

# *Crystallography News*

British Crystallographic Association



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## **BCA Spring Meeting 2007 - Canterbury** p8-15



**ECM Meeting** p16-19

**ACA - Honolulu** p21-22

**Awards of Medals** p25-26

**Meetings of Interest** p27



# Contents

From the President .....	2
Council Members .....	3
From the Editor .....	4
From Professor P Dolding Beedle .....	5
Puzzle Corner .....	6
Peter Main - Honorary Fellow .....	6
BCA 2007 Meeting .....	8-13
BCA 2007 Meeting Timetable .....	14-15
ECM .....	16-19
Groups .....	20
ACA .....	21-22
Books .....	23
His Worship Moreton Moore .....	23
Obituary: Desmond Cunningham .....	24
Awards of Medals .....	25-26
IUCr Wins Award .....	26
Meetings of Interest .....	27



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## *This month's cover:*

*Next year's Spring Meeting, in Canterbury, provides a contrast with this year's ACA in Honolulu.*



# From the President



**WHEN** you read this the Christmas vacation will be approaching rapidly so let me add my very good wishes for the festive season and wish you a peaceful and prosperous New Year.

This is my first chance to report on the ECM23 Leuven Meeting. I think that all who attended

will agree that it was a very successful and enjoyable meeting. At the Meeting **John Helliwell** was elected to the Presidency of the European Crystallographic Association, and I am sure that you would wish to join me in congratulating him on this prestigious appointment.

On the home front, the BCA Council met in September and discussed a wide range of issues pertaining to the development of the Association. For the future, perhaps the most important development is that it has been proposed that the "Young Crystallographers" are established as a separate "group" within the BCA. This will allow them to set up their own meetings and contribute to the BCA in a number of very positive ways that will strengthen the organisation. Secondly, I am particularly pleased that the Council has agreed that the BCA should formally elect an Education Officer who will sit on Council and be responsible all educational matters in which the BCA is involved. In this context, I am delighted to report that **Chick Wilson** who has been looking after education matters has organised a Brains Trust of eminent crystallographers who have agreed to go out and present lectures on crystallography to university science societies,

schools and colleges. The current members of the Brains Trust are **Mike Glazer, Elspeth Garman, Bill David, Garry Taylor,** and **Chick Wilson** himself. We are most grateful to them for giving up their very valuable time. If you would like to book any of them to give a talk at your institution please get in contact with Chick in the first instance.

As you will see later in this issue of Crystallography News Lindsay Sawyer and his team have done a splendid job organising the programme for the BCA Spring Meeting to be held at the University of Kent at Canterbury from 16-19 April, 2007. In addition to an outstanding list of "Named" and "keynote" lecturers there are sessions that should have something to spark everyone's interest. This year, we welcome back the X-Ray Fluorescence community who will be running parallel sessions throughout the meeting. As last year, the Young Crystallographers will be running a satellite meeting before the main meeting and this year we have the "Motherwell Event" to recognise **Sam Motherwell's** outstanding contribution to crystallography over the last four decades. I went on the site visit to Canterbury during the Summer and found it to be a very pleasant environment for the Meeting. So I encourage you all to come along and help to celebrate our 25th Anniversary Meeting.

Finally, at the AGM, at the Spring Meeting, we have to elect a new Vice President, and Secretary, as **John Finney** and **Christine Cardin** are coming to the end of their terms of service. So the Council officers and I look forward to receiving nominations for these key vacancies of Vice-President, Secretary and the new formal post of Education Co-ordinator.

**Paul Raithby**



# BCA Council 2006-07

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



## BCA Corporate Membership

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

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

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

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

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# From the Editor



**WELCOME** to issue 99 of *Crystallography News*! As we celebrate 25 years of the BCA, we will be seeing Issue 100 of this journal, which, like the BCA itself has grown and evolved greatly since 1981. We hope to have some special articles to celebrate this landmark, and suggestions would – as always – be most welcome!

Much of this issue is concerned with the Spring Meeting, and a considerable part of the details of the lecture programme as well as the overall timetable will be found around the centrefold. We are grateful to all those who have worked to get this information together, particularly the programme chair **Lindsay Sawyer**. The photographs of Canterbury were kindly supplied by **Jim Higham** of the University of Kent, and if you would like to see more photographs of this beautiful city and area, we recommend his website: [www.photoboxgallery.com/68220](http://www.photoboxgallery.com/68220)

We are also grateful to the **Arnold Beevers** Bursars who have written up their experiences at the ECM and the ACA. The standard of these reports is high, and they provide very refreshing insight into the parts of meetings other reports don't reach!

We are glad to say that our eponymous – and presumably pseudonymous – correspondent **Professor Dolding Beedle** has surfaced again. Observant readers will note that he seems to have come to terms with nanotechnology at last. He might appreciate a quote we will not attribute: "I didn't know a nanogram was so small – perhaps that's why it isn't always able to detect breast cancer!"

Also, the far from pseudonymous **Howard Flack** has not only sent his reply to a question raised about "arithmetic crystal classes", he has also kindly taken over Puzzle Corner for this issue. Howard is one of the few people we have come across who may be better known as a parameter than as a person, so we have included a photograph, which hopefully hasn't been inverted in the process.

**Henk Schenk**, former President of the IUCr, has an amusing demonstration in which a brick marked "crystallography" sits proudly atop the biology, chemistry, geology and physics bricks. Then, lest one gets too proud of being a central science, he shows what happens when funding becomes short. Crystallography gets many cack-handed compliments, but the headline in the November *Chemistry World* takes some beating. Commenting on the award of the Nobel Prize in Chemistry to **Roger Kornberg** for his work on DNA transcription, its headline reads: "Call that chemistry? This year's Nobel prize in chemistry was a *tour de force* for crystallography, underscoring the vital role chemistry plays across the sciences..." Maybe chemistry should have a turn at being the brick that falls into the hole!

And with that, we'll join the president in wishing all our readers a Happy Christmas and A Good New Year!

**Bob Gould**



# From Prof. P Dolding Beetle

## Building a Better Beamline User

**DESPITE** the brilliant promise of nanotechnology, reported in a previous edition of *Crystallography News*, the hoped for advances in nanobots necessary to replace central facilities have not arrived in the time expected.

Thus, for the short term at least, central facilities will play a useful place in world science, and the continuing evolution of ever higher brilliance sources, such as Diamond and the ISIS Second Target Station, with their emphasis on building high-flux beamlines that enable ultra fast data collection is laudable. It is, however, highly flawed, since improvements in the efficiency of utilisation of such sources has not kept up. Her Majesty's neutrons and photons cannot be wasted, and improvements in this area are long overdue. Unimaginative types might suggest the use of high reliability automation and high performance equipment, controlled via heartless, metal machines. But such a mundane approach lacks the necessary vision for the transformative science that will be required in the coming millennium. It has rightly been rejected at most modern X-ray synchrotron beamlines, where, thankfully, the mechanical and engineering talents of the users are still essential to build the beamlines when they arrive. Automation also removes the high drama of manual sample changing and the fascinating typing in of arcane command languages that is the most important and challenging part of beamline usage.

A second, previously unexplored, possibility will require people to perform at ever-increasing speeds and reliabilities, well beyond that of even exceptional current humans. However, using recent advances in the field of dance-rave technology, cheap, bathtub-made chemicals can be used to mould an improved synchrotron user. Despite the obvious benefits, under present European legislation, it would be illegal and highly unethical to use humans during the testing stages of this concept. Animal models capable of accurately describing both the physiological response, and the social behaviour of humans in a central facility are required. *Crystallography News* is an appropriate forum to report the findings of a preliminary EPSRC, ESRC and CCLRC-supported study, concentrating on the social response of users to psychoactive therapy, involving two thousand specially-trained howler gibbons, between the ages of 20 and 50, who modelled the response of a typical user program.

Troops of howler gibbons were released en masse into existing multi-beamline X-ray and proton synchrotrons. A small proportion of senior silverback gorillas, that closely model the response of the more distinguished users in the scientific community, were simultaneously released. Variable quantities of amphetamines were supplied to them in an effort to determine the optimal doses required both to

enter long streams of obscure Unix commands into control computers and to align single crystals within the millisecond time scales demanded by modern instrumentation. The silverbacks tended to take smaller doses, and it was observed that they were less physically active at the central facilities than the howlers, although a large retinue of more active, and naturally inquisitive, junior gibbons typically surrounded them. When suddenly removed from their natural environment of remote ivory towers and unnaturally confined in a synchrotron, silverbacks spent large quantities of time pacing apparently aimlessly in circles around the ring. When one of them sighted a rival silverback, a violent display of snarling, chest beating, and fake charging was frequently observed, as they attempted to determine which was dominant. Both silverbacks usually ended up withdrawing into their hutches without significant physical damage.

The silverbacks typically had access to more and higher quality food than the junior howler gibbons, which fought over the scraps remaining after the silverbacks had finished eating in the cafeteria. The gibbons were often highly active at night, when they were usually abandoned at the beamline by the silverbacks, and primitive hunter-gatherer behaviour was observed among them particularly in the vicinity of the few functioning vending machines. One particularly thorny question was of the right animal model for beamline staff. Eventually, the three-toed sloth was found to provide the best model. The sloths typically consumed no amphetamines at all, and were observed clinging motionless to comfortable chairs in the coffee lounge for hours at a time, or occasionally performing highly technical tasks on the beamline at imperceptibly slow rates of motion. Typical interactions between howlers and sloths saw the howlers emitting loud vocalisations associated with animated facial expressions and agitated body motions, while the sloths either stared blankly in return, or blinked very slowly in apparently total incomprehension. Subdivision of the howler gibbons into age classes was required during statistical analysis, since members of the younger age classes were frequently distracted by performing extended displays of elaborate courtship rituals, which tended to interfere with the concentration required during some of the more delicate experiments. A follow-on study has to address the interaction between amphetamines and the large quantities of alcohol consumed by this age class.

This promising, innovative avenue of research is soon expected to lead to better users, able to change samples at 100% reliability in milliseconds, disassemble and assemble ancillary equipment in seconds (that before took many hours), and analyse terabytes of data in minutes.

**Prof P Dolding-Beetle**  
**Nano-Innovation Platform for Primate Research Institute for Interdisciplinary Studies in Primate-Synchrotron Synergies**

# Puzzle Corner

GUEST EDITOR HOWARD FLACK



**INTERPRET** the following crystallographic sums:

- (a)  $92 + 65 + 73 = 230$  ( $11 + 11 + 10 = 32$ )  
(b)  $68 + 262 = 230$  ( $10 + 22 = 32$ )  
(c)  $207 + 22 + 1 = 230$

You have to answer (a) and (b) correctly to qualify for the prize. If anyone can answer (c) correctly, H. D. Flack has promised to contribute a complementary prize.

**FOLLOWING** the publication of the answer and results of the puzzle corner in the June 2006 issue of *Crystallography News*, there were some questions concerning space-group types and arithmetic crystal classes. These are clarified in the following paragraphs.

## Space groups and space-group types

The distinction between space groups and space-group types is the same as that between geometric crystal classes and crystallographic point groups. For the latter there are 32 geometric crystal classes but an infinity of point groups. A point group has the symmetry operations oriented in a specific and defined orientation. So an object with a two-fold rotation axis aligned along x has a different point group from one with the axis aligned along z. However these two point groups belong to the same geometric crystal class because they are equivalent to one another by rotation or rotoinversion. In like manner two crystals in Pmmm with cell dimensions  $a = 3, b = 5, c = 8$  and  $a = 7, b = 11, c = 13$  have different space groups but the same space group type. There are 230 space group types and an infinity of space groups.

## Arithmetic crystal classes

There are different ways of classify space group (types). One popular and useful way of doing this is to classify the space group by its geometric crystal class obtained by dropping all of the translational components in the symmetry operations composing the space group. These leads to 32 classes of space groups. Another way is to classify the space group by its Bravais lattice. This leads to 14 classes of space groups. If one classifies the space groups simultaneously on geometric crystal class and Bravais lattice, one obtains 73 classes which are known as the arithmetic crystal classes. H. Wondratschek has informed me that "arithmetic crystal class" seems to have been introduced by P. Niggli and W. Nowacki, "Der arithmetische Begriff der Kristallklasse und die darauf fussende Ableitung der Raumgruppen", *Z. Kristallogr.* 91 (1935) 321 - 335 (in German). "Geometric crystal class" appears to be natural if the term "crystal class" becomes ambiguous and the up to then unique "Crystal class" has to be specified.

## Peter Main – Honorary Member



**PETER**, who was chosen an honorary member of the BCA earlier this year, has been a member since our inception and a valuable and continuous member of the team that runs the CCG biennial school.

He was born in 1939 in Newbiggin-on-Sea. His B.Sc. and Ph.D. were from UMIST, where he began his research on Direct Methods with Michael Woolfson. He held a Post. Doc. at Purdue with

Michael Rossmann in 1964-67, and then joined Michael Woolfson in Physics at York in 1967; he is now a Professor of Physics there. He is probably best known as one of the developers of MULTAN and subsequent refinements thereof. MULTAN was one of the first programs that persuaded ordinary crystallographers that they could use direct methods. It is also a leading German industrial detergent and a large city in Pakistan, but Peter is not known to have connections with either of these. His current research is on improvements in electron density maps for proteins. Interested in cycling and music – he has cycled from Land's End to John O'Groats – he is normally a quiet man except when behind an organ console. He is married with three sons and one daughter.

**Bob Gould**

# BCA 2007 Spring Meeting

## Practical Information

**THE** BCA meeting starts at 11.30 on Tuesday 17 April, and concludes with a refreshment break at 15.00 on Thursday 19 April 2007. To enhance our already exceptional programme we are delighted to welcome back XRF and the Young Crystallographers to the University of Kent.

The XRF and XRD sessions will be integrated into the main scientific timetable and the Young Crystallographers session will commence on Monday 16 April. Following the successful **Mike Hursthouse** event organised in Lancaster this year we are pleased to announce that the **Sam Motherwell** lectures and dinner will follow the scientific programme on Thursday 19 April and will conclude at lunchtime on Friday 20 April. All scientific lectures including the Young Crystallographers and Sam Motherwell event will take place within the Keynes College Building.

We will have our traditional Commercial Exhibition, which will of course incorporate XRF and will be located within the dining hall of the Rutherford College. Due to the popularity of the Young Crystallographers session at the Spring Meeting in Lancaster the Commercial Exhibition will be open from 19.00 on Monday 16 April and will close after lunch on Thursday 19 April. As well as being open during all refreshment breaks delegates will have the opportunity to visit all stands during the poster and exhibition buffet dinner on Tuesday 17 April.

Registration and refreshment breaks during the main scientific programme will take place within the Rutherford dining hall, however registration and refreshments for the Young Crystallographers session on Monday 16 April and the Sam Motherwell event on Thursday 19 April/Friday 20 April will take place within the Atrium Foyer of the Keynes College Building.

For more information on the Exhibition and Sponsorship opportunities, or for any other enquiries about registration or accommodation, please contact **Elaine Fulton** at the BCA Administrative Office, 01355 244966 or email [bca@glasconf.demon.co.uk](mailto:bca@glasconf.demon.co.uk)

## Registration

### Early Registration Costs (before 12 March 2007)

<b>Full Registration</b>	<b>£150.00</b>
<b>Student/Unemployed/Retired</b>	<b>£75.00</b>
<b>Non-Member Surcharge</b>	<b>£30.00</b>
<b>One-Day Registration (no concessions)</b>	<b>£75.00</b>

### Late Registration Costs (after 12 March 2007)

<b>Full Registration</b>	<b>£200.00</b>
<b>Student/Unemployed/Retired</b>	<b>£75.00</b>
<b>Non-Member Surcharge</b>	<b>£30.00</b>
<b>One-Day Registration (no concessions)</b>	<b>£100.00</b>

**Accommodation**

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

<b>Standard B&amp;B</b>	<b>£30.00 per night</b>
<b>En-suite B&amp;B</b>	<b>£45.00 per night</b>

Accommodation is divided across three locations within the University campus. Standard accommodation is within the Rutherford College and en-suite accommodation is located within Keynes College and Becket Court. Breakfast and dinner will be served within the dining hall of the Eliot College.

Check- In time is from 14.00 and keys must be returned on day of departure no later than 10.00.

## Collection of Accommodation Keys

Delegates staying in Rutherford College collect their keys from Rutherford reception between the hours of 14.00 and 22.00.

Delegates staying in Keynes College collect their keys from Keynes reception between the hours of 14.00 and 22.00.

Delegates staying in Becket Court collect their keys from Eliot College reception between the hours of 14.00 and 22.00.

## Catering

Refreshments and lunch from Tuesday 17 April – Thursday 19 April will be served in the Exhibition area of the Rutherford Dining Hall. Refreshments and Lunch for the Young Crystallographers will be served within the Atrium Foyer of the Keynes College. Morning refreshments on Friday 20 April for the Sam Motherwell event will also be served within the Atrium Foyer of the Keynes College.

Breakfast and Dinner (including the Conference Dinner on Wednesday 18 April and Sam Motherwell Dinner on Thursday 19 April) will be served in the Eliot Dining Hall.

The Young Crystallographers Buffet Dinner on Monday 16 April and Poster and Exhibition Buffet Dinner on Tuesday 17 April will be served within the Exhibition area of the Rutherford Dining Hall.



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

<b>Packed Lunch</b>	<b>£6.00</b>
<b>Dinner on campus (Monday 16 April)</b>	<b>£15.00</b>
<b>Conference Dinner</b>	<b>£30.00</b>
	<b>£15.00 for concessions</b>
<b>Sam Motherwell Dinner</b>	<b>£15.00</b>

Please be aware that if packed lunches and evening meals are not selected on the registration form and paid for prior to attending the meeting it is the individual's responsibility to make alternative arrangements

## Social Events

On Tuesday 17 April, the poster and exhibition reception will be held in the early evening. Wine and a buffet meal will be served within the exhibition area. Delegates will have the opportunity to meet with the exhibitors and poster presenters in a relaxed and informal setting. There will not be an additional charge for attending this evening reception, however sponsorship is welcome.

The Conference dinner will be held on Wednesday 18 April in the Eliot dining hall at a cost of £30.00/£15.00 for concessions.

## Car Parking

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

## Email Facilities

Computer access will be available within the library at the University of Kent and wireless is also available in certain designated areas on campus. Logins must be purchased in advance on the registration form and are charged at £10.00 per login. More details regarding the wireless network at Kent University can be found on the Spring Meeting website [www.crystallography-meetings.org.uk](http://www.crystallography-meetings.org.uk)

## Abstract Submission

See details under Scientific Programme. All abstracts to be submitted to: [abstractbca@glasconf.demon.co.uk](mailto:abstractbca@glasconf.demon.co.uk)

## Deadline for poster abstracts

**Friday 16 February 2007** See details under Scientific Programme.

## BCA Bursaries

A limited number of bursaries are available from the Arnold Beevers bursary Fund to cover the cost of registration, two

nights **standard** accommodation, lunches from Tuesday 17-Thursday 19 April, evening buffet on Tuesday 17 and the Conference dinner on Wednesday 18 April. The bursary will not cover travel expenses and recipients will be expected to present a poster and produce a report on part of the meeting.

Council is again seeking commercial sponsors of Spring Meeting Bursaries at £175.00 per student and it is hoped that some Named Bursaries will be awarded at this meeting. Individual BCA members may also wish to give a living legacy by sponsoring their own named student bursary. All sponsors will receive a certificate of appreciation and be acknowledged in the annual bursary report.

The closing date for all applications is **Friday 16 February 2007**. Only on-line applications via the BCA website: [www.crystallography.org.uk](http://www.crystallography.org.uk) will be accepted.

## Insight into Canterbury, Kent

Canterbury, England's most famous cathedral city of Geoffrey Chaucer's Canterbury Tales and now a UNESCO world heritage site sits on the River Stour in one of the most attractive corners of rural Kent. It has been welcoming visitors for many years and provides the perfect backdrop for the 2007 Spring Meeting.

Canterbury is still very a popular destination with its many ancient buildings, shops, bars and restaurants and has retained both an old world charm and a cosmopolitan vitality.

The main campus at The University of Kent covers 300 acres and is located just over one mile from Canterbury's city centre.

## Travel Directions

### By Road:

#### To reach Canterbury from:

London: M2, A2 (56 miles; 89km) Dover: A2 (16 miles; 26km) Ramsgate: A253, A28 (18 miles; 29km) Ashford: A28 (14 miles; 22km) Maidstone (26 miles; 42 km) and Tonbridge (40 miles; 64km): M20, M2, A2. From the North or West: M25, M20, M2, A2

**Canterbury to the University:** Canterbury central ring road, A290 Whitstable Road, St Thomas Hill, approx 1 mile (1.6km) along the A290, University entrance on right (signposted) near top of hill.

The Visitors' car park on Giles Lane is a 'Pay and Display' car park. Parking elsewhere is very restricted and for permit holders only.

### By Rail:

#### Two rail routes from:

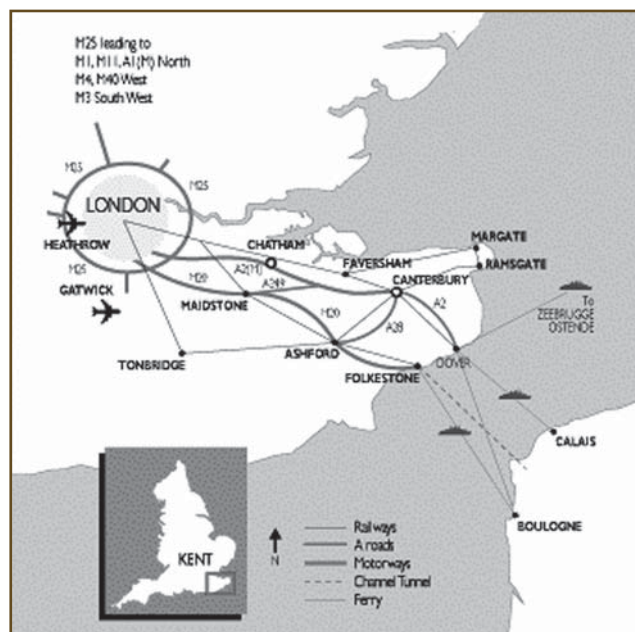
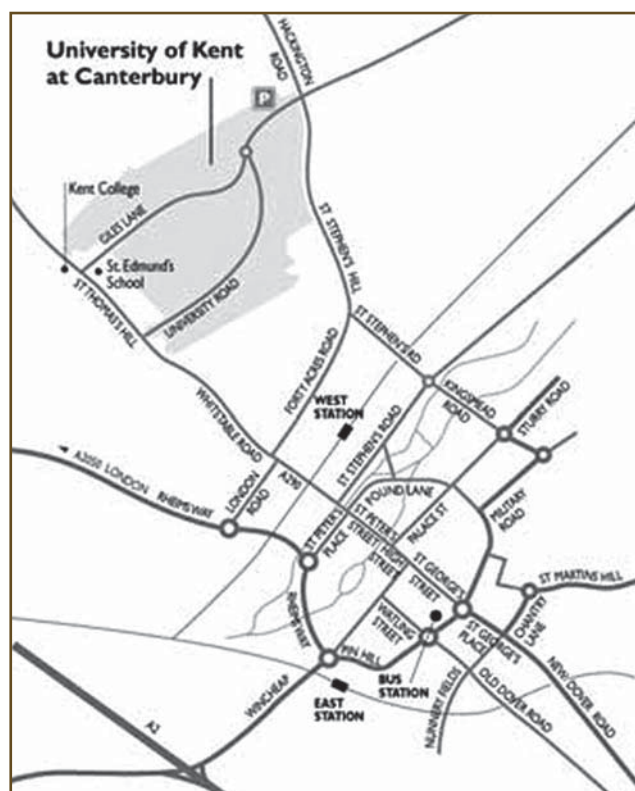
London (Victoria) to Canterbury East: Journey time approx 85 minutes. Mondays to Saturdays two trains an hour (one direct, one change at Faversham), Sundays – direct hourly service.

**London (Charing Cross or Waterloo East) to Canterbury West:** Journey time approx 90 minutes. Monday to Friday – direct hourly service through most of the day.

Taxis are available at both Canterbury stations.

**By Bus:**

Canterbury Bus Station to the University, regular bus service taking approximately 14 minutes. From Canterbury East follow path on City Walls to Bus Station (clearly visible by City Wall). From Canterbury West turn right out of the station, walk to main road, bus stop is on far side, approx 50 metres to left.



# Scientific Programme

## Spring Meeting Exhibitors Forum

**BECAUSE** of the continuing success of the Exhibitors Forum, presentation slots will be allocated on a strictly first come first served basis. However, those companies that select a 5 x 3 exhibition stand will automatically receive a dedicated slot on Tuesday 16 April prior to the exhibition and poster buffet.

The forum will provide each exhibitor with the opportunity to present their latest developments and encourage participants along to their stands in the Commercial Exhibition.

To register your interest in presenting, please contact Elaine Fulton at the BCA Administrative Office, 01355 244966 or email [bca@glasconf.demon.co.uk](mailto:bca@glasconf.demon.co.uk)

The overall theme for the meeting in April 2007 is “New Methods and Innovation”, a suitable portmanteau expression to cover the wide range of topics being dealt with this year. It is a pleasure to have the X-ray Fluorescence meeting running alongside that of the the Industrial Group and this year we have tried to arrange parallel sessions such that ‘discipline hopping’ will be possible, provided that Session Chairs keep their speakers in check! As ever, we hope that this will encourage interactions between the communities and make for a highly stimulating meeting.

We have continued the idea of keynote speakers, so successfully introduced last year, so that the four Keynote lectures should provide a chance for all of us regardless of our specialist interests to enjoy what are the hot topics in others’ fields. The Teaching Keynote this year is provided by Chick Wilson and will deal with thermal motion, something all of us have to consider. From the high fat content of the title, no doubt owing much to the geographical background of the speaker, we can look forward to an energetic presentation. The “Young Crystallographers” satellite meeting is with us once again and several slots exist in the main programme for them to share their results with the wider community. The Exhibitors’ Forum is designed to give our Exhibitors the chance to provide short, meaty presentations of their latest developments covering, as they do, both hardware and software, and fitting in nicely with the overall theme.

## Scientific Sessions

The sixteen scientific sessions spread over the two and a half day duration of the meeting contain a mouth-watering selection of topics. We decided this year not to have any specific workshops although time is available both before and after the main meeting should any wish to hold one. There is, however, a special event being organised by Frank Allen to honour Sam Motherwell in recognition of his considerable contribution to crystallography throughout the years. This year we are delighted to have three BCA named lectures, the Bragg, the Hodgkin and the Lonsdale Lectures

with recipients well known to us all. If you wish to attend any of the Motherwell event, please be sure to tick the relevant box on the main meeting registration form.

Thanks to the efforts of the programme committee and the session chairs the detailed scientific programme is nearly complete, and on the following pages the planned sessions and agreed speakers are outlined. We have once again managed to recruit a goodly selection of invited speakers from overseas so that the Meeting certainly has a real international flavour. Further details of the programme and registration can be found on the BCA Website at [www.crystallography-meetings.org.uk](http://www.crystallography-meetings.org.uk) as they become available.

Abstract submission, please, to [abstractbca@glasconf.demon.co.uk](mailto:abstractbca@glasconf.demon.co.uk) no later than the deadline of 16 February 2006 for poster presentations.

## Call for Abstracts

As for every BCA Meeting, much of the discussion of new science takes place around the posters. Please plan on showing a poster on your recent work, and encourage others in your group to do the same – remember: points are awarded and, in the words of Humphrey Lyttelton, 'What do points mean? Points mean prizes!'

Please submit your abstracts on-line to [abstractbca@glasconf.demon.co.uk](mailto:abstractbca@glasconf.demon.co.uk). Abstracts should fit on a single side of A4 and be in a font no smaller than 12 point Times Roman, 10 point Arial or equivalent. The preference is for Microsoft Word format.

**The deadline is Friday 16 February 2007.**

The lecture programme in the main meeting is now full and so it will not be possible for further oral presentations to be considered. Thanks to all who have already submitted abstracts.

Lindsay Sawyer

## Named Lectures

**Lonsdale Lecture: Tuesday 11.30-12.30**  
**Professor Bill David** (ISIS/RAL)  
*Combinatorial Studies of Hydrogen Storage Materials - Playing the Odds.*

**Bragg Lecture: Wednesday 12.00-13.00**  
**Professor Sir Roger Penrose** (Oxford)  
*Quasi-Crystals and Non-local Assembly: A Quantum-Theory Foundations Issue?*

**Hodgkin Lecture: Wednesday 17.45-18.45**  
**Professor Judith Howard** (Durham)  
*Looking Back, Leaping Forward.*

## Keynote Lectures

**Biological Structures Group: Wednesday 09.00-09.45**  
**Professor John Moulton** (Maryland) *Modelling SNPs in human disease.*

**Chemical Crystallography Group: Thursday 09.00-09.45**  
**Professor Chick Wilson (Glasgow)** *Beans, sausages and pancakes: a recipe for understanding thermal motion in crystals.*

**Industrial Group: Wednesday 14.15-15.00**  
**Professor R.L. Snyder (Georgia Inst. of Technology)**  
*Nano-Materials.*

**Physical Crystallography Group: Tuesday 14.00-14.45**  
**Professor Richard Catlow** (Royal Institution) *title TBA.*

## Parallel Sessions

### Tuesday 15.15-16.45



#### Expression to Data Collection

Chair: **K. Brown** (Imperial)

**Laurence Pearl** (Cancer research UK)  
*Combinatorial Domain Hunting.*

**Fabrice Gorrec** (SGC, Oxford) *Robotic & Protein Crystallization: Experimental Design, Application and New Developments.*

**Peter Moody** (Leicester) *Automation in a small Protein Crystallography Laboratory.*



#### New science from big facilities

Chair: **Jon Wright Simone**

Teichert (Max Planck Institute, Gottingen)  
*Time-resolved X-ray Diffraction: Possibilities and Limitations for Studying Light-activated Matter.*

**Simon Brown** (ESRF, Grenoble) *Science and Instrumentation on the XMaS beamline.*



#### Co-crystals of Pharmaceutical Materials

Chairs: **Anne Kavanagh** (AstraZeneca, Macclesfield),

**Roy Copley** (GSK, Harlow)

**Bill Jones** (Cambridge) *Strategies for designing and making cocrystals.*

**Keith Chadwick** (Manchester) *Co-crystals - does thermodynamics hold the secrets of drop grinding?*

**Chris Frampton** (Pharmorphix) *Panic to Panacea: Cocrystallisation in Pharmaceutical Development.*



## Wednesday 10.15-11.45



### Complementary and Emerging Developments in SR

Chair: **TBA**

**Bonnie Wallace** (Birkbeck) *Synchrotron Radiation Circular Dichroism Spectroscopy: A New Tool for Structural Biology.*

**Dmitri Svergun** (EMBL, Hamburg) *Analysis of Biomacromolecular solutions with Small-Angle Scattering.*

**So Iwata** (Imperial) *Diamond Membrane Protein Laboratory.*



### Solving Difficult Problems at Central Facilities

Chair: **John Warren** (CCLRC)

**Bill Clegg** (Newcastle) *Keeping British chemistry at the forefront with synchrotron single-crystal diffraction.*

**Alistair Lennie** (CCLRC Daresbury) *New Facilities for High Pressure at the SRS.*

**Kenneth Shankland** (CCLRC ISIS) *Small molecules, big facilities: some good reasons to write a Facility experiment proposal.*



### XRF / XRD Joint session on thin films

Chairs: **Dave Taylor** (ICDD), **Chris Staddon** (Nottingham)

**Tom Ryan** (Nanometrics, Oregon, USA) *Thin Films and Coatings by XRF and XRD: an Overview.*

**Joachim Voitok** (PANalytical) *Advanced solid-state X-ray detector for the analysis of thin-layered structures.*

**Hugues Guerault** (BrukerAXS) *Up-To-Date XRD-Techniques for investigating ultra-thin films and ultra-small features.*

**Brian Tanner** (Bede) *X-ray probes of the layer and interface structure of nano-scale films for opto-electronics and spintronics.*



### Computational methods in crystallography

Chair: **Dave Allan** (Edinburgh)

**Carole Morrison** (Edinburgh) *Finding the elusive hydrogen atoms - how computational chemistry can help.*

**Stewart Clark** (Durham) *Density functional methods in crystallography.*

**Mark Johnson** (ILL, Grenoble) *title TBA*

## Wednesday 15.30- 17.00



### Computational automation

Chair: **TBA**

**Julie Wilson** (York) *Alice's Adventures in Grenoble.*

**Andrew Leslie** (MRC, Cambridge) *title TBA*

**Randy Read** (Cambridge) *Likelihood and automation in PHASER.*



### Transport and Reactivity in Crystals

Chair: **Simon Parsons** (Edinburgh)

**Richard Jones** (Keele) *Zeolites Sorption Sites and Temperature.*

**Paul Raithby** (Bath) *Bright Ideas In Exciting Crystallography.*

**Kenneth Harris** (Cardiff) *Molecular transport in crystalline tunnel structures.*



### Diffraction from Surfaces and Two Dimensional Crystallography

Chairs: **Judith Shackleton** (Manchester),

**Richard Morris** (Morris Analytical X-ray)

**D. C. Arnold** (University College Cork) *Structural studies of ordered mesoporous silica in channelled substrates.*

**Tom Hase** (Durham) *X-ray characterisation of nanomagnetic materials.*

**Peter Laggner** (Graz) *TBA*

## Thursday 10.15-12.15



### Post-phasing and Beyond

Chair: **Randy Read** (Cambridge)

**Tassos Perrakis** (Netherlands Cancer Institute) *Algorithms and Ideas for Automated Model Completion.*

**Nick Furnham** (Cambridge) *RAPPER: Restraint Based Conformer Generation Using Crystallographic Data.*

**Kim Watson** (Reading) *GRID on the Grid: A New Workflow Environment for High-Throughput Biological Computing.*

**Paul Emsley** (York) *Model Building Tools in Coot NCS Tools, Helices and Strands.*



### One Hundred and One Ways to Prepare an XRPD Sample

Chairs: **Jeremy Karl Cockcroft** (UCL),

**Martin Gill** (Natural History Museum)

**Gordon Cressey** (Natural History Museum) *Random Diffraction Patterns (without really trying).* This session is scheduled to include an IG prize talk by a Young Crystallographer.



### Disordered materials and glasses II

Chair: **Matt Tucker** (Durham)

**Sylvia Mclain** (ISIS) *title TBA*

**Eugene Gregoryanz** (Edinburgh) *title TBA*

**Adrian Barnes** (Bristol) *title TBA*

## Thursday 13.30 – 15.00



### Dynamics in Crystals

Chair: **Chick Wilson** (Glasgow)

**John Evans** (Durham) *title TBA*

**Stewart Parker** (ISIS) *Vibrational Spectroscopy with Neutrons: Catalysts, Hydrides and Polyethylene.*

**Graeme Day** (Cambridge) *Dynamics in Molecular Crystals across the Crystal Packing Landscape.*



### A Standardless Future for Quantitative XRPD?

Chair: **Steve Norval** (ICI, Wilton)

**Gordon Cressey** (Natural History Museum) *Random Mounts and Reproducibility ? The Key to Standardless Q.P.A.*

**Christopher Gilmore** et al (Glasgow) *Quantitative Analysis of Mixtures Using High Throughput Instrumentation without the Use of Standards.*

**TBA** (BrukerAXS) *Quantitative analysis of cements.*

**TBA** (PANalytical) *Standardless Quantitative Analysis.*



### Disordered materials and glasses I

Chair: **John Loveday** (Edinburgh)

**Robert Newport** (Kent) title TBA

**Martin Wilding** (Aberystwyth) title TBA

## Young Crystallographers

### Monday

**11.30 - 12.30 Registration**

**12.30 - 15.00 Session 1**

**Roy Copley** (GSK) *Insights into pharmaceutical small molecule crystallography (Keynote) Followed by 5 YC short talks*

**15.00 - 15.30 Coffee**

**15.30 - 17.00 Session 2**

**Andres Goeta** (Durham) *Getting Hot Results from Cold Data (Keynote) Followed by 3 YC talks*

**17.00 - 17.30 Coffee**

**17.30 - 19.00 Session 3**

*Poster 'Flash' presentations*

**19.00 - Dinner + poster session + wine**

### Tuesday

**9.00 - 11.00 Session 4**

**Andrea Hadfield** (Bristol) *TBA Followed by 4 YC talks*

## XRF Session Details

### Tuesday Morning

**Tutorial / Workshop Session XRF: Where are we now?**

**Mark Ingham** is organiser and chair. We have secured two speakers of international renown to present the following sessions.

**10.00 Bruno Vrebos** (PANalytical) *XRF: What instruments have we got, or are likely to get soon?*

**11.15 Coffee**

**11.45 Rene Van Grieken** (Antwerp) *XRF: What can we do with them?*

### Tuesday Afternoon

**14.00 - 15.30 Semi-quantitative**

**Ros Schwarz** is organiser and chair.

**TBA** (British Geological Survey, Keyworth) *What on earth is this?*

**15.30 - 16.45 Calibration Samples**

**Ros Schwarz** is organiser and chair.

**David Beveridge** (ILFORD Photo) *No standards? No blanks? No standardless software? No problem!*

**Phil Russel** (PANalytical) *Normative Committees*

**TBA** (British Geological Survey, Keyworth) *Wide Range Oxide fused bead standards*

**17.00 - 18:30 XRF Exhibitors' Forum**

**Dave Taylor** is organiser and chair. Exhibitors will be allowed to give commercial talks aimed at encouraging delegates to visit their exhibition stand for further information. Exhibitors will be required to register in advance to give a presentation and the available time of 90 minutes will be divided equally to fit in all the talks.

### Tuesday Evening

Posters and Exhibition with buffet and wine.

### Wednesday Morning

**10.15 - 12.00 XRF / XRD Joint session on thin films**

**Dave Taylor and Chris Staddon** are the organisers.

**Tom Ryan** (Nanometrics, Oregon, USA) *Thin Films and Coatings by XRF and XRD: an Overview*

**Joachim Voitok** (PANalytical) *Advanced solid-state X-ray detector for the analysis of thin-layered structures*

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**Brian Tanner** (Bede) *X-ray probes of the layer and interface structure of nano-scale films for opto-electronics and spintronics*

## Wednesday Afternoon

**13.30 - 15.00 and 15.30 - 17.00 XRF Applications - including Cultural Heritage**

**David Beveridge** is organiser and chair.

**Luisa Carvalho** (Lisbon) *X-ray Fluorescence Analysis on paper characterisation*

**Clair Collins** (Oxford Instruments) *Analysis of archaeological artefacts by handheld XRF*

**Malcolm Haigh** (Spectro) *Analysis of Geological Samples using a Polarised-Beam Benchtop XRF Spectrometer*

**TBA** (British Geological Survey, Keyworth) *Mobile XRF and MCERTS analysis of soils*

## Thursday Morning

**10.00 XRF Foundation Lecture**

**Margaret West** is organiser and chair.

**Rene Van Grieken** (Antwerp) *Environmental Issues*

**11.00 - 12.30 Presentations on Environmental issues**

**Nick Marsh** (Leicester) *Climate Records - Lurking in the small print? What's at the bottom of your lake?*

**Chris Vanhoof** (VITO, Belgium) *Development and validation results of a new European Standard prEN 15309 for the determination of the elemental composition of waste and soil by XRF.*

**Stan Piorek** (Niton) *Screening of electronic products with a "small-spot" hand-held XRF analyser for compliance with RoHS Directive.*

**Ros Schwarz** (Oxford Instruments) *RoHS compliance testing - handheld and micro-spot XRF: performance and pitfalls*

**12.30 Closing Remarks**

## From the Secretary Elections to Council, 2007

**THIS** year there will be vacancies on the Council for the Offices of Vice-President and Secretary, and we will also be choosing for the first time an Education Co-ordinator. There will be more information in the March Issue, but please consider possibilities for these posts. Nominations, properly seconded should be with the Secretary at least two weeks before the date of the AGM, which is at 17.00 on Wednesday 18 April 2007.

**Christine Cardin**  
Secretary to Council



## The Motherwell Symposium

**THE** Symposium will take place at the Spring Meeting on Thursday afternoon and Friday morning. It comprises talks by both established and younger scientists. There will be a banquet in honour of Sam Motherwell on the evening of Thursday 19 April. The Symposium will be chaired by Frank Allen (CCDC) and Graeme Day (University of Cambridge).

**Frank Allen** (CCDC, Cambridge, UK)  
*Introduction: Sam Motherwell's science at the CCDC.*

**Robin Taylor** (CCDC, Cambridge, UK)  
*Using small-molecule crystal-structure data to validate protein-ligand structures.*

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

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

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

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

**James Chisholm** (CCDC, Cambridge, UK)  
*Searching the CSD for extended motifs and other challenging queries.*

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

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

**Peter Wood** (University of Edinburgh, UK)  
*Understanding High-Pressure Phase Transitions with Pixel Calculations.*

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

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



# BCA 2007 Spring Meeting -

	Monday 16th April		Tuesday 17th April									
	Satellite Mtg											
0900			YC Session 4 09.00 to 11.00		Possible Workshop?							
0915												
0930												
0945												
1000												
1015												
1030												
1045												
1100												
1115												
1130	Young Crystallographers Registration 11.30 to 13.00		Possible Workshop			Lonsdale Lecture 11.30 to 12.30 Professor William David (ISIS)						
1145												
1200												
1215												
1230												
1245	Young Crystallographers Session 1 13.00 to 15.00		Possible Workshop			Lunch, Exhibition & Registration 12.30 to 14.00						
1300												
1315												
1330												
1345												
1400												
1415												
1430	Tea & Coffee 15.00 to 15.30		Tea & Coffee 1445 to 1515			Keynote PCG Richard Catlow (London) 14.00 to 14.45						
1445												
1500												
1515	YC Session 2 1530 to 1700		Possible Workshop or special interest groups		BSG Session 1 1515 to 16.45							
1530					CCG Session 1 15.15 to 16.45		IG Session 1 15.15 to 16.45					
1545					Break 15 mins							
1600					Exhibitors' Forum 17.00 to 18.30							
1615												
1630												
1645												
1700												
1715					YC Session 3 17.30 to 19.00		Possible Workshop or special interest groups			Poster Exhibition Buffet Dinner 18.30		
1730												
1745												
1800												
1815												
1830	YC Dinner 19.00		Possible Workshop or special interest groups			Poster Exhibition Buffet Dinner 18.30						
1845												
1900												

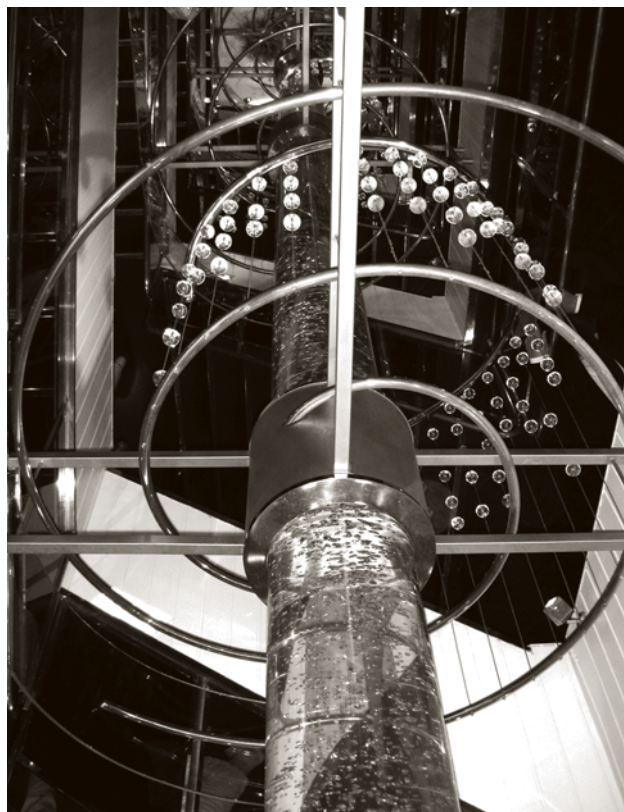
# Timetable

	Wednesday 18th April				Thursday 19th April			
XRF Regist	Keynote BSG John Moulton (CARB) 09.00 to 09.45				Teaching Keynote (CCG) Chick Wilson (Glasgow) 09.00 to 09.45			
	Tea & Coffee 09.45 to 10.15				Tea & Coffee 09.45 to 10.15			
XRF 1A	BSG Session 2 10.15 to 11.45	CCG Session 2 10.15 to 11.45	PCG Session 1 10.15 to 11.45	XRF 3 & XRD Thin Films	BSG Session 4 10.15 to 12.15	IG Session 3 10.15 to 12.15	PCG Session 2 10.15 to 12.15	XRF 5 Keynote
Coffee Regist	Break 11.45 to 12.00				Break			
XRF 1B	Bragg Lecture 12.00 to 13:00 Professor Sir Roger Penrose (Oxford)			Lunch & Exhib	Lunch & Exhibition 12.15 to 1330			XRF 5
Lunch	Lunch & Exhibition 13.00 to 14.15		PCG AGM	IG AGM				Lunch & Exhib
XRF 2A		BSG AGM	CGG AGM	XRF 4A	CCG Session 4 13.30 to 15.00	IG Session 4 13.30 to 15.00	PCG Session 3 13.30 to 15.00	
	Keynote Lecture IG R L Snyder (Georgia) 14.15 to 15.00							
Tea	Tea & Coffee 15.00 to 15.30				Tea & Coffee 1500 to 1530			
XRF 2B	CCG Session 3 15.30 to 17.00	BSG Session 3 15.30 to 17.00	IG Session 2 15.30 to 17.00	XRF 4B	Space for workshops, SIGs etc if required			
XRF Exhib Forum	BCA AGM 17.00 to 17.45				Sam Motherwell Event Talks Dinner Talks on Friday			
	Hodgkin Lecture 17.45 to 18.45 Professor Judith Howard (Durham)							
	Dinner 19.15 for 19.45							

## Twenty-third European Crystallographic Meeting Leuven, Belgium, August 2006

**THE** European Meeting in Leuven was well up to standard, as the pictures and the following reports by three of our bursars show!.

Ed.



The 23rd European Crystallographic Meeting grouped together crystallographers in the city of Leuven in Belgium in August. The 4-day conference at the Katholieke Universiteit Leuven held an impressive scientific programme with 16 plenary lectures, 46 microsymbosia and 2 poster sessions of 400 posters altogether. The social events, such as the walking tour of Leuven medieval city, the concert of the Kolacny brothers, the special lecture on the Belgian beers, the Marresearch Party at the Atomium and, last but not least, the congress dinner in the Chateau du Lac in Genval, made the conference even more enjoyable. It was

also possible to hang around the numerous exhibitions during the days as 30 exhibitors were present: Art Robbins Instrument, Axo Dresden, Axygen, Beevers Miniature Models, Bruker AXS, Cambridge Crystallographic Data Center, CCP4 Daresbury Laboratory, European Molecular Biology Laboratory, Fluidigm, Formulatrix Inc, Greiner Bio-one, Incoatec GmbH, International Union of Crystallography, Marresearch, MarUSA, MicroCal LLC, Mitegen, Molecular dimension Ltd, Oldenbourg Zeitschrift fur Kristallographie, Open Eye Scientific software, Oxford Cryosystems, Oxford Diffraction Ltd, Oxford university Press, PANalytical, Rigaku, RWTH-Aachen University, STOE&Cie, Taylor & Francis and XENOCs SA.

Monday morning started with a very interesting plenary lecture from **Thomas Schneider** (FIRC Institute of Molecular Oncology Foundation and The European Institute of Oncology in Italy) on the use of coordinate uncertainties in structure comparison. This technique can be used for proteins, for instance, it shows up the difference between the conformers by looking at the distances between the atoms.

The following micro-symposia on *Instrumentation and Experimental Techniques for Applications to Symmetry, Charge and Orbital Studies* was presented by **Vladimir E. Dmitrienko** (Institute of Crystallography in Moscow, Russia); **Yves Joly** and **Emilio J. Lorenzo** (Grenoble) and **Helen F. Gleeson** (Manchester). Yves Joly concentrated on the study of charge ordering by resonant diffraction. Atoms with closely related site symmetries but with almost no difference in charges exhibit resonances at different energies, and that sensitivity allows estimations of charge disproportion.

During the afternoon, **Gautam R. Desiraju** (Hyderabad); **Enrique Espinosa** (Dijon); **E. James Milner-White** (Glasgow); **Frederic Arod** (Lausanne) and **Ivan Glukhov** (Moscow) gave talks in *The Understanding Molecular Interactions* session. Gautam emphasised Halogen... Halogen interactions and explained that there were two types of these. In the case of hexachlorobenzene, the molecule forms Cl...Cl contacts and  $\pi \dots \pi$  stacking interactions but when the crystal is compressed along the needle length, it deforms and bends, because of the weak Cl...Cl interactions as opposed to the stronger  $\pi \dots \pi$  stacking.

On the Tuesday morning, **Gustaaf van Tendeloo** (Antwerp) gave a plenary on electron crystallography which was a very good and useful overview of the technique. After introducing the basics of the method, Gustaaf discussed the problem of dynamical scattering, which is not a real problem according



to him once you know you have to take it into account. He explained that, these days, electron microscopy is able to do detailed structure analysis by combining information from reciprocal space with information from real space and that modern software is now able to perform dynamical calculations very quickly.

Also on Tuesday, **Gastone Gilli** brought a few smiles to people's faces with his sense of humour despite the little technical problems at the beginning, and gave a great chronological talk on *Modern hydrogen bonding theory*. He proposed a nice explanation of the evolution of the previous hydrogen bond theories: if we accept the idea that previous theories may have been erroneous because they were based on insufficiently accurate experimental data, nowadays the existence of crystallographic and thermodynamic databases, which allow a more accurate collection of data from the most reliable H-bonds, would give a new scope on the study of the true nature of the H-bond, a broad research field which continues to attract interest from many researchers worldwide.

**Lee Brammer's** lecture on *Halogen-mediated supramolecular chemistry* in the solid state described a new class of halogen bonds (M-X...X'-C) obtained using two complementary properties of halogens: acting as effective and directional hydrogen bond acceptors when they are bonding to metal centres (M-X), and, in contrast, very poor hydrogen bond acceptors in the case of organic halides (C-X). Brammer discussed the use of this interaction as a supramolecular synthon in the construction of supramolecular assemblies in crystals, and he presented a range of visual solid state reactions using these compounds.

**Christer Aakeröy** spoke on *Constructing co-crystals with molecular sense and supramolecular sensibility*. Aakeröy gave an interesting lecture on the development of synthetic methods for the directed assembly of co-crystals. By using a broad range of examples with different hydrogen bond donors and acceptors, he designed binary and ternary supermolecules and co-crystals (It is amazing how easy everything was when he was explaining it!).

**Ronald Ruth** (Lyncean Technologies, USA); **Thomas Tschentscher** (Hamburg); **Shinya Hosokawa** (Hiroshima) and **Richard Tyrrel** (Texas) presented works in a session on *New X-ray Sources and New Possibilities*. Ronald Ruth showed us the compact light source (CLS), a miniature synchrotron source for the home lab. It has up to three beamlines and can be used like the X-ray facilities at the synchrotron but is 200 times smaller. It uses a laser undulator and a miniature electron beam storage ring.

On the Wednesday, a session on *Structures by Electron Crystallography* was proposed by **Vidar Hansen** (Stavanger); **Stavos Nicolopoulos** (Valencia); **Wim Tirry** (Atwerp); **Zhanbing He** (Stockholm) and **Holger Klein** (Grenoble). Stavos said that the precession method can be used for nanocrystals and that this method gives a solution to the strong dynamical scattering problem by increasing the

kinematic character of the electron diffraction. With electron beam precession, few reflections are simultaneously excited in dynamical condition and the diffraction pattern obtained can be interpreted as close to kinematical conditions.

On the Thursday morning, **Loic Bertrand** (Gif-sur-Yvette) gave quite an uncommon talk in the *Crystallography in Art and Archaeology Sciences* session. He explained that applications of synchrotron diffraction techniques cover a large range of heritage and archaeology needs, such as ageing characterisation of ancient human and animal hairs. He also presented SOLEIL, the new synchrotron radiation source near Paris that will be fully opened in 2009.

The session *New Crystallographic Softwares* was on the last afternoon. **Artem R. Oganov** (ETH Zurich) spoke on the prediction of unknown crystal structures with algorithms using the USPEX method, which can be really useful for instance for studies at high pressure. **Dylan Jayatilaka** (Western Australia) described the program Crystal Explorer, which uses the Hirshfeld surfaces of molecules to analyse how the molecules pack in a crystal by means of differing shapes and colours of the surface. This software would be a useful tool for researchers interested in the packing of organic molecules and the type of interactions involved.

**Chris Gilmore** (Glasgow), presented the computer program dSNAP, and its applications to the search for structural data in the Cambridge Structural Database. Gilmore showed that the program could be used to group similar structures from the CSD using cluster analysis, thus reducing the time required to analyse a large hit-list compared to manual browsing using Conquest.

We would like to thank the BCA for the bursaries which permitted us to participate to the 23rd ECM 2006, a good conference that gave us the opportunity to meet and listen to very interesting crystallographers in a nice city.

**Kathy Guille**  
Newcastle University

**Noelia Sanchez Ballester**  
Loughborough University

## Report on the visit to the ECM, Leuven, Belgium.

**THINK** of Belgium and a number things come immediately to mind (mine at least); Hercule Poirot; Tintin; rain; chocolate and beer. During my time at ECM 23 I was treated to a fair amount of the latter three and thankfully none of the former. Having chosen the interesting method of travelling to Leuven, first by plane to Amsterdam and then by train across the Low Countries, we arrived very tired and slightly fed up with the precipitation falling from the sky. This mood was deepened when we inexplicably completely failed to see the notice indicating which door we



were supposed to be using to enter the student accommodation. Cue lots of walking backwards and forwards looking for a lock that accepted our keys. At least we weren't alone and eventually someone more intuitive than we (he was already inside) spotted our conference bag marker and showed us the way.

My French co-worker was slightly aggrieved to discover that we were in the Flemish part of Belgium and would thus be unable to put her translating skills to good use. This is a good tip - make sure you have an international group so that its members are able to translate for you at international conferences. In the event, a sound knowledge of French proved highly useful when attempting a little detour to Brussels.

On to the conference itself. The opening ceremony surpassed the IUCr congress in its bizarreness as we were treated to an introduction from the local dignitaries and mighty members of the ECM interspersed with an *cappella* boy band belting out 80's hits and ballads. The attempts at getting a bemused audience of crystallographers to join in were admirable but ultimately doomed to failure. Surely that was impossible to follow, but a brave attempt was made by **Eleanor Dodson**, who gave her Max Perutz prize lecture *Issues for the refinement of macro and micro molecules*. The opening ceremony completed, we departed for a welcome reception, where in true conference style, there was a lot of wine but not a lot of food.

The first day kicked off with a choice of plenary lectures, mine being that of **Thomas Schneider**, who described an elegant method for the comparison of structures of the same macromolecular species, many of which have been determined numerous times to different degrees of resolution. Choosing between the six microsymbiosia proved difficult, as with the remaining days; however, I flitted between *Crystal design and functional materials*, initiated by

an excellent talk by **Kitigawa** who described the synthesis and structural properties of metal organic frameworks, and *Molecular crystallography under non ambient conditions*, which included an entertaining talk by **Ross Angel** on the use of high pressure techniques.

The afternoon session was set firmly in the realms of crystal engineering, or *Understanding molecular interactions*, the highlight of which was the ever engaging **Gautam Desiraju**, who described the complexity of halogen:halogen interactions and the interesting physical properties displayed by the crystals of species forming such interactions.

Monday and Tuesday were the allocated days for my poster presentation, with Monday being the day to stand next to the poster. It seemed to receive a fair amount of attention and was read by a number of people. The poster sessions were fortified by the provision of free beer to all delegates, a feature of the whole week. This was a nice touch, if a little odd with the later plenary lectures still to be held.

Monday night's entertainment was provided by the local **Kolacny brothers**, who played a number of pieces on the piano, both separately and together on the same piano. This was an excellent experience and thoroughly enjoyed by all.

My choice for Tuesday morning's plenary was the talk given by **Gastone Gilli**, who discussed modern hydrogen bonding theory, essentially the existence of the resonance assisted hydrogen bond which is related to the pKa-values of the species involved in the hydrogen bond. This was a new concept to me and one that I found fascinating. The highlight for the remainder of Tuesday was the introduction of the 'home synchrotron'. Although described as compact and miniature, it was nevertheless still quite enormous, and beyond the scope of most departmental laboratories. It was still a very interesting experience and the first orders have been made! Other talks attended focussed on the hydrogen bonding theme, with **Len Barbour's** being particularly interesting, as usual.





Tuesday night was the pinnacle of the entertainment provided and surely ideal for the crystallographic community; a lecture on beer. Interesting as the fellow from **Inbev** was, the main interest was in the beer itself; 400 litres of it. Delegates of past BCA meetings will no doubt be aware of the tragedies that have occurred in many of the bars the length and breadth of Britain, where they have, on average, been drunk dry within the first two nights. Imagine my shock when the waiters were literally forcing glasses of beer on those hardy souls who stayed to the bitter (or should that be lager) end.

There seemed to be a paucity of talks (as well as delegates) on Wednesday, although a couple of lectures on polymorphism and perusal of the exhibition whiled away the morning. The afternoon was made of sterner stuff, consisting of a session on advanced methods for computer simulation of molecular crystals. This was essentially the employment of high powered computers in the prediction of unknown crystal structures or the refinement of 1- or 2-dimensional data sets. I am afraid that the high maths lost me in a few talks but the presentation by **Natalia Panina** on the crystallisation of pigments was pitched at just the right level.

Having no real interest in the evening plenary lectures, and finding ourselves with a free evening (no room at the Mar inn), we decided to take a short journey to Brussels, centre of Europe. Sadly it wasn't quite as grand as we had expected, with the main tourist attractions ruthlessly exploited by shops selling all manner of junk. Having said that, we might have enjoyed it more if it hadn't poured with rain. So a quick jaunt on the underground later found us at the Atomium, designed way ahead of its time in the 50's, and a quite extraordinary building, where we looked on in envy at the lucky people who managed to get Mar tickets. So on to Thursday, and I was beginning to flag, I must admit. The morning kicked off with an impromptu talk by **Hans Burgi**, standing in for **Israel Goldberg**. Given the short notice, this was a very good talk and was a nice introduction

to the concept of spin crossover complexes. Following on from this was a new concept in the determination of absolute configuration of structures containing light atoms, even using data obtained via molybdenum radiation. Its simple concept seems to work and should be available in *Platon* now. I will certainly be giving it a go. Next, on recommendation, I attended **Joel Bernstein's** talk on polymorphism, and it was certainly the excellent talk I was promised. I spent most of the rest of the day trying to work out if I would actually be able to get back to Britain on the Friday, as the terror alert was just making itself known. I decided to attend the afternoon session on communicating and educating crystallography, which was slightly knocked out of joint by one of the speakers failing to show up. Nonetheless, the parts of **Gordon Barr's** talk that I was able to see suggested a worthwhile project that certainly attracted attention, with the *eCrystals* concept delivered by **Simon Coles** providing insight in to one of the possible future directions of the role of crystallography.

The conference was completed with the conference dinner, held in a prestigious hotel on the banks of a lake. Although the service was excellent and the food very good, I was dismayed by the lack of opportunity to mingle with other tables, as there was very little time at the end of the evening to mix and say my goodbyes. Nonetheless, I think an enjoyable evening was had by all.

This was certainly an enjoyable conference, although perhaps not reaching the dizzy heights of the IUCr congress (by which I think I was spoiled), and I would like to thank the BCA bursary committee for giving me the opportunity to attend.

**Ross Harrington**  
University of Newcastle



# Groups



## PCG Winter Meeting:

### Physical Crystallography in the UK

**THE** physical crystallography group held its winter meeting on the 25th October at the Centre for Science at Extreme Conditions (CSEC) at the University of Edinburgh. The title of the meeting was 'Physical crystallography in the UK'. Whilst it was not possible to have speakers from all the relevant institutions in the UK, a broad cross-section was provided by six speakers from five institutions. The talks covered techniques from high pressure studies to total scattering; and topics from Fullerenes in solution to novel multiferroics. The meeting was organised by **John Loveday**, hidden behind the six speakers.



**Lars Lundegaard** (Edinburgh), **Chris Howard** (UCL), **Andrew Goodwin** (Cambridge), **Dean Keeble** (Warwick), **James Smith** (Warwick) and **Lauren Chapon** (ISIS). It was a very interesting meeting and was enjoyed by all those that attended with considerable discussion and questions being generated by each of the talks. The PCG committee would like to thank all the speakers for their excellent contributions

**Matt Tucker**

## Young Crystallographers' Group

**BREAKING NEWS:** The YCG is in the process of becoming the fifth group of the BCA!

The YCG is for 'starting out' crystallographers, i.e. PhD students and first term PDRA's, and is open to members of the four current groups (CCG, BSG, PCG and IG). Membership of the YCG will be automatic, if applicable, and is **in addition** to membership of any of the other groups.

The YCG committee would like to invite announce our upcoming meeting as a satellite to the BCA Spring meeting in Canterbury, Kent on the 16–17 April 2007. Registration for this meeting is alongside registration for the main BCA meeting and will be **free of charge**. This meeting is designed to give the younger generation of crystallographers an opportunity to present their research to their contemporaries in a relaxed and informal atmosphere.

**PRIZES:** There will be a prize donated by the Industrial Group to the best talk (loosely) related to Industry. If you wish to be considered for this please indicate when submitting your abstract.



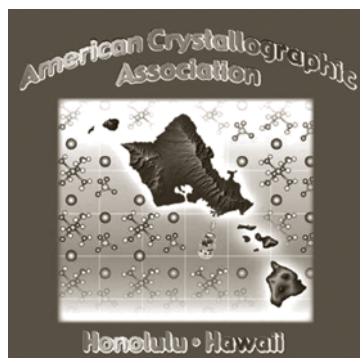
YC06: Lancaster University

**LOGO:** Get creative! We need a permanent logo for the YCG, so send us your designs. You can surely do better than the one shown!

**COMMITTEE NEWS:** Due to the new status of the group, we will be looking for members to join the YCG committee which currently consists of **Simon Coles** (Southampton), **Alexandra Griffin** (Bristol) and **Mike Probert** (Durham). If you are interested in being considered, especially those from the PCG, IG and BSG, please contact Alex.

Alex Griffin: ([a.griffin@bris.ac.uk](mailto:a.griffin@bris.ac.uk))

## American Crystallographic Association Honolulu 2006



**THE** 2006 meeting of the American Crystallographic Association was held at The Sheraton Hotel on Waikiki Beach, Hawaii. Honolulu International Airport was my first introduction to Hawaii where

travellers are greeted with the relaxing sound of Hula music as they wait for their luggage: an extremely effective way of reducing post-flight stresses. I was particularly happy to discover that the post-doc accommodation was in a hotel approximately one minute from both the beach and the shops – perfect. The following day I made my way to the conference hotel and discovered that it was situated right on the seafront with wonderful views of blue seas and palm trees; coffee breaks could be spent on the boardwalk overlooking the sea where you could often see sea turtles swimming, and all around there were many

crystallographers embracing the laidback Aloha spirit in Hawaiian shirts and leis.

The first day of the conference brought a session on *International Macromolecular Crystallographic Advances* with a wide selection of talks covering many different proteins and highlighting a wide range of methods. I was particularly interested to hear **Bostjan Kobe's** talk where they had phased by cobalt SAD on their home source, and **Zihe Rao's** talk on the structure of a number of proteins from the SARS virus. In the afternoon I attended the Buerger Award Symposium where the award was presented to **Helen Berman** who gave an interesting talk on some historical aspects of crystallography, particularly concentrating on the emergence of the Nucleic Acid Database and the Protein Data Bank and the uniformity of pdb and mmCIF formats. The following talks by **Paula Fitzgerald, Stephen Neidle, Jordi Bella, Wah Chiu** and **Stephen Burley** highlighted the impact Helen has had in many diverse areas from nucleic acid and protein structures to cryoEM and drug discovery.

On Day 2, I attended the session on *Biomacromolecular Assemblies* which was aimed at trying to get crystallographers interested in using Small Angle X-ray Scattering to complement their crystallographic studies. This session was particularly interesting to me as someone who is currently trying to obtain information about protein-



protein complexes in solution. An introductory talk by **Dmitri Svergun** from Hamburg provided a very good overview of the technique with examples of how it had been used to observe complex shapes as in the case of ATPase, how it can be used in conjunction with individual solved structures to define how complexes are formed in solution (e.g. growth factor and receptor complex), how it can be used to define missing loops and regions which are disordered in crystal structures, and also how it can determine monomer/heteromer equilibria and the stoichiometry of complexes. **Jack Johnson** (not the Hawaiian singer) gave a stunning talk showing how his group had followed the maturation of virus particles by time-resolved SAXS with impressive movies of their results. The afternoon session focused on neutron crystallography and how the boundaries of this area are being pushed forward with smaller crystals and larger molecules being studied.

Day 3 brought a session on *Proteins involved in Host Immune System and Pathogenic Interactions* with talks on Toll-like receptors, Down Syndrome Cell Adhesion Molecule and a TCR-superantigen-peptide/MHC complex. **James Sacchettini** explained some of the problems associated with current anti-tuberculosis drugs and his current work in identifying new drug targets and lead compounds. In the afternoon's *Computational Methods* session we had talks on the use of TLSMD to define TLS groups, as well as updates on RAPPER, BnP, LAFIRE, ARP/WARP and PHENIX.

The fourth day started with a session on *Complementary Techniques*. **Alexander McPherson** told us about atomic force microscopy and showed some impressive movies of a large crystal incorporating a small surface crystal into its lattice as it grew, and work on single virus particles. **Quan Hao** spoke about methods used to obtain molecular envelopes

and subsequent phasing from these, and **Clare Peters-Libeu** spoke about her interesting work on lipoproteins where she was looking at both Bragg diffraction and diffuse scattering from crystals of protein-lipid complexes. In the afternoon a session on *Large Macromolecular Assemblies* consisted of talks on ribosome-antibiotic complexes, RNA polymerase II and fungal and mammalian fatty acid synthases. Finally, **Jianwei Miao's** talk on diffraction microscopy provoked much discussion.

The final day of talks started with *Membrane Proteins* and addressed a number of different methods for growing crystals. In more than one case it was vital to not purify the protein too much as that was shown to strip away lipids which proved essential for crystallization. The final session of the meeting on *Difficult Structures* started off by **Zbigniew Dauter** telling us how to make a structure difficult by doctoring some of his own data. **Wim Hol** spoke about many difficulties which had been encountered and overcome in his group's work on tropical diseases, and finally **Michael Sawaya** spoke about a technique he had used in the scaling of severely anisotropic data which had lowered his  $R_{\text{free}}$  from 43% to 31% and which will be implemented in Scalepack in the future.

With over 400 posters packed into 3 sessions, there was no shortage of reading material on a wide range of subjects and it was a great environment in which to present my own work on a coiled coil protein. I have come back to the lab with a renewed interest in complementary techniques to crystallography, a number of new ideas to try out and, most importantly, a big dose of inspiration. Thanks to the **Arnold Beevers** Bursary Fund for help towards my travel.

**Rebecca Conners**  
University of Bristol





## Books

### The Jahn-Teller Effect

Isaac B. Bersuker, *University of Austin, Texas*

*Cambridge University Press, 2006*

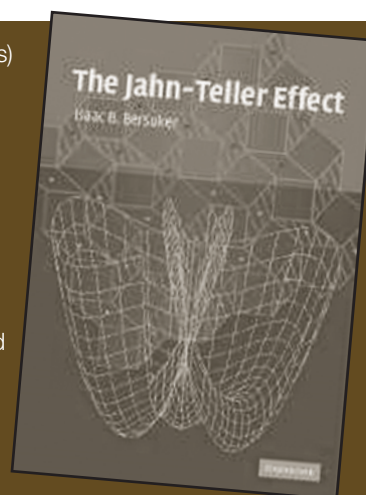
Price: £100.00 (hardback)

ISBN-10: 0521822122, xvi+620 pages

**FOR** all those chemists whose understanding of the Jahn-Teller effect involved explaining why 6-coordinate copper(II) complexes are never regular octahedra, or why the U.V./visible spectra of octahedral titanium(III) complexes show a shoulder on the side of the main peak, this text is a real eye opener. It is certainly a book for the purists, but it does cover aspects of physics, chemistry and biology. It treats the subject at a high level, and employs quite a rigorous mathematical approach.

For the general reader Chapter 1 is very helpful, as in it the author provides a general historical introduction to the subject; explains the general principles, putting Jahn-Teller vibronic coupling effects in the context of molecular and array structural science; and outlines the aims and objectives of the book. In Chapter 2 the fundamental physics leading to the development of the theory are explained, while in Chapter 3 the basic formulations for different symmetry systems are discussed, and the methods used to deal with multicentre systems explained. In Chapter 4 pseudo-Jahn-Teller, product Jahn-Teller and Renner-Teller (which

deals with linear molecules) effects are discussed. In Chapter 5 the solutions to the vibronic equations are described, as are the energy spectra showing dynamic Jahn-Teller effects. In Chapter 6 the general theory relating to electronic spectra, infrared and Raman spectra and magnetic resonance spectra is covered. In Chapter 7 the geometry and spectra of molecular systems ranging from diatomics up to pentaatomic  $\text{MX}_4$  systems, and benzene and cyclopentadienyl families, are discussed. Finally, in Chapter 8, Jahn-Teller effects in solid-state systems are described.



This is probably not a book that a crystallographer would sit down and read cover-to-cover but for the general reader this book is certainly useful as a reference volume, and for experts in the area the text would be a useful addition to a library. The material is very well and clearly presented, and it is apparent that the text has been written by an expert in the field. There are references at the end of each chapter which provides a useful source of the original literature and provides a source for further reading.

Paul Raithby

## His Worship Moreton Moore

**CRYSTALLOGRAPHERS** get involved in many things, but not everyone will know that after many years as a councillor, Moreton became Mayor of Runnymede. Congratulations to the original editor of this journal! Runnymede is, of course, looking forward to 2015 when it will be celebrating the octocentenary of the Magna Carta.



# Obituary

## Desmond Cunningham (1942-2006)



**DES CUNNINGHAM**, who died on 18th September 2006, was a Chemistry Professor at the National University of Ireland, Galway (Ollscoil na hÉireann, Gaillimh). He was a much loved academic and his passing represents a sad loss for the chemistry and crystallographic community in Ireland. His research, (with more than 175 papers),

principally focused on the synthesis and characterisation of Group 14 derivatives using Mössbauer spectroscopy and X-ray diffraction techniques, makes him a key figure in the development and promotion of inorganic chemistry in Ireland from the 1970s.

He was born on March 6th 1942 and grew up in Mountcharles in County Donegal, where his father was a school principal. In his early years both music and painting competed with his interest in science. He chose chemistry when a career decision had to be made and was educated at University College Dublin. He studied synthetic inorganic chemistry (1965-1968) on 'Studies on Chromium(III) Alkoxides' under the supervision of Dr. W. K. Glass and was awarded a Ph.D. degree for this research from the National University of Ireland.

Post-doctoral research in London, in the then Northern Polytechnic, introduced Des to the chemistry of tin which subsequently became a lifelong interest in conjunction with Mössbauer spectroscopy. In 1971 he moved to a lectureship in University College Galway and established a thriving research group engaged in the study of Group 14 and transition metal complexes. Research included synthetic and structural studies on metal phenylphosphonates/phenylarsonates, heterobimetallic Schiff bases and metal oxides.

Des had a strong interest in solid state chemistry and had often dreamed of establishing a crystallography group in Ireland. In the late 1970s he spent a year on sabbatical leave in Oklahoma, USA, where he gained considerable expertise in using diffraction equipment and running a crystallography laboratory. From this experience, the Crystallography Centre in Galway was established with collaboration from Patrick McArdle and Tim Higgins. Initially a Hilger & Watts Y290 4-circle diffractometer was used for data collection (from George Ferguson, University of Guelph, Canada). The positive impact of this diffractometer

was immediate, driving research in new directions in synthetic and structural chemistry both in Galway and in collaboration with other Irish research institutions. Two successive HEA large equipment grants followed and provided further funding for more modern equipment to pursue and expand research in chemical crystallography, powder diffraction and biological crystallography.

Des had extensive collaborations with industry in Ireland. A pharmaceutical company had a major problem with a tin catalysed reaction using a process that produced the desired drug in 1h but left a tin oxide 'mess' that took many hours to clean up. Production runs were limited to only one per day. Des and co-workers overcame the problem using inexpensive chemicals by turning the 'mess' into a white powder that was easier to handle. Production was tripled in all plants in which the drug was produced (which represented >20% of the company's worldwide profits). More recently, he together with co-workers developed a process for coating glass (and other materials) with tin and other metal oxides. This process has been patented and is superior to existing methods. These very thin oxide coatings make plate glass windows and glass bottles much stronger than uncoated glass.

During his recent illness he was always optimistic and continued to involve himself in much chemistry, correcting theses and suggesting reactions from his hospital bed. Several fascinating compounds were synthesised by his research students and their crystal structures solved and examined by him in the days before he died.

The funeral Mass for Des was celebrated in Moycullen Church, Co. Galway. In a ceremony that was punctuated by anecdote, verse and song, the congregation were moved from tears to laughter. Afterwards, Des was laid to rest in the graveyard beside Moycullen Church.

Des thought well of everyone and thus had more friends than most. The wonderful atmosphere he could create with his personality, his music and his love of painting will long be remembered by all who knew him. He was very friendly and sociable, and he appreciated a well poured pint of stout amongst friends - a lifelong interest which hadn't diminished with age. He was an excellent teacher, mentor and friend to the many students that he taught as undergraduates or supervised as postgraduate students as well as his colleagues and friends. He will be missed by the many people that he met throughout his life.

Des was a dedicated family man and is survived by his wife Patsy, his daughter Aileen, his brother Conal and his sisters Sheila and Catherine.

**Patrick McArdle (NUI Galway), John Gallagher (Dublin City University) and John McGinley (NUI Maynooth)**

# Awards of Medals

## Award of Medals by the Institute of Physics

### GLAZEBROOK MEDAL:

**Colin Carlile**

*The Institut Laue-Langevin, Grenoble*



The Glazebrook medal and prize, for outstanding contributions to the organisation, use or application of physics in an industrial, commercial or educational environment, has been awarded to Colin Carlile for his contributions to neutron science, in particular through his leadership of the Institut Laue- Langevin.



Colin Carlile has pursued a highly successful career in neutron science, conducting both original research and designing novel neutron instruments, as

well as managing instrumentation suites at the ISIS neutron source near Oxford. The pinnacle of his career has been his leadership over the last seven years at the Institut Laue-Langevin (ILL) - the world's premier source of neutron beams for research.

A European research centre, the ILL includes the UK, France and Germany as principal partners as well as nine other national scientific partners.

During his time at the ILL, Carlile has revolutionised the outlook of the institute. He has pushed through a programme of instrument upgrades, which has increased their average performance by a factor of seven, and further advances are on the way. He has also created an environment in which highly motivated staff -- and new initiatives such as the deuteration laboratory -- can flourish. In addition he has introduced a series of new security measures and initiated the design of an improved fuel element, ensuring that the long established ILL neutron source will remain competitive with other sources that are due to be built.

As a result the ILL has a secure long-term future and will continue to contribute to our understanding of everything from unconventional superconductors to biological macromolecules, from nuclear reactions to the origin of matter in the universe, and from the binding of bio-molecules to tests of quantum mechanics.

### DUDELL MEDAL:

**Richard Nelmes**

*University of Edinburgh*



The Duddell medal and prize, for outstanding contributions to the advancement of knowledge through the application of physics, has been awarded to Richard Nelmes for pioneering new techniques and instrumentation that have transformed high - pressure structural science.



Richard Nelmes has pioneered techniques and instrumentation that have transformed international high-pressure structural science. Where earlier results were often

somewhat qualitative, his work from the 1980s led to the production of quantitative diffraction data that can now be analysed to pressures beyond a megabar, revealing remarkable structural complexity in many materials.

From 1989, he led developments of powerful new methods for synchrotron X-ray powder diffraction that fully exploited 2D detectors and overcame the effects of pressure cells on data quality. This has since become the way that all such work is done worldwide. His own group's research has achieved striking new structural insights, first in semiconductors like Si, Ge, InSb and GaAs under pressure, and more recently in elemental metals. For example, at very high pressures the group discovered an extraordinary new structure in Ba, and then in several other metallic elements, of a type previously known only in binary systems. He has since developed new single-crystal X-ray techniques to address the complexity of some high-pressure metal phases.

Nelmes has also made extensive use of neutron diffraction methods. These were limited to much lower pressures than X - ray studies for many years but, through collaboration with colleagues in Paris since 1988, he has achieved an order of magnitude increase in pressure and spurred international efforts to take neutron techniques to a megabar. His group's research with neutrons includes numerous studies of high-pressure structures in ice and water, as well as discoveries about methane hydrate that are important for understanding the atmosphere of Saturn's moon Titan. He also led the recent establishment of the Centre for Science at Extreme Conditions at the University of Edinburgh.



## MOTT MEDAL:

**Andre Geim**

*University of Manchester*



The Mott medal and prize, for distinguished research in condensed-matter or materials physics, has been awarded to Andre Geim for his discovery of a new class of materials - free-standing two-dimensional crystals, in particular graphene.



During the last two years Andre Geim has played a crucial role in opening up a new field of condensed-matter physics through his discovery of a new class of materials - strictly two-dimensional atomic crystals.

Among them graphene - a free-standing single layer of graphite - occupies a very special place due to its truly remarkable properties.

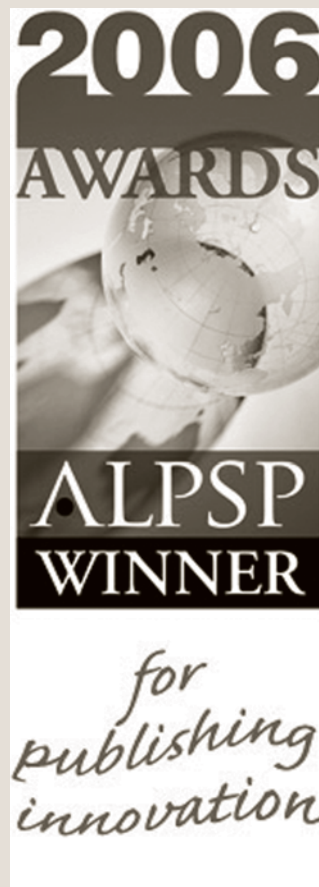
Graphene is only one atom thick but highly stable under ambient conditions and exhibits nearly perfect crystal quality. It is also highly conductive so electrons confined within this atomic gauze travel submicron distances without scattering. Geim has demonstrated a ballistic ambipolar transistor based on graphene, which has significantly improved the prospects of carbon-based electronics, although major applications of graphene and other two-dimensional materials await further development.

There is, however, no doubt about the exceptional new physics that graphene offers. Quasiparticles in graphene are not like normal electrons described by the Schrödinger equation but behave as massless relativistic fermions described by the Dirac equation.

Geim and colleagues have proven this in a series of elaborate experiments in which they reported two new types of the quantum Hall effect (dubbed as half-integer and chiral) as well as the minimum (or Mott's) quantum conductivity in the limit of no charge carriers. The latter discoveries have opened a new paradigm of "relativistic-like condensed matter" in which quantum relativistic phenomena can now be studied in bench-top experiments.

Geim works extensively to embed science in society, with educational demonstrations on magnetic levitation (the "flying frog" experiment) as well as research on biomimetic adhesives exploiting the same physical mechanism as that used by geckos when they climb ("geckotape"). Through this, and his discovery of graphene, Geim has attracted worldwide media attention.

## IUCr wins prestigious international award for publishing innovation



**THE International Union of Crystallography (IUCr) has won the 2006 Award for Publishing Innovation of the Association of Learned and Professional Society Publishers (ALPSP).**

The Award, for Data Exchange, Quality Assurance and Integrated Data Publication (CIF and checkCIF), recognises the involvement of the IUCr in the development of the Crystallographic Information Framework and its applications, e.g.

- Standard data definitions for crystallographic information archive and interchange.
- Submission format for structure report articles in crystallographic journals.
- Standard format for depositing supplementary structural data accompanying publications.
- Automated checking of the integrity and self-consistency of crystal structure models (the web checkCIF service).
- Use of checkCIF as a peer review tool.

Dissemination of crystal structural models in online publications and automated visualization.

Read more in

[www.iucr.org/docs/alpsp\\_award2006](http://www.iucr.org/docs/alpsp_award2006)

# Meetings of interest

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

## 7-8 December 2006 25th

BESSY Users' Meeting, Berlin, Germany  
[www.bessy.de/cms.php?idcatar](http://www.bessy.de/cms.php?idcatar)

## 9 December 2006

James D. Jorgensen (1948-2006)  
Symposium on "Opportunities in Neutron Powder Diffraction", Argonne National Laboratory, Illinois USA  
[www.msd.anl.gov/groups/nxrs/workshop](http://www.msd.anl.gov/groups/nxrs/workshop)

## 7-10 January 2007

PCG Rietveld Refinement School, Durham  
[www.dur.ac.uk/john.evans/webpages/pcg\\_rietveld\\_school\\_2007](http://www.dur.ac.uk/john.evans/webpages/pcg_rietveld_school_2007)

## 10-12 January 2007

International Workshop - Current Challenges in Liquid and Glass Science, The Cosener's House, Abingdon  
[www.isis.rl.ac.uk/disordered/SpencerFest/SpencerFest](http://www.isis.rl.ac.uk/disordered/SpencerFest/SpencerFest)

## 14-19 January 2007

International School on Mathematical and Theoretical Crystallography. The University of Havana, Cuba  
[www.lcm3b.uhp-nancy.fr/mathcryst/havana2007](http://www.lcm3b.uhp-nancy.fr/mathcryst/havana2007)

## 21-24 January 2007

5th European Conference on Computational Biology - ECCB '06, Eilat, Israel  
[www.eccb06.org](http://www.eccb06.org)

## 23 January 2007

Modern Protein Drug Target Crystallography Training Course, South San Francisco CA, USA  
[www.selectbiosciences.com/conferences/Rupp/index.aspx](http://www.selectbiosciences.com/conferences/Rupp/index.aspx)

## 31 January - 2 February 2007

International Workshop on Dynamic of Molecules and Materials, Grenoble, France  
[www.ill.fr/Events/DMM](http://www.ill.fr/Events/DMM)

## 19-22 February 2007

6th Pharmaceutical Powder X-ray Diffraction Symposium, sponsored by ICDD, Barcelona, Spain  
[www.icdd.com/ppxrd](http://www.icdd.com/ppxrd)

## 5 - 9 March 2007

Annual meeting of the Deutsche Gesellschaft für Kristallographie, Bremen, Germany  
[www.dgk-dgkk-2007.uni-bremen.de/](http://www.dgk-dgkk-2007.uni-bremen.de/)

## 9-13 April 2007

Materials Research Society Spring Meeting, San Francisco CA, USA  
[www.mrs.org/spring2007](http://www.mrs.org/spring2007)

## 15 - 20 April, 2007

LDSO 2007: The Sixth International Conference on Low Dimensional Structures and Devices, San Andres, Colombia  
[www.fis.cinvestav.mx/lbsd2007](http://www.fis.cinvestav.mx/lbsd2007)

## 16-20 April 2007

Latin American Workshop on Applications of Powder Diffraction and satellite mini-course "Methods of Powder Diffraction", Campinas, Brazil  
[www.lnls.br/lawpd17](http://www.lnls.br/lawpd17)

## 16-19 April 2007

BCA Spring Meeting, University of Kent, Canterbury  
[www.crystallography.org/](http://www.crystallography.org/)

## 9-11 May 2007

GISAXS - an advanced scattering "method", [HASYLAB@DESY](mailto:HASYLAB@DESY), Hamburg, Germany [indico.desy.de/conferenceDisplay.py?confId=111](http://indico.desy.de/conferenceDisplay.py?confId=111)

## 23-25 May 2007

14th BENSC Users' Meeting, Hahn-Meitner-Institute, Berlin, Germany  
[www.hmi.de/bensc](http://www.hmi.de/bensc)

## 7-17 June 2007

Engineering of Crystalline Materials Properties: the 39th crystallographic course at the Ettore Majorana Centre, Erice, Italy  
[www.crystalalice.org/futuremeet.htm](http://www.crystalalice.org/futuremeet.htm)

## 11-17 June 2007

First school and workshop on X-ray micro and nanopores: instruments, methodologies and applications Erice, Italy  
[www.ifn.cnr.it/XMNP2007/home.hfm](http://www.ifn.cnr.it/XMNP2007/home.hfm)

## 1-6 July 2007

"School on Materials Applications of the Organic Solid State" (SMAOSS), Mérida, Venezuela  
[www.ula.ve/eventos/iccoss](http://www.ula.ve/eventos/iccoss)

## 8-13 July 2007

XVIII International Conference on the Chemistry of the Organic Solid State (XVIII-ICCOSS), Mérida, Venezuela  
[www.ula.ve/eventos/iccoss](http://www.ula.ve/eventos/iccoss)

## 11-13 July 2007

Neutrons in Biology, ISIS, RAL  
[www.isis.rl.ac.uk/conferences/nib2007/](http://www.isis.rl.ac.uk/conferences/nib2007/)

## 21-26 July 2007

ACA Annual Meeting - Salt Lake City, UT, USA  
[www.hwi.buffalo.edu/ACA/](http://www.hwi.buffalo.edu/ACA/)

## 23-31 July 2007

ICNX 2007 (the International Conference on Neutron and X-Ray Scattering 2007), Indonesia  
<http://centrin.net.id/~nslbatan/icnx>

## 29 July - 3 August 2007

15th International Conference on Vacuum Ultraviolet Radiation Physics, Berlin, Germany  
[www.bessy.de/VUVXV/front\\_content.php](http://www.bessy.de/VUVXV/front_content.php)

## 12-17 August 2007

ICCG-15 / ICVGE-13 / OMVPE-13: International Conference on Crystal Growth, Salt Lake City, UT, USA  
[www.crystalgrowth.org/conferences/iccg15/index.php](http://www.crystalgrowth.org/conferences/iccg15/index.php)

## 13-17 August 2007

BSR2007 - Ninth International Conference on Biology and Synchrotron Radiation. Manchester, UK  
[www.srs.ac.uk/bsr2007/](http://www.srs.ac.uk/bsr2007/)

## 22-27 August 2007

ECM-24, European Crystallographic Meeting, Marrakech, Morocco  
[www.ucam.ac.ma/fssm/ecm24](http://www.ucam.ac.ma/fssm/ecm24)

## 7-9 October 2007

Size-Strain - Diffraction Analysis of the Microstructure of Materials Garmisch-Partenkirchen Germany  
[www.mf.mpg.de/ss-v](http://www.mf.mpg.de/ss-v)

## 31 May - 5 June 2008

ACA Annual Meeting - Knoxville, TN, USA,  
[www.hwi.buffalo.edu/ACA/](http://www.hwi.buffalo.edu/ACA/)

## 9-14 June 2008

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