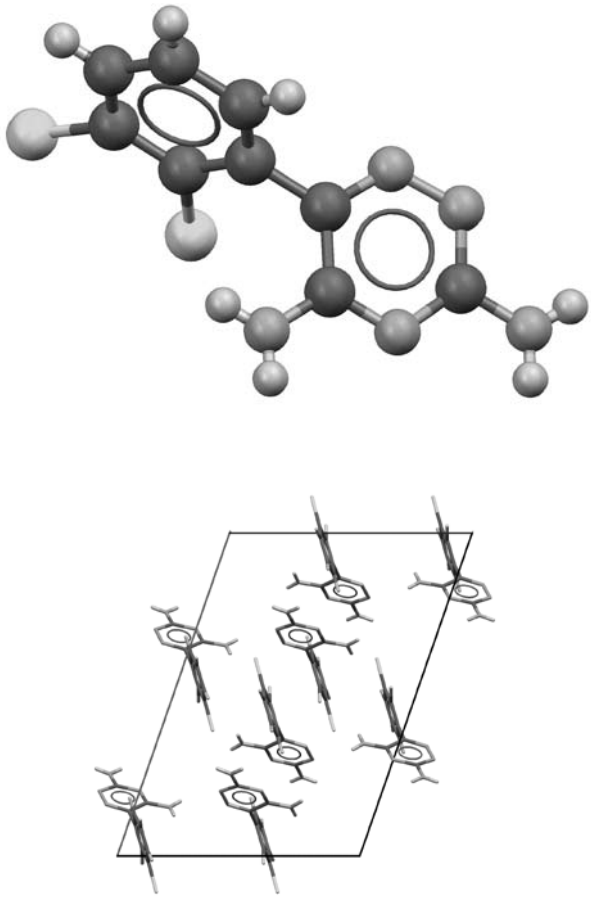


Fig. 1 Crystal structure of Lamotrigine (CSD reference code EFEMUX01). The structure can be viewed using WebCSD - the online search interface to the CSD at **www.ccdc.cam.ac.uk/halfmillionthstructure**

Gary M. Battle
Cambridge Crystallographic Data Centre

The Fankuchen Award

WE are delighted to learn that David Watkin (pictured left) will receive the 2010 Fankuchen Award from the American Crystallographic Association. This prize was established in 1971 in memory of Dr. Isidor Fankuchen (pictured left below), Professor of Physics at the Polytechnic Institute of Brooklyn from 1942 to 1964. Born in Brooklyn in 1904, as a young man Fankuchen earned his living by repairing and installing radio sets. (His obituary does not record whether these were crystal sets.)

After obtaining a BSc from Cooper Union and a PhD from Cornell University he spent a year in Manchester working on crystal structure determination by Patterson methods at the invitation of **W. L. Bragg**, followed by two years at Cambridge where he took part in early virus crystallography. Returning to Brooklyn, during his long career he established a reputation as "the Apostle of X-ray Diffraction", admired by his regular students at the Polytechnic Institute and those at the "summer clinics" he held. He also published 95 papers and became the first American Co-Editor of *Acta Crystallographica*. His outstanding accomplishments in both teaching and research are reflected in the prize that bears his name, and who could be a more suitable recipient than David? Because it is only awarded every three years and there are no geographic or age restrictions, this recognition is a very high honour indeed.

Seizure: Crystals in Modern Art

ALTHOUGH crystals are a means to an end for crystallographers, most of us still pause for a moment to admire a particularly beautiful specimen that appears under the microscope. The success of jewellers through the ages proves that macro-sized crystals have even wider appeal. Recently crystals played an essential part in a work, unexpectedly bearing the name "*Seizure*", nominated for that high-profile celebration of modern art, the Turner Prize.

In its introduction to the nominees for the 2009 Turner Prize the www.tate.org.uk website describes one of the nominees, **Roger Hiorns**, as follows: "Hiorns creates arresting sculpture and installation combining unusual materials. His exploration of chemical processes took spectacular effect in *Seizure*, in which a derelict flat in South London was filled with liquid copper sulphate, which after a period of time encrusted every surface of the space with blue crystals. Roger Hiorns has been nominated for his solo exhibition at Corvi Mora, London and for *Seizure, Artangel commission*, Harper Road, London."

We have **David Watkin** to thank for sending in the photographs of this installation taken by **Keith Waters**. David and his cultured coterie of art-lovers viewed the exhibition in London just before Christmas. This work was created by pumping 75,000 litres of $CuSO_4$ solution into an abandoned bed-sit, eventually leaving it entirely covered with crystals of copper sulphate - some several inches long. What interested David was that by and large, the long physical axis to the crystals pointed downwards. Sadly, this entry did not win but was a runner-up; and no more of us can see it because, according to David, it has subsequently been broken up.

I am left pondering a question. If this installation were re-created aboard the International Space Station, would the crystals point every which way?

Carl Schwalbe

Customs Absurdistan

Customs Absurdistan: with Crystals to America

EVERYBODY knows that education and research are highly valued in Germany, especially by politicians during election campaigns. To be sure, perspectives change at 1 minute after the close of voting, but we scientists have long since become accustomed to it. Notwithstanding that fact, we try our best, as is fashionable, to achieve new discoveries by interdisciplinary and international efforts, in large federations, clusters and focus areas whenever possible, since individual research is no longer worth anything. A certain Mr. Einstein, who came upon the theory of relativity in the loneliness of his Berne patent office, would not be worthy of any support today.

Being aware of this, a while ago we applied for synchrotron beam time on the Small Molecule Beamline of the Advanced Photon Source (APS) at Argonne near Chicago, which has an outstanding reputation for high-resolution experiments in electron density research (and which was later confirmed in every respect). Naturally, as with all large research facilities, a project application was required. In the ranking that is customary in the United States it was awarded the top grade and even brought us a bit more beam time than we had requested. Thus our proposal cannot have been all that bad.

Now it is well known that in order to measure crystallographic data one needs crystals, and here the real problem started. We had prepared quite a few samples of more than 20 compounds. In view of the strict security measures, especially for air travel to the USA, we did not dare to take along our samples in checked baggage and certainly not in hand luggage. Therefore we hired a courier service to ship by air freight to Argonne everything that we thought we needed (crystals, preparation tools, glassware, sample holders, etc.). For a halfway acceptable fee this was all supposed to happen within a few days. “Supposed to”, because on the outward journey the customs office intervened, this time the American customs. We first learned that our freight had an inadequate declaration. We had truthfully declared that the contents were “non toxic”, “non explosive” and “harmless”, but now we made the effort to describe every single compound by structural formula and properties. However, this was still insufficient because we had neglected to give a valuation. That could not be. One is not allowed to bring anything into the United States that lacks commercial value. Now we had to think about the price of the few crumbs that we or our preparative colleagues had produced. We could easily have come up with a value of zero since surely nobody would want to buy our crystals from us. Instead we began to guess the value of the chemicals that were used to synthesise our samples, added the price of the glassware and other equipment and with a good conscience arrived at a figure which the American customs finally deemed satisfactory. After several telephone calls across the Atlantic (many thanks to the people from the courier service for their very professional help with this!) our freight was released and still landed on the desk of our APS beamline scientist before we arrived.

Following this first act there naturally had to be a second, since our stuff had to go back again. Therefore we turn to the courier service once again, this time immediately giving a non zero valuation. In spite of this, the German customs grab our package, and now their intention to collect some duty becomes truly absurd. First we point out that we have not imported any wares from the USA, but that it just involves our own property, or that of our own university, which we brought to the USA a couple of days ago. We are informed that this would make no difference. If this were to be taken into account, we should have kept our shipment sealed up while in the USA and sent it back unopened. We object that under these conditions we could not have measured our crystals in Argonne, and our trip would have been pure tourism, which in view of the travel costs would surely have displeased our employer. However, for the customs that is not relevant.

Now our valuation is also questioned. We should accurately report the quantity of our samples. Stupidly we did not previously weigh them. Our entry of a few milligrams per sample is not sufficient for the customs. In an attempt to help us out of this difficulty, we are advised that the valuation could also be derived from the number of items. We confess, by now barely audibly, that we also have never counted our crystals, and that with dimensions in the tenths or hundredths of a millimeter per crystal we cannot reliably estimate how many crystals there are in a few-milligram sample. It must be a few hundred to a few thousand.

We don’t know what to do next. Now the customs officers take action with a firm hand. Our old valuation is suddenly at the races once again. From it an official customs duty in high Euro double figures is calculated and sent to us as a bill. Cautiously we ask our legal staff if we can use resources from the University’s budget to pay it. As soon as the word “Customs” is mentioned, with a wave of the hand they advise “Pay up and shut up.”

Therefore we pay duty for things that were never manufactured or modified abroad, have no commercial value and have always been the property of a German government institution (our university). Absurd, or what?

My advice: if you intend to do something similar, first learn about international customs regulations or leave your crystals at home!

P.S.: To our relief, we obtained outstanding data at Argonne.

Peter Luger, FU Berlin

Translated by Carl Schwalbe

Meetings of interest

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

3-5 March 2010
Dynamics in Confinement, Grenoble, aFrance
http://www.ill.eu/news-events/events/confit2010/

3-5 March 2010
EMBO Workshop on Visualizing Biological Data, Heidelberg, Germany
http://www.embl.de/training/courses_conferences/conference/2010/VIZ10-01/

8-12 March 2010
International Collaboration on Advanced Neutron Sources (ICANS-XIX), Grindelwald, Switzerland
http://www.iucr.org/news/notices/meetings/meeting_2009_127

11-13 March 2010
Sixth International Workshop on X-ray Radiation Damage to Biological Crystalline Samples, Stanford Synchrotron Radiation Laboratory, Stanford, USA
http://smb.slac.stanford.edu/news/workshops/rd6/index.shtml

11-19 March 2010
31st Berlin Neutron Scattering School, Helmholtz Centre, Berlin, Germany
http://www.helmholtz-berlin.de/events/neutronschool/

15-17 March 2010
Polymorphism & Crystallisation 2010, London, United Kingdom
http://www.polyandcrys.com/Event.aspx?id=244544

15-17 March 2010
High-Resolution X-ray Spectroscopy: Past, Present, and Future. Symposium, Utrecht The Netherlands
http://www.sron.nl/index.php?option=com_content&task=view&id=2156&Itemid=1986

15-19 March 2010
International Centre for Diffraction Data, Spring Meeting, Newtown Square, PA, USA
http://www.icdd.com/

17-19 March 2010
NOP2010. International Workshop on Neutron Optics, Alpe d'Huez, France
http://www.ill.eu/news-events/events/nop2010/

18-20 March 2010
Discussions in Structural Molecular Biology, Nove Hrady, Czech Republic
http://www.structbio.eu/Current_Meeting.html

21-25 March 2010
American Chemical Society Spring 2010 National Meeting & Exposition, San Francisco, CA, USA
http://www.acs.org/meetings

27-31 March 2010
Small-Angle Scattering Short Course 2010, "Beyond RG", Argonne, IL, USA
http://small-angle.aps.anl.gov/courses/short_course_2010.html

7-10 April 2010
POLYCHAR18. World Forum for Advanced Materials, Siegen, Germany
http://www.uni-siegen.de/fb8/polychar18/

12-13 April 2010
Young Crystallographers satellite meeting, University of Warwick
http://www.chem.gla.ac.uk/yc/

13-15 April 2010
BCA Spring Meeting: Data Matters, University of Warwick
http://www.crystallography.org.uk/

18-22 April 2010
PCG Rietveld School, Durham
http://www.crystallography.org.uk/

18-23 April 2010
Adsorption, Absorption and Crystal Growth, Gargnano, Italy
http://www.imem.cnr.it/deptecpro.html#cg

19 April 2010
CPOSS: Characterisation and Computational Modelling of Complex Behaviour
http:// www.cposs.org.uk/

21-25 April 2010
International Workshop DyNano 2010 "Structure and Dynamics of Nano-objects using short wavelength radiation ", Corsica, France
http://www.synchrotron-soleil.fr/Soleil/ToutesActualites/Workshops/2010/DyNano2010

26 April - 7 May 2010
School on Synchrotron and Free-Electron-Laser Sources and their Multidisciplinary Applications, Trieste, Italy
http://cdsagenda5.ictp.trieste.it/full_display.php?ida=a09142

28-29 April 2010
Data Analysis for Quasielestic Neutron Scattering with FRIDA, Garching, Germany
http://www.jcns.info/DataAnalysis2010

2-7 May 2010
European Geosciences Union. General Assembly 2010, Vienna, Austria
http://meetingorganizer.copernicus.org/EGU2010/sessionprogramme

2-7 May 2010
3rd ILL Annual School on Advanced Neutron Diffraction Data Treatment using the FullProf Suite, Grenoble, France
http://www.ill.eu/news-events/events/fpschool-2010/

12 May 2010
BCA Industrial Group XRF users' meeting, British Geological Survey. Keyworth, Nottingham
http://ig.crystallography.org.uk/ig.htm

13 May 2010
BCA Industrial Group minerals meeting, Between the Sheets! British Geological Survey. Keyworth, Nottingham
http://ig.crystallography.org.uk/ig.htm

24-28 May 2010
ISC. 2nd Granada International School of Crystallization: Foods, Drugs and Agrochemicals, Granada, Spain
http://www.iscgranada.org/

24-30 May 2010
Diffraction at the Nanoscale Nanocrystals, Defective & Amorphous Materials, PSI Villingen, Switzerland
http://user.web.psi.ch/powder2010/

25-28 May 2010
ISDSB 2010. 3rd International Symposium on Diffraction Structural Biology, Paris and Orsay, France
http://www.synchrotron-soleil.fr/Workshops/2010/ISDSB

3-13 June 2010
International School of Crystallography. 42nd Course: Structure and Function from Macromolecular Crystallography: Organisation in Space and Time. Erice, Sicily
www.crystalerice.org/erice2010/2010.htm

6-11 June 2010
Gordon Research Conference in 'Crystal Engineering', Waterville Valley, NH, USA
http://www.grc.org/programs.aspx?year=2010&program=crystaleng

7-11 June 2010
Fundamentals of X-ray Powder Diffraction, ICDD Headquarters, Newtown Square, PA, USA
http://www.icdd.com/education/xrd.htm

7-11 June 2010
Graduate Course - Neutron Scattering techniques in Structural Biology, Oak Ridge National Laboratory, TN, USA
http://neutrons.ornl.gov/conf/gcnb2010/

8-11 June 2010
COHERENCE 2010. International Workshop on Phase Retrieval and Coherent Scattering, Rostock-Warnemünde, Germany.
https://indico.desy.de/conferenceDisplay.py?confId=2327

14-18 June 2010
Advanced Methods in X-ray Powder Diffraction, ICDD Headquarters, Newtown Square, PA, USA
http://www.icdd.com/education/xrd.htm

21-24 June 2010
IWPCPS12. Twelfth International Workshop on Physical Characterization of Pharmaceutical Solids, Lille, France.
http://www.assainternational.com/workshops/iwpcps_12/iwpcps_12.cfm

21 June - 2 July 2010
MathCryst Summer Schools: Topological Crystal Chemistry & Irreducible representations of space groups, Nancy, France
http://www.crystallography.fr/mathcryst/nancy2010.php

26-28 June 2010
ECRS-8 - the 8th European Congress on Residual Stresses, Riva del Garda, Italy
http://events.unitn.it/en/ecrs8

4-9 July 2010
IZC16 and IMMS7. 6th International Zeolite Conference and 7th International Mesostructured Materials Symposium. Engineering of New Micro- and Meso-Structured Materials, Sorrento, Italy.
http://www.izc-imms2010.org/index.php

5-8 July 2010
MOLMAT2010. IVth International Conference on Molecular Materials, Montpellier, France
http://www.molmat2010.fr/

5-8 July 2010
PNCMI2010: 8th international workshop on Polarised Neutrons in Condensed Matter Investigations, Delft, The Netherlands.
http://www.tnw.tudelft.nl/live/pagina.jsp?id=3f2f14d1-c18b-4276-aa94-90d5d52fc337&lang=en

5-9 July 2010
Combined Analysis Using X-ray and Neutron Scattering, Caen, France.
http://www.iucr.org/news/notices/meetings/meeting_2009_222

11-14 July 2010
7th International Conference on Synchrotron Radiation in Materials Science (SMRS-7) and 6th International Conference on Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation (MEDSI), Oxford.
http://www.diamond.ac.uk/Home/Events/MEDSI.html

11-16 July 2010
Gordon Research Conference in 'Electron Distribution & Chemical Bonding', South Hadley, MA, USA
http://www.grc.org/programs.aspx?year=2010&program=elecdist

18-23 July 2010
Gordon Research Conference in `Diffraction Methods in Structural Biology', at Bates College, Lewiston, Maine, USA. Chair: Andrew Leslie. Co-chair: Ana Gonzales.
http://www.grc.org/programs.aspx?year=2010&program=diffrac

24-29 July 2010
American Crystallographic Association Meeting, Chicago, Illinois, USA
http://www.amercrystalassn.org//meetingspg_list/futuremeetings.html

21-27 August 2010
20th General Meeting of the International Mineralogical Association, Budapest, Hungary
http://www.ima2010.org/

22-26 August 2010
240th ACS National Meeting & Exposition, Boston, MA, USA
http://portal.acs.org/portal/acs/corg/content

23-27 August 2010
FEL 2010. 32nd International Free-Electron Laser Conference, Malmö, Sweden
http://fel2010.maxlab.lu.se/

27-30 August 2010
EPDIC12. 12th European Powder Diffraction Conference, Darmstadt, Germany
http://www.epdic12.org/

27-29 August 2010
MaThCryst Satellite Conference of ECM26, Darmstadt, Germany
http://www.crystallography.fr/mathcryst/darmstadt2010.php

29 August - 2 September 2010
26th European Crystallographic Meeting, Darmstadt, Germany
http://www.ecm26.org/

5-10 September 2010
BCA/CCP4 Summer School XV, Oxford.
http://crystallography.org.uk/bca-ccp4-summer-school-2010

20-23 September 2010
XTOP2010, the International Conference on High-resolution X-ray Diffraction and Imaging. University of Warwick, UK
http://www2.warwick.ac.uk/go/XTOP2010

3-4 November 2010
BCA Industrial Group Autumn Meeting, Diamond Light Source, Harwell
http://ig.crystallography.org.uk/ig.htm

25-29 August 2013
28th European Crystallographic Meeting, University of Warwick
http://www.crystallography.org.uk/

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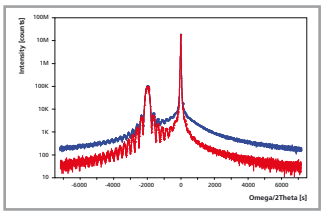

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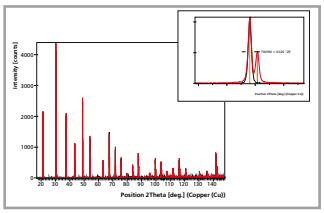

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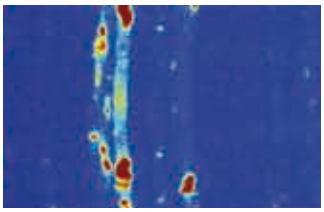

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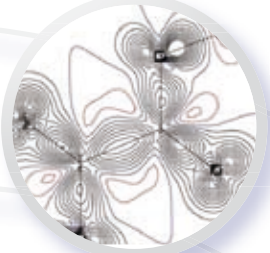

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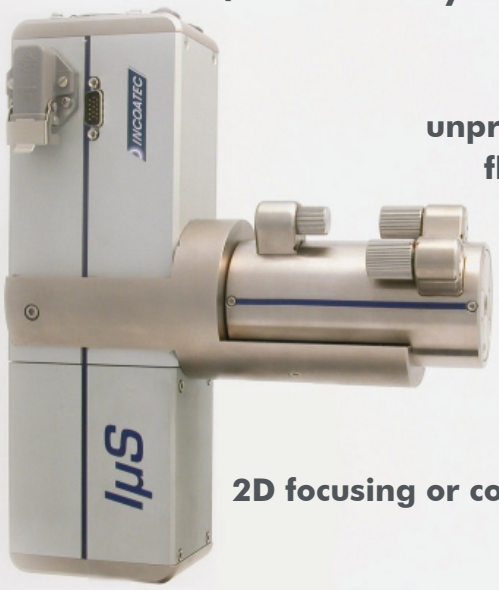

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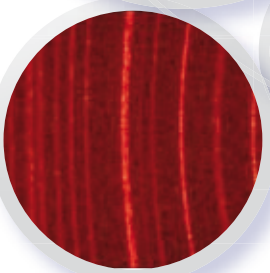

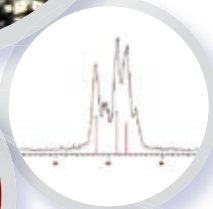

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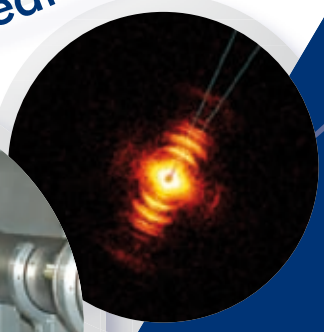

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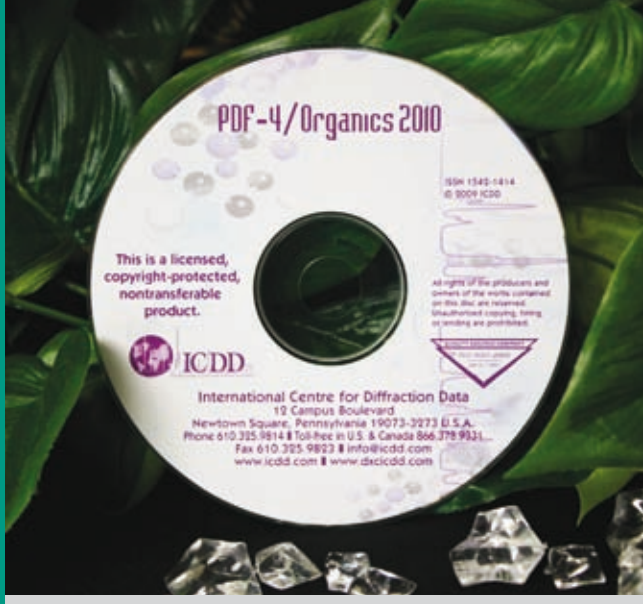

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