

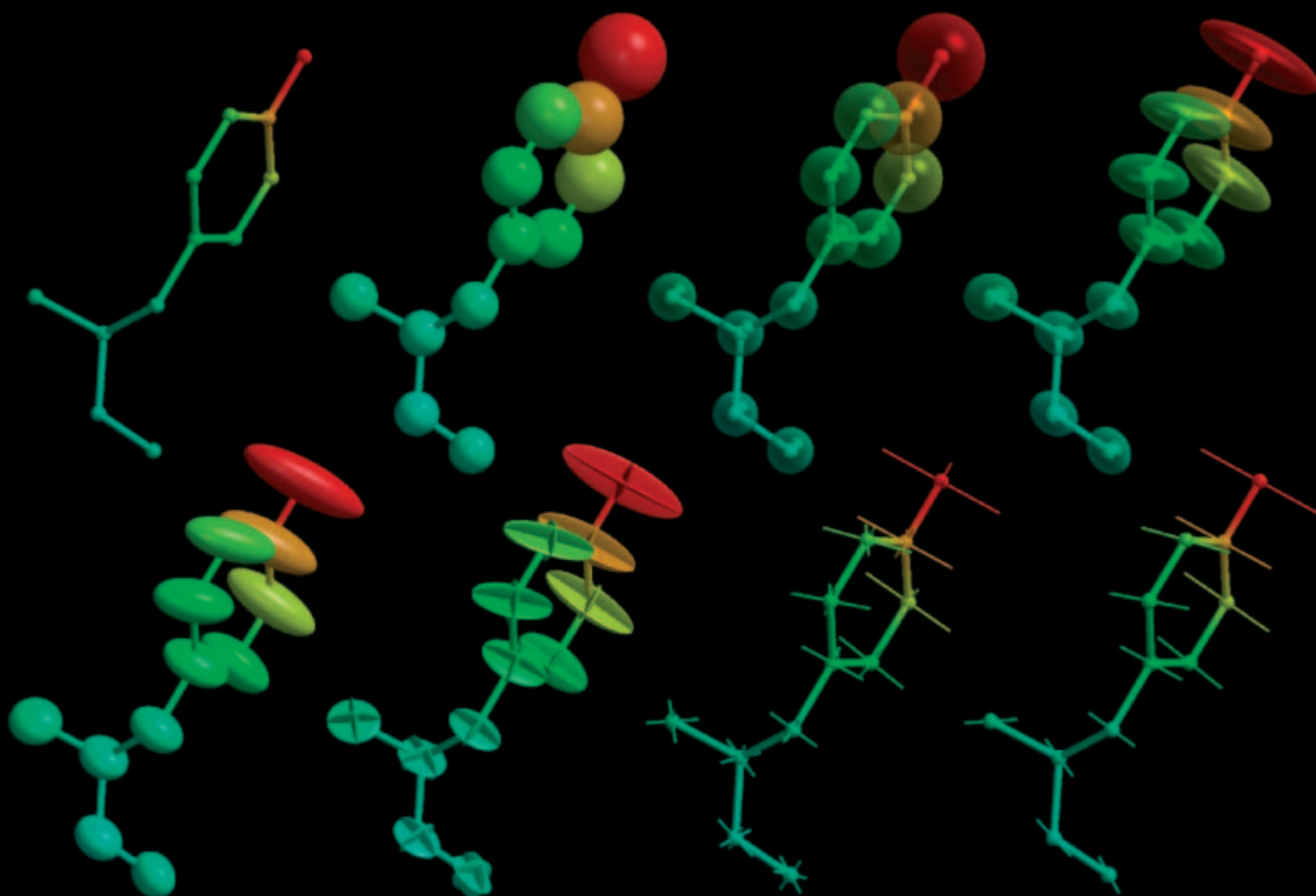
# Crystallography News

British Crystallographic Association



Issue No. 88 March 2004

ISSN 1467-2790



**BCA Spring Meeting–UMIST** p8-17

**CCP4 in Leeds** p18-21

**News from the Groups** p21-30

**Forthcoming Meetings** p31-32





**BCA Administrative Office,**  
Northern Networking Ltd,  
1 Tennant Avenue,  
College Milton South,  
East Kilbride, Glasgow G74 5NA  
Scotland, UK  
Tel: + 44 1355 244966  
Fax: + 44 1355 249959  
e-mail: bca@glasconf.demon.co.uk

CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association.

Text should preferably be sent electronically as MSword documents (any version - .doc, .rtf or .txt files) or else on a PC disk.

Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files.

Items may include technical articles, news about people (e.g. awards, honours, retirements etc.), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews.

Please ensure that items for inclusion in the **June 2004** issue are sent to the Editor to arrive before **25th April 2004**.

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

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

## BCA News March 2004

# Contents

From the President .....	2
Council Members .....	3
From the Editor/Corporate Members .....	4
To the Editor/Puzzle/Stop Press .....	5
Bursary Report.....	6
Diamond Building Construction .....	7
Secretary's Report to Council.....	8
Commercial Exhibition .....	9
Minutes of 2003 AGM.....	10
Scientific Sessions .....	12
Timetable of Spring Meeting .....	16
CCP4 Leeds.....	18
CCG Autumn Meeting .....	21
CCG AGM.....	23
IG Forum II Birkbeck.....	23
IG AGM .....	27
PCG Winter Meeting .....	28
PCG AGM.....	29
Meetings of Interest.....	31



**UMIST:**  
Renold Building - home of the BCA 2004.



### Cover Pictures from CCP4

**Main image:** Different representations of co-ordinates and anisotropic displacement parameters in BobScript.

**Inset picture:** R. Esnouf with a solid solid (sic) model of bluetongue virus core.

# From the President



**SO, here I am almost at the end of my first year as BCA President, and an anniversary is always time to look back, but also forward. In my opinion the organisation remains successful and is operating smoothly.**

The hard work of the BCA Officers and members of Council and the strong interactions with our efficient BCA Administration Office at Northern Networking ensures this. Of course, we have to evolve, but any evolution in a successful organisation should be planned and carried out in a suitably considered manner. This I hope is our ongoing philosophy in the BCA and over the coming months some of that evolution will hopefully become apparent, notably in consideration of our Web identity, enhancing the support of our Education remit and in continuing to broaden our appeal to UK structural scientists in general.

I mentioned the hard work of the BCA Officers, and record here that two of these, Vice-President Paul Fewster and Secretary Christine Cardin, have each served a three-year term. Their hard work and great support of the BCA and its aims and objectives is very much appreciated by myself and all on Council. On a similar note, I would like to record my thanks and appreciation to two retiring Council members: Paul Barnes and our Past-President Chris Gilmore. Both have served BCA Council with distinction and I would note particularly the contribution over many years of Paul, often in the background, who served as Exhibition Convenor and latterly as an active co-opted member of Council. I am sure all will remain active and strong supporters of the BCA.

The Spring Meeting approaches (Manchester, early April) and Paul Fewster and the Programme Committee have been working hard at putting together a strong, vibrant and diverse programme. The job of Programme Chair for a BCA Spring meeting is always "interesting", and in particular this year we have had so many suggestions (timely, delayed, very delayed and late) for sessions that at times the evolving timetable has seemed maze-like. This is healthy of course, but to me strengthens the case for the Spring Meeting

Programme Committee to meet earlier in the cycle to allow the Programme to be finalised and publicised at an earlier stage, to attract more attendees. The evolving Programme is available on the Web ([www.crystallography.org.uk](http://www.crystallography.org.uk)), and the Abstracts will also be displayed prior to the meeting ([www.isis.rl.ac.uk/BCA2004/](http://www.isis.rl.ac.uk/BCA2004/)). The Review Symposium - to be published in Crystallography Reviews - at this year's Spring Meeting revolves around the Plenary session on "Catalysis: from Metals to Macromolecules" and will also encompass papers from several other sessions.

It is a pleasure to note that three Prize lectures will be delivered at the Spring Meeting. The Bragg Lecture will be given by John Finney, and the Dorothy Hodgkin Lecture by George Sheldrick. The Kathleen Lonsdale Lecture is being staged as part of the Young Crystallographers' meeting immediately prior to the Spring Meeting, and returns that lecture to its original aim of being presented to a largely young audience. Less young attendees are also of course encouraged! Also on the Monday, we will have the Young Crystallographers' Mixer and Open Exhibition evening, to which all are again invited.

I have been encouraged by the positive response to the idea of establishing a network of Departmental/Regional BCA Representatives, and work on setting up that network continues. One of the aims of having these local representatives is to encourage colleagues working in crystallography or related areas to join the BCA. Although it is still to my mind remarkably inexpensive to join, I remain somewhat concerned over an apparent drop in our membership. The regional representatives will play an important role in helping to remind lapsed or intending members of the benefits of being part of the BCA, and the reliance our organisation has upon a strong membership base in representing the needs of all crystallographers in the UK. On a related topic, in Durban I was elected onto the Executive Committee of the European Crystallographic Association, now under the Presidency of Hartmut Fues. In that capacity, can I also remind BCA members that individual membership of the ECA is available - details on the BCA website.

I look forward to seeing many of you in Manchester at the Spring Meeting.

**Chick Wilson**

# Council Members

## 2003-04



### COUNCIL MEMBERS

#### President (2006)

**Prof. Chick Wilson**

Rutherford Appleton Laboratory  
ISIS Facility  
CHILTON OX11 0QX  
Tel: 01235 82 1900 ext 5137 or  
01235 44 5137  
C.C.Wilson@rl.ac.uk

#### Vice President (2004)

**Professor Paul F Fewster**

PANalytical Research Centre  
Sussex Innovation Centre  
Science Park Square  
University of Sussex  
Falmer, BRIGHTON BN1 9SB  
Tel: 01273 704422  
Paul.Fewster@PANalytical.com

#### Secretary (2004)

**Dr. Christine Cardin**

University of Reading  
Dept of Chemistry  
Whiteknights  
READING RG6 6AD  
Tel: 0118 9318215  
c.j.cardin@reading.ac.uk

#### Treasurer (2006)

**Mr. David J. Taylor**

35 Birchley Road,  
Billinge  
WIGAN WN5 7QJ  
Tel: 01744 893108  
djtaylor@lineone.net

#### Immediate Past-President (2004)

**Prof. Chris J. Gilmore**

Department of Chemistry  
University of Glasgow  
GLASGOW G12 8QQ  
Tel: 0141 330 3716  
chris@chem.gla.ac.uk

### ORDINARY MEMBERS

**Dr Alexander J. Blake (2006)**

School of Chemistry,  
University of Nottingham  
University Park  
NOTTINGHAM NG7 2RD  
Tel. 0115 9513488  
a.j.blake@nottingham.ac.uk

**Dr Elspeth F. Garman (2006)**

Laboratory of Molecular Biophysics  
Rex Richards Building  
University of Oxford  
South Parks Road  
OXFORD OX1 3QU  
Tel. 01865 275398  
elspeth@biop.ox.ac.uk

**Dr Peter C.E. Moody (2006)**

Department of Biochemistry  
Adrian Building  
University of Leicester  
University Road  
LEICESTER LE1 7RH  
Tel. 0116 2523366  
pcem1@leicester.ac.uk

### GROUP REPRESENTATIVES

#### Biological Structures

**Dr. Andrea Hadfield**

Department of Biochemistry,  
University of Bristol  
BRISTOL BS8 1TD  
Tel: 0117 928 7436  
A.T.Hadfield@bris.ac.uk

#### Chemical Crystallography

**Dr Harry Powell**

MRC Lab. of Molecular Biology  
MRC Centre  
Hills Road  
CAMBRIDGE CB2 2QH  
Tel: 01223 402423  
hrp1000@cus.cam.ac.uk

#### Industrial

**Prof. Christopher S. Frampton**

Crystallography Strategic  
Marketing Manager,  
Bruker Nonius B.V., Oostsingel 209  
2612 HL Delft, The Netherlands.  
Tel: +31 (0)15 215 25 19  
chris.frampton@bruker-nonius.com

#### Physical Crystallography

**Dr John Evans**

Department of Chemistry  
University of Durham  
DURHAM DH1 3LE  
john.evans@durham.ac.uk

### CO-OPTED MEMBERS

**Prof. P. Barnes,**

Department of Crystallography  
Birkbeck College  
Malet Street  
LONDON WC1E 7HX  
Tel: 020 7631 6817  
barnes@img.cryst.bbk.ac.uk

**Professor John Helliwell**

Department of Chemistry,  
University of Manchester,  
MANCHESTER, M13 9PL  
Tel. 0161 2754686  
john.helliwell@man.ac.uk

### EX-OFFICIO MEMBERS

**Editor "Crystallography News"****Dr Robert Gould**

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

**Education Officer****Mrs K.M.Crennell**

'Fortran Friends'  
P.O.Box 64  
DIDCOT OX11 0TH,  
Tel: 01235 834 357  
bca@isise.rl.ac.uk

**Webmaster****Dr Jeremy K. Cockcroft**

School of Crystallography  
Birkbeck College  
Malet Street  
LONDON WC1E 7HX,  
Tel: 020 7631 6849  
cockcroft@img.cryst.bbk.ac.uk

### GROUP CHAIRMEN

**Biological Structures Group****Dr. Richard Pauptit**

Protein Structure Lab  
AstraZeneca,  
Mereside,  
Alderley Park,  
MACCLESFIELD SK10 4TG,  
Tel: 01625-516135  
richard.pauptit@astrazeneca.com

**Chemical Crystallography Group****Dr Alexander J. Blake**

School of Chemistry,  
University of Nottingham  
University Park  
NOTTINGHAM NG7 2RD  
Tel. 0115 9513488  
a.j.blake@nottingham.ac.uk

**Industrial Group****Prof. Christopher S. Frampton**

Crystallography Strategic  
Marketing Manager,  
Bruker Nonius B.V., Oostsingel 209,  
2612 HL Delft, The Netherlands.  
Tel: +31 (0)15 215 25 19  
chris.frampton@bruker-nonius.com

**Physical Crystallography Group****Dr P.A. Thomas**

Department of Physics  
University of Warwick  
COVENTRY CV4 7AL  
Tel. 0113 233 2538  
p.a.thomas@warwick.ac.uk

Full committee details on the BCA website <http://bca.cryst.bbk.ac.uk/BCA/>

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



# From the Editor



**WELCOME** to issue 88.

We hope you like the new, brighter format, which we trust answers some of the criticisms we had last year. I am indebted to Mick Reilly and Barry Brown of Anderson's, our printers in Glasgow, who designed it. Please don't hesitate to tell us what you think about it! We

have returned to the older tradition of a single large photograph on the front cover, which should have more impact than our row of "postage stamps".

The emphasis in this issue is naturally on the forthcoming Spring Meeting in Manchester, and the spreadsheet in the centrefold gives the up to date timetable as we go to press, along with the commercial exhibitors who help to make our meetings possible. Be sure, though, to take the President's advice and keep up-to-date on the BCA Website.

Also in this issue are reports of lively meetings sponsored in the autumn/winter by all our four groups. The interaction between the groups and the association makes the BCA what it is, and I hope that we can continue to communicate with one another through Crystallography News.

We note with respect the death of the eminent French Crystallographer Erwin Felix Lewy-Bertaut on 6 November, 2003. His was a remarkable life – including the way he obtained his double name. An obituary will appear in our next issue.

Finally a plea from your editor. I am delighted with the manuscripts I get from you all – mostly even on time! In order to make Crystallography News readable, though, it is essential to have pictures. I am often driven to dragging up old pictures of where a meeting was. If you are writing a report, please try to get a few pictures too – crystallographers are best, but local animals, tramcars and food are also welcome! I can handle most formats – including hard copy. I will also be photo-active at the Spring Meeting, so please smile when you see me!

**Bob Gould**



## BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
- A 10% discount on exhibition stands at the annual 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 **£600.00** per annum

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

### BCA Administrative Office

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

## Corporate Members

Astex Technology  
Bruker/Nonius  
Chemical Computing Group  
Cambridge Crystallographic Data Centre  
deCODE genetics (Emerald Biostructures)  
Fluidigm Europe/EMEA  
Hampton Research  
International Centre for Diffraction Data  
Oxford Cryosystems  
PANalytical  
Rigaku MSC

# To the Editor...

Dear Sir,

I wish to raise concern about a great body of scientific knowledge that has been lost. It was available as archaic parchments, but this format is not new enough to be referenced in modern computer based science citation systems, and is not compatible with on-line journals. Thus it is unavailable to the modern world, where the IUCr on-line crystallography journals back to 1948 are but a strange, bizarre exception. Some naïve simple folk would say that this lost knowledge exists but a short walk away. However they do not realise that in the age of on-line journals, a walk to the library is a "bridge too far". A new law of science sayeth, "it is forbidden to know of, cite or read scientific literature that is not one computer-click away"; here endeth the new law of science. Like the scholars of the middle ages, we have lost the knowledge of the ancients. Though unlike them, we dare not admit this in public.

Back in that now mythical time (pre 1990's, but especially pre 1970's) there were allegedly a race of scientific giants that roamed the earth. They blazed trails on how to do science intelligently and succeed on difficult problems, often in the laboratory with affordable equipment. Their gradual passing is such that now billion dollar central facilities are often required to obtain routine results. Some say. "Nay, they were not giants, but gods, and their like will never be seen again in this forsaken nano-drive and bandwagon driven age". Such inane rantings are but the folklore and tall tales of a past time, where faint echoes are revealed in on-line science citation searches. While we may admire past science by their use of strong legs, strong hearts and strong minds, we ourselves have but knuckles that can do no more than scar the land. Many are reduced to mediocrity, as the experience of those before us is not easily available to guide and enlighten. We sense the cup of knowledge they poured, but we have not the reach to grab and drink heartily thereof.

Will we ever be able to do such things as they? We lack the experience of this old race of scientists. On our seats of computer power, where "information" is but one click away, within our superficial fortresses of administrivia, our armour a thin veil of vision statements and a weak shield of "quality documentation". Too distracted by the sounds and sights of tapping keyboards, we don't know how to, and we don't have the time to find out.

Yours sincerely,

**P. Dolding-Beedle**

**Egregious and Regal Professor of Honesty in Science.**  
(Alternative name and address supplied!)

## Puzzle Corner



Sadly, last month's caption competition had no entries at all. I hope the distinguished seekers after truth in the picture weren't too disappointed! I had better put in my best efforts which were:

*Oh, you mean a Dutch keyboard isn't the same as a Polish one!*

or

*Ton and Richard enjoying a game of "Simon says".*

And no one but me would award a prize for those!

So this month here's a really easy one for you. The three little pigs, having gone to a macromolecular school, decided to build houses from genetically modified peptides. The first used ser-thr-arg-ala-trp, and the second chose the slightly more complex: ser-thr-ile-cys-lys-ser. The third little pig had problems. Explain why, and suggest a suitable alternative for what he had in mind. The usual £10 book token for the best entry!

Editor

## Stop Press

**All: I am delighted to say that Elspeth Garman (University of Oxford) has accepted our invitation to deliver the 2004 Kathleen Lonsdale lecture, as part of the Young Crystallographers' day at the forthcoming BCA meeting in Manchester.**



Chick Wilson

# Treasurer's Bursary Report 2003

**GENEROUS** membership donations have boosted the **Arnold Beavers Bursary fund** by over **£250** this year. The **BSG** has transferred interest on its reserves of **£455** to the fund and a **GIFT AID** refund of **£1,145** has also been allocated to the fund.

The **York Spring Meeting** saw the award of bursaries totalling **£4,960** to 31 students from 16 Universities. Six of these Bursaries were commercially sponsored. The **BCA** is grateful to the following organisations for this valuable support: **Bruker AXS**, **ICDD**, **PANalytical**, and **Syngenta**. For the first time a certificate of appreciation was presented to each sponsor.

Through the year there were 17 applications for **Arnold Beavers Bursaries** and all were accepted. However, four **£200** awards for **ECM21** were returned when sufficient funding from other sources could not be mustered. So, in 2003 13 bursaries totalling **£2,660** were taken up.

Through the year "good works" have benefited from **BCA** funding. **£800.00** went to the **Eighth Oxford School** on **Neutron Scattering**.

## **IUCr Congress Bursary fund.**

The **£25,000** loaned for the **Geneva Congress** helped towards setting up and funding 164 bursaries totalling **\$110,000** to applicants from 31 countries with the **UK** receiving 31. **£22,241** (the dollar equivalent of the original loan) was returned in **June 2003** and has been offered to the organisers of the **2005 Congress** in **Florence**.

Details of the Bursary scheme can be found under **Membership** on the **BCA** web site. In **2004** only web based bursary applications will be accepted.

NAME	UNIVERSITY	CONFERENCE	AWARDED
Miss Sophie Dale*	Univ. of Loughborough	ECM-21 (South Africa)	£200.00
Miss K Line	University of Exeter	VII International School on the Crystallography of Biological Macromolecules. (Italy)	£160.00
Miss Jennifer Kirkhouse	University of Strathclyde	39th IUPAC Congress (Canada)	£200.00
Dr Simon Coles*	University of Southampton	ECM-21 (South Africa)	£250.00
Mr Robin Owen*	University of Oxford	ECM-21 (South Africa)	£200.00
Dr Shabir Najmudin*	University of Warwick	ECM-21 (South Africa)	£250.00
Dr Helena Wright	University of Warwick	ECM-21 (South Africa)	£250.00
Dr Tatiana Novoselova	The Queen's University of Belfast	10th World conference on Titanium (Germany)	£200.00
Mr Gary Nicol	University of Newcastle	Younger European Chemist Conference (Grenoble)	£150.00
Mr Luco Russo	University of Newcastle	Younger European Chemist Conference (Grenoble)	£150.00
Mr Kostas Beis*	University of St Andrews	2nd International Conference on Structure Dynamics...(Switzerland)	£200.00
Miss Anne Blewett	University of Warwick	29th Lorne Conference on Protein Structure & Funtion (Australia)	£200.00
Mr Raja Mondal	University of Durham	33rd National Seminar on Crystallography (India)	£250.00

\*Reports from these bursars have appeared in *Crystallography News*.

# Diamond building construction



**Fig1.** On 11 November 2003, local secondary school teachers toured the construction site to gain some idea of what type of careers were available in civil engineering with some presentations (indoors!) on the research which will be done with diamond. Here one of the project engineers is explaining to some of the party about the methods of construction; the 'portable' concrete mixer in the background is able to use special 'barium rich' rock to produce concrete with much greater shielding ability than normal concrete, which should reduce background radiation at the samples at the same time as allowing the building to leave more room for experiments by needing much thinner walls. Moving this heavy concrete by conventional 'ready mix' concrete lorries would add an unacceptable amount of heavy traffic to the already crumbling Oxfordshire roads, especially as the weight of the concrete means that the usual lorries could only cope with half a load, so there would have to be twice as many of them!



**Fig2.** Misty view of the site in November 2003 where building continues in all weathers.

I am grateful to the diamond Press and Public Relations team for allowing me to tour the construction site with the local teachers.



**Fig3.** (taken 21 January 2004). After all these weeks of preparing foundations, this last week has seen a few girders lifted into place, including what looks like the first one for the roof; at last we can see the start of the construction of the machine building itself, let us hope the snow and freezing temperatures forecast do not cause much delay.

Kate Crennell

## Book Review

### Rotational Spectroscopy of Diatomic Molecules

John Brown (Oxford) and  
Alan Carrington (Southampton)  
Cambridge University Press, 2003

Price: £100 (hardback), £39.95 (paperback)  
ISBN 0-521-81009-4 (hardback)  
0-521-53078-4 (paperback)  
1013+ xxxi pages.

This book is a huge piece of work, containing, among other things, more than 2500 equations with numerous references and tables of data. It is strongly based on the 1950 work Spectroscopy of Diatomic Molecules by G. Herzberg, The book deals mainly with work done since then, and has itself been some 30 years in the making. For those interested in this topic, it should provide a definitive sourcebook for many years to come.



# BCA Spring Meeting

## Secretary's Report to Council 2003- 2004

**THERE** have been several changes to the Council this year. Most obviously, we have a new President, Chick Wilson, who has already done a huge amount on behalf of members. We also welcome three new Ordinary Members. Elspeth Garman (Oxford) is well known to the biological community for her superb lectures on cryocrystallography, data collection, radiation damage and similar essential subjects. Peter Moody (Leicester) has been a member of the BSG committee and organised previous Spring Meeting sessions. Sandy Blake (Nottingham) is, among other things, Scientific Director and a lecturer on the BCA/EPSRC Crystallography School, as well as the Chairman of the CCG. We also have Chris Gilmore as former President, and have co-opted John Helliwell as runner-up in the Presidential election. Council met immediately after the Spring Meeting in York (agreeing that this was the last time that it would meet at 5 p.m. on Maundy Thursday!) and held a full day meeting in Birkbeck College in September.

The current (January 2004) membership figures are 564 Ordinary, 87 Corporate, 99 Student, 36 Retired, 3 Unemployed, 11 Honorary and 30 Life members, giving a total membership of 830. In terms of subject group interests these break down into 271 BSG, 247 CCG, 116 IG and

115 PCG, with 81 members declaring no particular affiliation. Members can update their details online through the Membership page of the website. It should be said that these membership figures are lower than those reported at the last AGM, when the total number of members on the database was given as 1106. We felt a year ago that 1000 was a good membership target and felt pleased with ourselves at that stage. It now seems that the database itself needed some tidying up and that the Administrative Office were somewhat optimistic. In fact, we should be concerned about these figures, particularly the number of student members. Please let me have any thoughts on this. Current membership figures will be presented by Northern Networking at the AGM.

Four excellent issues of the Newsletter have appeared, thanks to the hard work of our capable Editor. Council is very proud of Crystallography News, both its professional appearance and its worthwhile content. It now needs to reach a wider audience, through an increased membership. The website has undergone some changes, and more are proposed, although this represents a lot of work. The changes should make it easier for individuals to update their own parts of the website, and ideally the website should always be the most up to date information. We also plan to make greater use of email mailing lists for mailshots to members, bearing in mind that everyone gets far too many emails and that we must be careful here. The opinions of members on the best ways of improving communication would be very useful. For example, at the moment the

limited publicity for the Spring Meeting goes only to Members in Crystallography News and we could make much more use of posters and emails.

**The Group meetings this year were as follows:**

**The Biological Structures Group Winter Meeting,** "Protein Complexes" was held on 19th December 2003 in the New Lecture Theatre, Birkbeck College, local organiser Richard Pickersgill.

**The Chemical Crystallography Group Autumn Meeting 2003** - "Beyond Refinement; What Happens Next?" was held in the Accelrys Center of Excellence, Cambridge, on Wednesday November 12, 2003. The local organiser was Vanessa Hoy.

**The Physical Crystallography group** held a two day joint meeting with the Institute of Physics Condensed matter Physics Group on 8-9th December 2003 at the Cosener's House, Abingdon, on the subject "Probing Structure at the Nanoscale:- Fact, Fiction or Hype?", local organisers J.C. Wasse and P. Radelli

**The Industrial Group** held a two day meeting entitled "Industrial Group Forum II" in Birkbeck College on 13-14th November 2003. The local organiser was Dave Taylor.

It is a pleasure to record that in 2003-4 Eleanor Dodson, Richard Nelmes and Venki Ramakrishnan were all elected to Fellowship of the Royal Society. Louise Johnson was made a Dame and appointed Life Sciences Director of Diamond. Council have elected four new Honorary Members of the BCA, David Blow, Durward Cruickshank, Michael Hart and Judith Howard. George Sheldrick was chosen as Dorothy Hodgkin Lecturer, and will be presented with his prize at the Spring Meeting. Sadly we have to record the death of Bill Cochran, one of our Honorary Members. All these events have been recorded in Crystallography News.

In conclusion, as I said last year, we are a voluntary educational charity, and we could not exist without the hard work of all the people who give their time and expertise so generously to support crystallography and crystallographers in the UK.

**Christine Cardin (Secretary to Council)**

## Announcement of Election to Council

This year we have vacancies on the BCA Council for Vice-President and for Secretary. The current Vice-President, Paul Fewster, does not wish to seek re-election. Please send your properly seconded nominations to me as soon as possible. I will accept nominations until two weeks before the date of the AGM on 7th April 2004. If you nominate someone, it is your responsibility to make sure that the person you nominate is willing to stand for election.

**Christine Cardin (Secretary to Council)**

## Commercial Exhibition



**ANOTHER** record-breaking commercial exhibition will be a feature of the Spring Meeting. At Manchester, so far, we have 16 exhibitors and sponsors confirmed with some exhibiting for the first time. A new publishing zone is being developed to create an area dedicated to firms publishing in your field.

### Exhibitors include:

Beevers Miniature Models  
Bruker AXS  
Douglas Instruments  
Fluidigm Europe  
Genomic Solutions  
Hiltonbrooks  
ICDD  
IUCr  
Marresearch  
Molecular Dimensions  
Nextal Biotechnologies  
Oxford Cryosystems  
Oxford Diffraction  
PANalytical  
Perkin-Elmer Ltd  
Rigaku/MSC

This is the only meeting in the UK this year which gives you the opportunity to update your product knowledge from such a diverse range of suppliers. Registration, refreshment breaks, lunch and the posters are all in the exhibition area.

Check out the Spring Meeting WEB pages for the latest information and to download an Exhibition Plan. With one day registrations on offer, can you afford to miss this exhibition? The excellent scientific sessions are the bonus that warrant the full three days of your time! Don't miss out on the early bird registration fee – deadline is the 5th March.

# Minutes of Annual General Meeting

**HELD** on Wednesday, 16th April 2003 at 4.30 p.m. in the University of York. The President (Chris Gilmore) in the Chair.

89 voting members were present. One minute's silence was observed in memory of Hal Taylor, John Robertson and Ron Jenkins of ICDD.

- 1. Approval of agenda.** The agenda was approved
- 2. Apologies for absence.** There were no apologies for absence.
- 3. Minutes of the previous AGM.** These had been published in the March 2003 issue of Crystallography News. They were approved as a correct record of the meeting.
- 4. Secretary's Report.** The secretary, Christine Cardin, presented her report, which had been published in the March 2003 issue of Crystallography News.
- 5. Northern Networking report.** This report was presented orally. Gill Moore said that there were now 1106 members on the database. There are 861 ordinary members, 65 retired members, 175 student members and 5 unemployed members. There are also 31 Life Members and 9 Honorary Members. By subject group these break down as 340 BSG, 287 CCG, 127 PCG and 161 IG, with none specified as 191. There are 12 Corporate members. She reported that the Newsletter flourishes, and that the Spring Meeting had 282 registered participants (up 30 on last year). There were five new exhibitors and 12 corporate members. She was asked about the cost of the newsletter, which is under discussion by Council. She was thanked by Chris Gilmore.
- 6. Renewal of the Northern Networking contract.** The meeting voted unanimously to renew the contract for three years until June 2006. The contractual terms had previously been approved by Council.
- 7. Treasurer's report.** The Treasurer, David Taylor, presented a detailed report, which was subsequently published in the June 2003 Crystallography News. In questions, David was asked about the £25,000 lent to the IUCr after the Glasgow meeting. The Treasurer 'feared bad news' and said any debate should be deferred. Chris Gilmore thanked David for his tireless work on behalf of members, and Mike Hursthouse proposed that the accounts be accepted. This was seconded by Sandy Blake.
- 8. Elections to Council.** There were two candidates for President, John Helliwell and Chick Wilson, whose manifestos has been published in the March 2003 edition of Crystallography News. After a secret ballot, Chick Wilson was deemed elected. The President thanked both candidates for their willingness to stand for election.

## 9. Appointment of Examining Accountant for 2003.

David Taylor recommended that the Young Company be reappointed. Harry Powell proposed that the meeting accept this, seconded by Steve Maginn.

## 9.AOB.

1. The Vice-President proposed a change to the Statutes and Bye-laws to allow the creation of a membership category to be known as Fellows. The BCA is too small an organisation to use Direct Debit as a method of adjusting the subscription, and there is currently no simple method of keeping the subscription income flexible. Members who had been Fellows for ten years on reaching 65 would subsequently become Life Fellows and pay no further membership subscriptions, although as Fellows they would pay a premium rate to be decided by Council. Durward Cruickshank asked what the purpose of this proposal was. In his opinion the BCA could not go down the RSC route of accreditation, and the felt the proposal was divisive. Mike Hursthouse said he thought the accounts seemed healthy and could not see why the BCA needed to raise more money in this way. He would rather give his spare cash to charity. Mike Glazer said the proposal smacked of 'rich men buying honours'. He would rather see the subscription go up. David Taylor said that there was a big administrative cost of increasing the subscription. Richard Pauptit said it was a pity to focus on the impact on finances. He thought the question was whether the BCA liked the idea of having Fellows, and this core principle was one we could vote on. After a show of hands it was clear that the meeting was largely opposed to the idea of Fellows as proposed. There were a few abstentions, and the proposal was NOT PASSED.

## 2. Presentation of prizes.

The Industrial Group poster prize was awarded to Francesca Fabiani, presented by Jeremy Cockcroft. The PCG poster prizes were awarded to Pam McGregor (PP11) and C. Hejny (PP2), presented by Pam Thomas. The CCG poster prizes were awarded to Cheryl Doherty (CP37) and to Amber Thompson (CP2), presented by Sandy Blake. The David Blow BSG poster prize was awarded to Jim Pflugrath with second place going to Tom Oldfield and a honourable mention going to CCP4, presented by Richard Pauptit.

There being no further business the meeting closed at 17.15.

**Christine Cardin Secretary to Council**



## 2004 Annual General Meeting of the BCA

The Annual General Meeting of the British Crystallographic Association will be held at 16.35 on Wednesday 7 April 2004, at UMIST.

### AGENDA

1. Approval of Agenda
2. Apologies for absence
3. Minutes of the last AGM (published in this issue of Crystallography News).
4. Secretary's Report to Council (published in this issue of Crystallography News).
5. Northern Networking's Report.
6. Report of the Treasurer to include Presentation of the Accounts for 2003 and the Examining Accountant's Report.
7. Acceptance of the Accounts
8. Elections to Council  
Vice-President  
Secretary
8. Appointment of Examining Accountant for 2004.
9. Any other business

Christine Cardin  
Secretary to Council



# Scientific Sessions:

**THE** scientific sessions for the 2004 BCA Meeting will again concentrate on “hot-topics” in the field of crystallography.

The main theme and Plenary Session is on **Catalysis: from Metals to Macromolecules**, this will lead into a sub-theme on **Molecules in Medicine** covering both chemical and biological aspects and **Catalysis in Industry**. There will be sessions on **Small Angle X-ray Scattering**, which will include a workshop on the subject, thus offering a good introduction to this subject and an indication of the state-of-the-art. Similarly, **Incommensurate Structures** will be covered with sessions and a workshop. Another topic of importance to all crystallographers is **The Use of International Tables**. The emphasis will be on symmetry, for those interested in a deeper insight, this will be followed by a session on The Use of International Tables: **Advanced Aspects** of Symmetry. There will be other more specialized sessions including **Non-Bonded Interactions, Methods in Macromolecular Crystallography** and **Instrument Calibration** as well as workshops on the practical use of MSD databases and the CRYSTALS software suites. There will be a Special Interest Group session on **DIAMOND** that should be of interest to a large proportion of the crystallographic community.

The **Bragg Lecture** will be incorporated into the UMIST BCA as well as the **Dorothy Hodgkin Prize Lecture**. The Prize Lectures for the Physical and Chemical Crystallography Groups will take place as usual, as well as the general **Poster Sessions**. Prior to the main meeting there will be sessions organized by the **Young Crystallographers** and this will include the oral poster sessions as well as the **Lonsdale Lecture**.

Some additional details of speakers are given over the following pages:

Further more up to date details are available via the main BCA Webpage or specifically at:  
<http://bca.cryst.bbk.ac.uk/bca/meets/bca04/bca04.htm>

## Plenary Session: Catalysis: from metals to macromolecules

**James Naismith (St Andrews)**  
Activation of Inorganic fluoride

**Guy Orpen (Bristol)**  
Structural systematics of phosphine ligands for homogeneous catalysis

**Jim Kaduk (BP Chemicals, USA)**  
Extraframework Species in Zeolite Y at Non-Ambient conditions

**Philip Woodruff (Warwick and FHI Berlin)**  
Surface Crystallography and its Relation to Catalysis

## Plenary Session: Bragg Lecture

**John Finney (UCL)**  
Beyond Bragg's Law: crystallography without a lattice

## Plenary Session: Dorothy Hodgkin Prize Lecture

**George Sheldrick (University of Göttingen)**

## **Plenary Session: Diamond SIG**

Chair  
Paul Raithby

John Evans  
(Southampton/Diamond)

Liz Duke (Diamond Light Source)

General Discussion

---

## **Parallel Session: Instrument Calibration – how to be a star!**

Dave Taylor et al (ICDD)

Manfred Kreichbaum  
(Austrian Academy of Sciences)

Steve Norval (ICI plc)

Martin Vickers (Birbeck)

Judith Shackleton (Manchester)

David Beveridge  
(Ilford Imaging UK Ltd.)

## **Parallel Session: Molecules in Medicine**

Gary Parkinson (London)

Neil Feeder (Pfizer)

J P Derrick (UMIST)

Carl Schwalbe (Aston)

---

## **Parallel Session: Incommensurate Structures**

Vaclav Petricek (Czech Republic)

Gervais Chapuis (Switzerland)  
– to be confirmed

Kenneth Harris  
(Birmingham /Cardiff)

Clivia Hejny (Edinburgh)

Rob Hooft (Bruker-Nonius)

---

## **Parallel Session: Incommensurate Structures Workshop**

The Jana software package

**Parallel Session :**  
**Use of International Tables -  
Symmetry**

Session Leader:  
Bill Clegg (Newcastle)

---

**Parallel Session:**  
**Use of International Tables:  
Advanced Aspects of  
Symmetry**

Session Leader:  
Mike Glazer (Oxford)

**Parallel Session:**  
**Methods in Macromolecular  
Crystallography**

Kim Henrick (EBI)

J Hadden (Leeds)

M A Walsh (MRC-France, ESRF)

---

**Parallel Session:**  
**Non-bonded Interactions**

A Parkin (Glasgow)

L. Infantes (CCDC)



*Then and now: Manchester trams.*





## Parallel Session: Small Angle Scattering

Mary Vickers (Cambridge)

Richard Clapperton  
(Huntsman Surface Sciences)

Manfred Kreichbaum  
(Austrian Academy of Sciences)

Peter Laity (Cambridge)

Mark Farnworth (Pilkington Glass)

Andrew Harrison (Edinburgh)

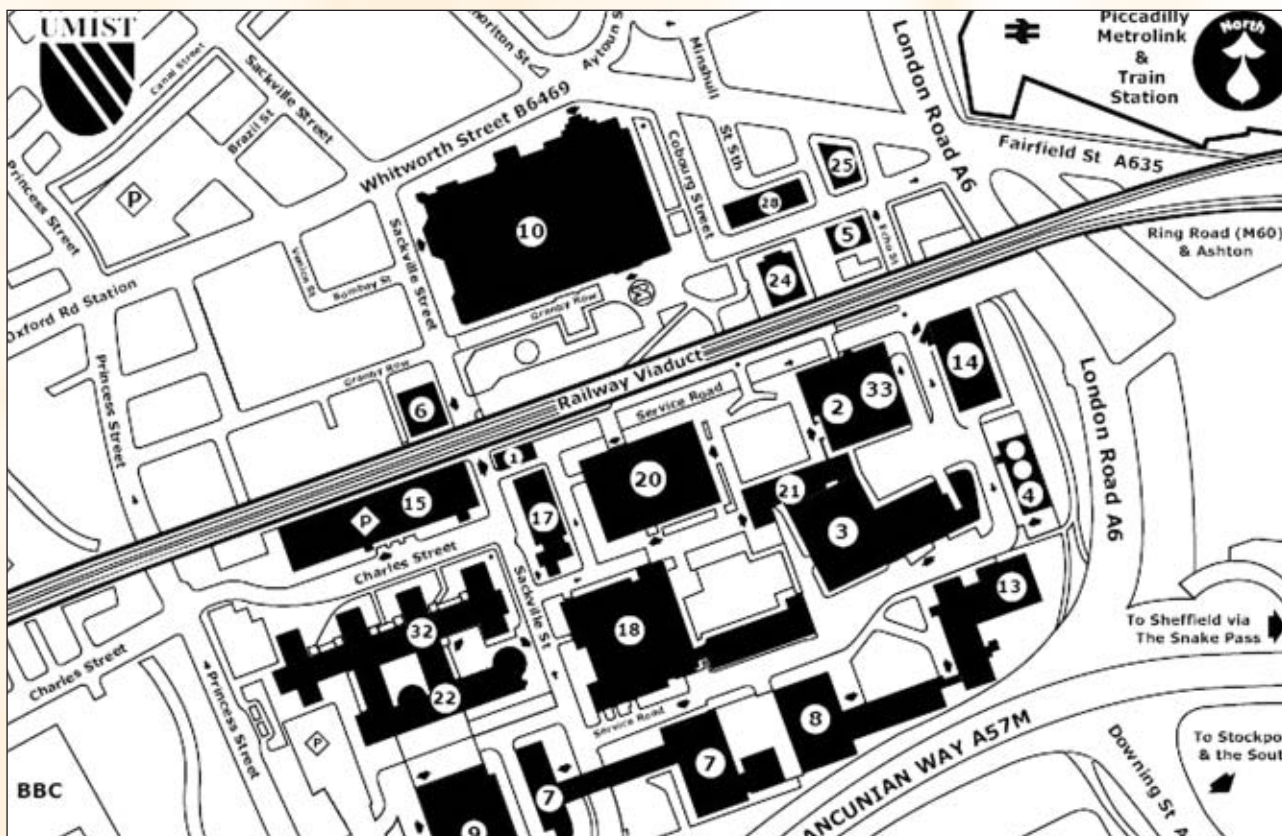
Richard Morris  
(Huntsman Surface Sciences)

## Parallel Session: MSD database services a practical session

Session Leaders:  
Kim Henrick and John Tate (EBI)

## Parallel Session: CRYSTALS Workshop

With David Watkin (Oxford)



*The UMIST Campus: The Renold Building is No. 20.*



	Monday 5 April	Tuesday 6 April	Wednesday 7 April		
08.30 hrs		Young Crystallographers Sessions	BCA Council Meeting 09.30 hrs - 10.30 hrs		
10.00 hrs		Coffee/Registration 10.30 hrs - 11.00 hrs			
10.30 hrs		11.00 hrs - 12.30 hrs - Plenary Session : Catalysis: from metals to macromolecules James Naismith (St Andrews) Guy Orpen (Bristol)	Parallel Session: Molecules in Medicine	Coffee/Exhibition	
12.00 hrs		Lunch & Exhibition: 12.30 hrs - 13.30 hrs	Parallel Session: Biomolecules in Medicine	AGM: Chemical Crystallography Group 12.00 hrs - 12.30 hrs	
12.30 hrs				Lunch & Exhibition will run	
13.00 hrs	Young Crystallographers Sessions	Plenary Session : Catalysis: from metals to macromolecules Jim Kaduk (BP USA) Phil Woodruff (Warwick)	Parallel Session: Methods in Macromolecular Crystallography		
13.30 hrs				Tea/Exhibition: 14.30 hrs- 15.00 hrs	Parallel Session: Molecules in Medicine: Chemical Aspects
14.30 hrs			Tea 15:00 hrs - 15:30 hrs		AGM: Chemical Crystallography Group 12.00 hrs - 12.30 hrs
15.00 hrs				Tea/Exhibition: 15.00 hrs - 15.30 hrs	Parallel Session: Small Angle Scattering
15.30 hrs	Young Crystallographers Sessions	Plenary Session : Bragg Lecture: John Finney (UCL) 15.30 hrs - 16.35 hrs	Parallel Session: Methods in Macromolecular Crystallography	Tea	
16.30 hrs			Oral Posters	DIAMOND SIG 16.40 hrs - 18.00 hrs	Prize Lectures: PCG & CCG
17.00 hrs	Dinner 18.30-22.30 hrs	AGM: Biological Structures Group 16.20 hrs - 16.30 hrs			BCA AGM : 1
17.45 hrs			Kathleen Lonsdale Lecture 18.30-19.30 hrs	Posters/Exhibitors 18.30-22.00hrs	Dorothy Ho George Sheldrick (Go
18.00 hrs					Young Crystallographers Mixer and Exhibition 19.30-21.30 hrs
18.30 hrs					
20.00 hrs					

Wednesday 7 April			Thursday 8 April			
Parallel Session: Incommensurate Structures	Parallel Session: Instrument Calibration: How to be a star!	Plenary Session: Use of International Tables				Parallel Session: MSD database services a practical session
10.00 hrs - 10.30 hrs			Coffee/Exhibition 10.00 hrs - 10.30 hrs			
Parallel Session: Incommensurate Structures	Parallel Session: Instrument Calibration: How to be a star!	Parallel Session: Non- bonded Interactions	Parallel Session: Small Angle Scattering	Parallel Session: Advanced Aspects of Symmetry		Parallel Session: MSD database services a practical session
	AGM:Industrial Group 12.00 hrs - 12.30 hrs	Lunch & Exhibition: 12.00 hrs - 13.00 hrs				
		Parallel Session: Non- bonded Interactions	Parallel Session: Small Angle Scattering	Parallel Session: CRYSTALS Workshop with PCs.		
Parallel Session: Incommensurate Structures Workshop		Tea/Exhibition: 14.30 hrs - 15.30 hrs				
AGM:Physical Crystallography Group 14.30 hrs - 15.00 hrs						
Tea/Exhibition: 15.00 hrs - 15.30 hrs			BCA Council Meeting: 16.00 hrs - 18.00 hrs			
16.35 hrs - 17.20 hrs						
Edgkin Prize Lecture: (Göttingen) 17.30 hrs - 18.30 hrs						
Dinner: 19.30 hrs						

# Meeting Reports

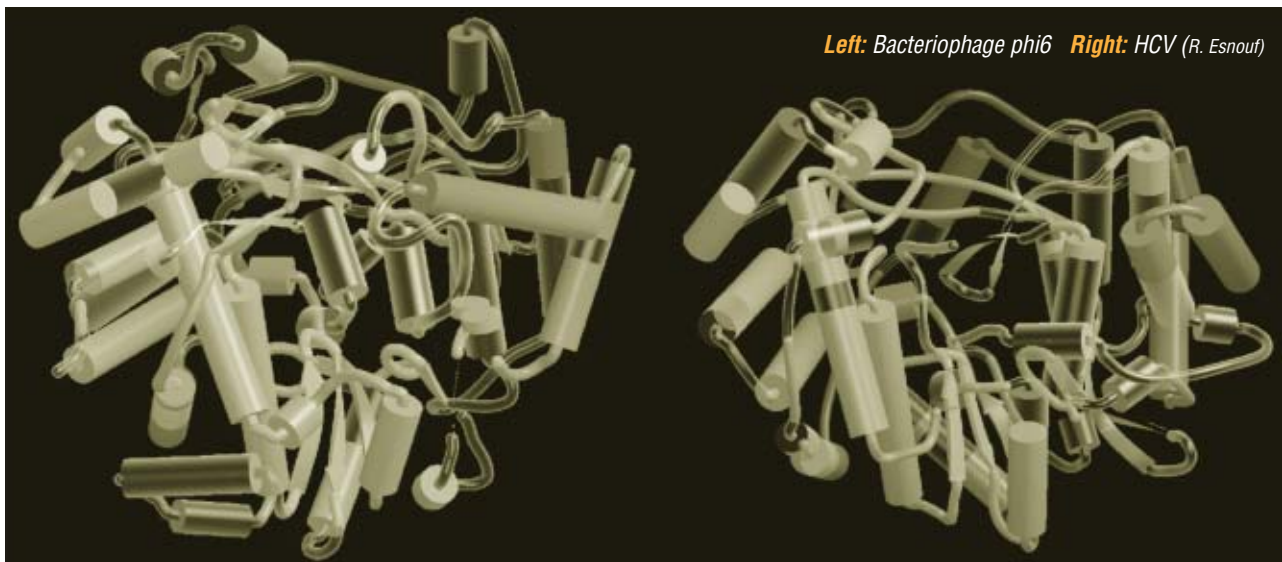
## CCP4 Meeting - Leeds 2004

**THE** New Year brings us to the annual **Collaborative Computational Project in Macromolecular Crystallography (CCP4)** meeting which was moved a bit westward from its recent home in York to the home of Tetley's brewery – Leeds! Held on the University of Leeds campus from January 4th to 5th, the meeting focused on “Model building and refinement” with a scientific programme organised by Martin Noble (University of Oxford) and Anastassis Perrakis (Netherlands Cancer Institute, Amsterdam, The Netherlands). This popular event was attended by 394 registered delegates coming not only from Europe and the USA, but also from Israel, India, China and Japan.

**Alwyn Jones** (Uppsala University, Sweden), a self confessed dinosaur, began the meeting with a talk on “Interactive electron density map interpretation”, which covered the development of interactive molecular graphics over the last the 25 years or so. Much of the talk was based around developments in his laboratory such as “Frodo”, released in 1979, which marked a major leap forward in the field. This programme rapidly became the tool of choice for many. Frodo had many useful features, e.g. flexible viewing of the molecule, the freedom to tear the molecule apart, interactive regularization of geometry, precontoured maps, etc.. These features were further developed, and a successor appeared about a decade later in the form of “O”, which is widely regarded as the “gold

standard” of molecular graphics. This programme, as well as others like it, illustrates how many of the developments in model building have been concerned with providing tools for easy correction of errors. Two types of errors which are particularly common are: 1) out of register errors (where the sequence is not aligned correctly with the structure); and 2) mis-assignment of sidechains. Principal reasons for the occurrence of these model-building errors are related to phasing errors, lack of high resolution data, and inexperience of the crystallographer. Newer tools helping to eliminate these errors include autotracing, which uses dynamic programming algorithms to allow rapid assessment of the quality of a model during the building process, involving corrections to alignments of the sequence and structure.

Session 2 opened with **Paul Emsley** (University of York, UK) who talked about the “Model building tools for molecular graphics” which are being incorporated into his programme “COOT”, which will provide the model building tools for the CCP4 Molecular Graphics project, “CCP4 MG”. COOT is free software built on free libraries. In particular, the use of the CLIPPER libraries means that the maps generated using COOT are essentially infinite and always map back into the asymmetric unit. Paul pointed out that no-one reads the manual, users like to use graphics programs in full-screen mode, and that users hate typing commands. As a result, COOT has “sophisticated defaults” which allow for these preferences. COOT is available from <http://www.ytbl.york.ac.uk/~emsley/coot>.



*Left: Bacteriophage phi6 Right: HCV (R. Esnouf)*

In “Overcoming the Ffear of Buccaneers”, **Kevin Cowtan** (University of York, UK) talked about the use of simulated maps in phase improvement programmes with particular emphasis upon “Pirate” and “Buccaneer”. He stressed the need for the development of optimal statistical targets for map simulation. Both Pirate and Buccaneer use a noisy map (generated from a refined model) to match a target noisy map (generated from an unknown structure). Phase errors are estimated and transferred from the target to the simulated map, then the data are rescaled and the process repeated. Reliable Figures of Merit (FOMs) are required. Pirate is a phase improvement programme which removes the limitations generated by the application of a solvent mask. These limitations arise from the way that ordered solvent or disordered protein are dealt with, or the fact that some value for the solvent content must be used for other methods of density modification. Buccaneer improves on this by using a log likelihood gain target in the transfer process. The results obtained are highly dependent on tuning the program parameters appropriately, and so should be viewed with some caution. However, bearing this in mind, the two programs do seem to give improved phases over other approaches.

After lunch, **Richard Morris** (European Bioinformatics Institute, Hinxton, Cambridge, UK) briefly overviewed some important pattern recognition techniques and classification methods, and provided some ideas about decision theory, linear programming and graph theory. Special attention was given to those approaches that have been employed with success in macromolecular crystallography, especially in the area of automated protein model building. His final take-home message was that Pattern recognition techniques are “very” cool.

**Tom Terwilliger** (Los Alamos National Laboratory, Los Alamos, NM, USA) described the Pattern-based probabilistic identification of protein sidechains, which has been successful in automated model building for maps with resolution as low as 3 Å. He demonstrated how tripeptides can be used in model building iteratively combined with statistical density modification to improve the quality and completeness of atomic models of macromolecules.

**Zbyszek Otwinowski** (Texas Southwestern Medical Center, Dallas, TX, USA) discussed the main features of his fragment-based model-building developments. Data mining techniques were used to identify the clusters of similar three-dimensional shapes in connected carbon alpha-traces. The resulting library is then used in a search based on a fast-rotation function, which is faster and more flexible than a translation function based search. Bayesian analysis of known structures based on maximum entropy approach is applied to build sidechains using conformational preferences that depend on the main chain structure.

**Vito Calderone** (University of Siena, Italy) followed with a more practical presentation to close the Session, targeting mainly the younger audience. He described key examples from his

own research project which demanded that he switch between various phasing and density modification program packages in the right sequential order to solve the structures.

Session 3 opened with an authoritative overview of refinement by **Dale Tronrud** (University of Oregon, Eugene, OR, USA). He explained the differences between maximum likelihood, least squares and empirical energy refinement and search, and 1st and 2nd derivative minimisation methods. Relatively new methods of torsion angle refinement and TLS refinement have allowed better residuals at low and medium resolution respectively. Dale pointed out that all packages use agreement of test set to calibrate error and increasingly other parameters such as the weighting of restraints and X-ray terms, and suggested that a second test set might be required to get a true free residual if more and more parameters are to be estimated from the ‘free’ set. In true Las Vegas-style, our croupier **Airlie McCoy** (University of Cambridge, UK) next had us shaking virtual dice of many sides in an extension of her well known review to make comprehensible more facets of maximum likelihood. In the middle of her presentation she explained that the probability of the Resurrection occurring has been calculated as 0.97 by Professor Swineburne (ask Airlie for the reference!). She then pointed out that uses of Bayes theorem have to be appropriate and require that the priors are properly assessed. In principle in maximum likelihood you do not need to weight the priors (chemistry) and the likelihood of the data (X-ray terms), given your model, but in protein crystallography you have to overweight the X-ray terms to get convergence.

**Garib Murshudov** (University of York, UK) then updated us on the developments in REFMAC (the main refinement program in CCP4) by explaining the intricacies of the dictionaries used to restrain the refinement and advising us on how to deal with a new ligand. He then outlined the Fisher Information Matrix which he has implemented as the minimiser in Refmac 5.2.

**Gerard Bricogne** (Global Phasing Ltd., Cambridge, UK) next explained how his programme BUSTER, in combination with TNT, can be used to deal with refinement of a very partial model which could arise, for example, from a molecular replacement solution of complex based upon one component part. The session closed with **Navraj Pannu** (Leiden University, The Netherlands) who pointed out that the assumption in phased refinement targets that the phases are independent of the model is not valid. To overcome this he has implemented a new likelihood function in his programme BP3. Navraj presented some encouraging preliminary results of where this approach has been used to deal with the difficult single wavelength anomalous dispersion where the bimodal phase distribution is particularly problematic.

The following morning saw the start of session 4, “Phase recycling, Model completion and ligand fitting”, and opened with **Piet Gros** (Utrecht University, The Netherlands) who



discussed a procedure he calls “Conditional Optimization” which combines molecular dynamics methods with fragmentary models composed of loose atoms as a means of improving the model-quality generated the initial stages of refinement, particularly in cases where only low to medium resolution data are available. The advantages of the procedure include a large radius of convergence which may prove useful when attempting *ab initio* phasing.

**Pietro Roversi** (Oxford University, UK) then followed. He expanded on the earlier presentation by Gerard Bricogne showing an example of how maximum likelihood methods in the BUSTER-TNT package can be used to refine a larger structure from an incomplete molecular replacement solution. The example discussed in detail showed how interpretable electron density could be obtained for a four domain fragment of the CD55 protein based upon a molecular replacement solution using only two of the four domains. Although care must be taken to obtain high quality low resolution data to use in this approach, the method seems to hold promise for aiding the solution of multiprotein complexes, for example, in the future. More details about the programme can be found at <http://www.globalphasing.com/buster/>.

**Serge Cohen** (Netherlands Cancer Institute, Amsterdam, The Netherlands) then brought us up to date with a description of the new model completion capabilities of the popular ARP/wARP package which is widely used for automated modelling of both protein and water molecules in electron density maps. A new event-driven control system was discussed which relies on an iterative approach to enable the modelling protocol to adapt during the execution of the process itself. This should lead to the automatic generation of models with even higher completeness and the generation of better models when only medium to lower resolution data are available. Other features discussed included procedures to give improved interpretation of loop regions and a reference to an electronic version by Alwyn Jones for structure validation.

**Petrus Zwart** (European Molecular Biology Laboratory Hamburg Outstation, Hamburg, Germany) closed the session with a complementary talk about the capabilities of ARP/wARP in the automated modelling of substrates, inhibitors and other ligands within a protein crystal structures. Given the variety of chemical structures involved this is a very challenging area for modelling in any case. Preliminary data were shown which demonstrated how difference electron density maps were being used to automatically identify objects within a crystal structure, and how procedures are being developed with appropriate scoring functions to provide enough pattern recognition so that complex ligand structures can be modelled in with improved confidence.

Session 5 on “Validation and Analysis” was held after coffee. First, **Gerard Kleywegt** (Uppsala University, Sweden) stressed the importance of depositing structure factors to allow users of the Protein Databank to view electron density, rather than just the refined interpretation

available from coordinates. He described the Uppsala Electron Density Server, which automatically calculates electron density and calculates R-factors for comparison with deposited values. Gerard appealed for help in discovering the reasons for those cases where significant differences arise, so that the methodology can be improved or errors corrected. It appears that not everyone is pleased about this.

**Duncan McRee** (ActiveSight Inc., San Diego, CA, USA) followed with a description of his new fitting program MI-fit. Although this is a commercial program, it is available free as a “demo” version for 60 days. His talk started with a memorable comparison of some CCP4 members with the characters of the Harry Potter books, and then described this very useful-looking successor to the very popular XtalView.

**Eugene Krissinel** (European Bioinformatics Institute, Hinxton, Cambridge, UK) went into hardcore details of the new coordinate libraries to be included in the next CCP4 release. These libraries will not only improve existing programs but will also simplify the development of new applications. Eugene went on to show how these libraries have been included in the SSM server at EBI and gave examples of protein structure alignment using SSM.

**Thomas Schneider** (FIRC Institute of Molecular Oncology, Milan, Italy) concluded the session by describing the programme ESCET and showed how coordinate uncertainties can be included in the comparison of structures to find the subsets to superpose or define as a rigid region. The program uses a generic algorithm to interpret large matrices. Examples of how the results gained can be used to provide biological insight were discussed.

The final session of the meeting addressed the topics of visualisation and illustration. **Warren DeLano** (DeLano Scientific LLC, San Carlos, CA, USA), author of PyMol, discussed in depth the philosophies of generating truly open source software to provide a ubiquitous tool in all arenas of science. He also discussed the frustrations of finding a suitable environment in which to provide freeware, and (almost apologetically) introduced his company DeLano Scientific, which survives on over 100 sponsorship contributions from individuals, companies and labs. He described use and applications of PyMol, which appears particularly suited to animated illustrations of biological interactions and morphing.

**Robert Esnouf** (University of Oxford, UK) related how BobScript was born as an enhancement of Per Kraulis’ program MolScript. MolScript underwent a transformation in version 1.4 when ray-tracing using Ethan Meritt’s Raster3D was introduced. BobScript added a number of features to MolScript 1.4, including the all-important ability to depict electron density. Details of the syntax (e.g., atom selection) were described as well as current capabilities, including generation of surfaces, movies and solid objects that can be POV-Ray rendered in ways that are only limited by your imagination. Robert delighted the audience by showing

physical virus models that had been generated sheet by sheet on a printer using BobScript map/surface output.

**Martin Noble** (University of Oxford, UK) suggested that graphics could be an important tool in relating form to function. Together with Paul Barrett, he developed a public web-interface called "Dynamite" <http://biop.ox.ac.uk/www/Dynamite.html> which will generate simulations from a set of coordinates. The user provides a coordinate file and presses start – and various results can then be down loaded including very attractive animations which illustrate the dynamic flexibility of your molecule: this can often be extremely revealing in terms of function. The dynamics techniques are well established but take time to master, and it is hoped this web-based tool will prove useful to those who desire a quick dynamic analysis. Martin finished his presentation showing a movie of a molecule that had escaped the confinement of a graphics program: it had landed on his desk. They're very friendly, really, though a bit shy.

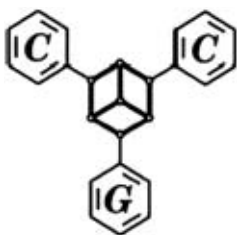
The last talk of the meeting was presented by **Liz Potterton** (University of York, UK) and discussed progress in the CCP4mg project: release version 1.0 is expected in February. This version will have continuous map and molecule generation, various modes of molecule display, selection tools, and some functionality. The labelling capability looked impressive. There will much further development but this should include user feedback from v1.0. We look forward to it!

In addition, a really excellent meeting dinner was held on the University of Leeds campus, which included a decently priced bar and a live band performing a repertoire to rival Pop Idol! As always, the smooth running of the meeting was guaranteed by the CCP4 organisation (Daresbury, UK) which includes **Maeri Howard-Eales, Charles Ballard, Pat Broadhurst** and **Liz Kennedy**. Without doubt their efforts guarantee that next year's event will be as popular as ever. One word of advice to next year's organisers...buy at least two bottles of whiskey to prevent any "punch-ups" in the future as Maeri really looked determined to take Charles Ballard's bottle of whisky instead of her bouquet of flowers!!

#### Members of the BSG

## CCG Autumn Meeting, 12 November 2003, Accelrys

"After Refinement – What Comes Next?"



**THE** CCG Autumn Meeting for 2003 was hosted in Cambridge by Accelrys and sponsored by MSC Rigaku. There was an excellent turnout with about 80 attendees.

After short welcomes by **Sandy Blake** (CCG Chairman) and **Vanessa Hoy** (local organiser), the programme began with **Tony Linden** (Zurich) describing "CHECKCIF 2003 - a general structure validation tool". Tony is Data Validation Editor for Section C of Acta Crystallographica, and was able to draw on a wide range of examples of incorrect or problem structures. He described the history of automatic validation which is now an integral part of every crystal structure analysis, helping authors to improve the quality of their structures and speeding the publication of results. The new version of the CHECKCIF program has a unified validation report and a clearer layout, and provides explanation of and possible solution to its various alerts. Tony detailed the validation procedure for Acta C papers, and also alluded to the procedures adopted by chemical journals. Finally, he gave several examples of mistakes which validation would not pick up, reinforcing the need for further checking.



**Speakers at CCG Autumn Meeting.** (l to r): *Kirsty Anderson, Richard Cooper, Frank Allen, Tony Linden, Mike Hursthouse, John Davies, Claire Wilson, Peter Murray-Rust.*

**Richard Cooper** (Oxford) continued the validation theme, but concentrated on "Validation as you go", where mistakes are avoided by carrying out validation at each stage of the structure analysis. In contrast to most structure analysis software, CRYSTALS provides guidance and validation throughout the process, essential because analyses are more and more being done by scientists with little or no formal crystallographic training. There are graphical analyses for hkl data, checks on the initial model and the placement of hydrogen atoms, and for effects such as extinction and twinning. Richard gave a further example in the link to MOGUL, a library derived from the main CSD which because of its design allows very fast retrieval of molecular geometries. Comparing these to the crystallographic model under refinement will immediately reveal errors or "interesting features". There is potential for extending this to chemically similar, and not just identical, geometries.

In her contribution, "Publishing crystallography in chemical journals", **Kirsty Anderson** (RSC) pointed out that most crystal structures are published in chemical journals, and described how her organisation publishes 20 primary chemistry journals, many of which contain articles with crystallographic content. The majority of the assessment is

done by Kirsty as the RSC's in-house Crystallographic Data Editor, working closely with the journal's Editorial teams. Most of her work (3500 structures per year) is for articles submitted to Dalton Transactions and Chemical Communications. Normally the manuscript is accompanied by a CIF, which goes to CCDC for initial checking, then back to Kirsty for further examination. In problem cases she may consult an external referee. Her main concern is to establish whether the structure analysis really does support the chemical conclusions drawn from it, and to this end she uses PLATON, ORTEP, Mercury and other software to check the CIF, the correctness of the molecular assignment, the stereochemistry, the intermolecular interactions and the detailed molecular geometry. The main problems she encounters are raw CIFs, disagreement between the manuscript and the CIF, missing crystallographic footnotes, suspiciously short intermolecular contacts and wrong absolute configuration. The structures she sees fall into three categories: the good, the bad and the ugly, the latter being structures of generally low precision. The rejection rate is about 2%, usually because of mis-assigned atoms or incorrect space groups.



*The local organisers: Anne McCloskey and Vanessa Hoy.*

After lunch **John Davies** (Cambridge) addressed the thorny subject of "Unpublished structures". His laboratory possesses two CCD area detector instruments which have provided datasets for 2652 complete, publishable structures in the last five years. However, while the time to determine a structure has reduced from months to under a day over the past 40 years, the time to publication has not changed greatly. He estimated that only about 20% of his structures have reached the public domain and he extrapolated from this to give a world-wide total of 444,000 unpublished structures (compared to 300,000 in the CSD!) He then addressed various possible solutions to the problem. Hiring more crystallographers was impractical, not least on financial grounds, and external deposition seemed the most promising route. This would require the permission of the owner of the data, but if a structure remained unpublished after 2-3 years it should be entered into a database. The procedure would have to be easy and automatic, involving no human refereeing but instead relying on freely-available evaluation software. John favoured deposition of the hkl data as well as the CIF, as this would require an average of only 500 kb per structure.

**Peter Murray-Rust** (Cambridge) then spoke on "e-Science in Crystallography and Chemistry: CIF and CML", describing the revolutionary impact of the Web and the GRID, where tools and knowledge are freely and openly available and disciplines can interoperate. While conceding that crystallography had pioneered data validation, electronic publication and data management through standard CIF syntax and dictionaries, he stated that other disciplines were now more advanced in their treatment of data. Where information is well understood it is possible to delegate much of its management to robots. Where there are multiple domains, common ontologies or mappings can be created so that information can be shared and aggregated. By using a common XML architecture - Chemical Markup Language (CML) - it is possible to integrate chemical and crystallographic information. CML is able to manage both the primary molecular crystallographic information and the wider set of properties (observed and calculated data, spectra, etc). A major loss of information occurs when results are published on paper, but if conventional chemical publications can be held entirely in XML, management tools will allow the journal article and/or supplemental data to be accessible by computer.

In addressing "The future of crystallographic 'publication'", **Frank Allen** (CCDC) noted that every crystal structure is important, its value extending well beyond the original motives for the analysis. By September 2003, the CSD had reached 300,000 structures, in line with earlier predictions, and although the advent of CCD area detectors had not yet had a major impact 75% of all determined structures remains unpublished. This lack of data is a drawback for users of the CSD: their awareness of current work will be incomplete, as will scans for known unit cells. Deductions will be less reliable: studies carried out now would not have been possible on a smaller number of entries. The impediments to publication include the question of who owns the structural data; what happens to structures that do not turn out as expected; what happens when the chemistry is rejected; and questions of academic recognition. The proposed solution is for data deposited at submission to be held in a secure CIF archive for three years, and then distributed. Frank acknowledged that this raised several questions, including those of validation and quality control, and what constitutes a publication.

The Meeting finished with a lively discussion session, covering many of the topics raised in the lectures as well as the archiving of data, the copyright status of numerical information, the content of databases and the ownership of results.

Finally, the Chairman thanked the speakers and session chairs, MSC Rigaku and Accelrys for generously sponsoring and hosting the Meeting, and the local organisers for their efforts in making it so successful. Pfizer was thanked for sponsoring free registration for student members of the BCA.

**Sandy Blake, University of Nottingham**

# CCG AGM



The Annual General Meeting of the Chemical Crystallography Group will be held on Wednesday 7th April 2004 during the BCA Spring Meeting in Manchester, starting at 12 noon.

Final details of the agenda and venue will be published on the CCG website  
<http://www.crystallography.org.uk/CCG/agm04.html>.

Items for inclusion in the agenda should be sent to the Secretary of the CCG to be received no later than Wednesday 31st March 2004.

## CALL FOR NOMINATIONS

Elections will be held for the posts of Secretary/Treasurer and one ordinary member of Committee. The present incumbents (Secretary/Treasurer, Dr Harry Powell; Member of Committee, Dr Simon Coles) will have each served a full term and are not eligible for re-election to the same posts (see rules 12 and 15 of the Constitution).

The deadline for nominations is Wednesday 31st March, i.e. 7 days before the AGM. Nominations may be made by e-mail; they must be supported by no fewer than two members of the CCG and should be accompanied by the written consent of the nominee.

## CURRENT OFFICERS (TERM OF OFFICE):

### CHAIRMAN

Dr Sandy Blake, (2003 - 2005)

### DEPUTY CHAIRMAN

Dr Simon Parsons, (2003 - 2005)

### SECRETARY/TREASURER

Dr Harry R. Powell, (2000 - 2004)

### COMMITTEE

Dr Simon J. Coles, (2001 - 2004)

Dr Richard Cooper, (2002 - 2005)

Dr Michaele J. Hardie, (2002 - 2005)

Dr Mary F. Mahon, (2003 - 2006)

Dr Georgina M. Rosair, (2002 - 2005)

Dr Simon J. Teat, (2002 - 2005)

Ms Katharine Bowes

(co-opted Student Representative) (2003 - 2005)

Dr Vanessa Hoy

(co-opted local organizer Autumn Meeting 2003) (2002 - 2004)

## BCA IG Forum II Birkbeck College London 13 & 14th November 2003



### THURSDAY 13th am

**THE** meeting started with a brief introduction by Jeremy Cockcroft who also thanked Dave Taylor for all his hard work in organising the meeting. Unfortunately, Dave could not be present as his wife Ann was recovering from hospital treatment. We all wish you a speedy recovery Ann.

### Opening session – Non-ambient Diffraction + Amorphous Pharmaceuticals.

#### 1. In-situ Diffraction From Materials and Macromolecules Under Microwave Irradiation – Andrew Harrison, University of Edinburgh.

The design and construction of equipment to drive solid-state reactions using microwave radiation and the monitoring thereof using X-ray or neutron scattering was discussed. Andrew described how fundamental information could be obtained from in-situ studies for e.g. the direct synthesis of magnetite from microwave hydrolysis of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$ . The original microwave source was a commercially available microwave oven, which was attacked with a hacksaw and a soldering iron! However, it was soon discovered that these units are unsuitable for sensitive heating control because they always run at full power - only the time of the irradiation can be varied. This experimentation led to the development of a purpose built instrument in which the microwaves could be "broadcast" by use of an antennae inside a high-pressure reaction bomb. Issues with thermometry, uneven heating and hotspots were also discussed as were the measurement of cell parameters including lattice expansion. Future work will include in-vivo studies of biomolecules for e.g. protein "wringing" modes.

#### 2. Non-Ambient Laboratory Powder Diffraction Studies – Synthesis, Kinetics and Phase Transitions – John Evans University of Durham.

In this presentation John described some of the laboratory experiments, which have been made possible by new developments in non-ambient powder diffraction technology including the synthesis of materials, the study of reaction kinetics and phase transitions. The equipment used was a Bruker D8 Advance diffractometer combined with a 1500 K furnace, a Cryofurnace (77 – 723 K) and a Cryostat (11 – 300K). Variable temperature powder diffraction gives lots of new information about the properties of materials for e.g. expansion rates, phase transitions, kinetics, crystallisation, chemistry, order-disorder transitions. Structural phase



transitions of inorganic oxides, for e.g. framework materials such as  $ZrW_2O_8$ , in which the unit cell is found to have a negative coefficient of thermal expansion. Following the change of width of the diffraction peaks enables the monitoring of domain changes as a function of time. (This work is available via the RSC website – a “Hot” article). Synthesis of  $ZrW_2O_8$  has also been performed in the diffractometer.

### **3. A Review of Methods Used to Quantify Amorphous Content in “Crystals” – Graham Buckton, The School of Pharmacy, University of London.**

Graham started his presentation by asking the question – “Is amorphous material important?” to which the answer is – “Yes – very”. Amorphous material is usually thermodynamically unstable, its presence is not normally intentional (e.g. it is introduced during the milling process) and it acts as sites for the absorption of water. Normally present at about the 1-2% level.

How does one study / quantify it? Various techniques available;

- DSC
- XRPD
- Spectroscopies
- Inverse Phase Gas Chromatography

For example amorphous lactose and amorphous raffinose. Both may contain 1-2% amorphous material, which effect inhalation efficiency and the solubility of drugs for oral delivery. Amorphous content may be viewed in two different ways. There may be crystals with a 99% crystalline core and a 1% amorphous surface or 99% of the particles may be crystalline and the remaining 1% is amorphous. If the product starts at 100% crystalline physical manipulations such as milling will disrupt the surface and introduce an amorphous phase(s?), which will vary with time so the properties of your product are not constant and will vary from batch to batch.

### **THURSDAY 13th pm**

#### **4. Standardless Phase Quantification of Industrial Coatings – Susan Etok, RMCS Cranfield University.**

Susan described the process of plasma spraying of hydroxyapatite onto titanium substrates compared to direct, low temperature electro-deposition for use in prosthetic coatings. It is important to measure the amount of amorphous calcium phosphate in these coatings and this is done using XRD.

#### **5. Understanding Gear Performance with X-ray Diffraction – Brian Shaw, Design Unit, University of Newcastle.**

Submarine Gearboxes – makes a change (sorry!). Statement – “gears fail mainly from fatigue”. Brian described the importance of how gear design and mechanical alignment can be improved from residual stress XRD measurements.

#### **6. Use of Intense Radiation Sources in the Study of Functional Materials – Paul Barnes, Industrial Materials Group, Department of Crystallography, Birkbeck College.**

Paul described how neutron and synchrotron sources are enhancing rapid time resolved observation of functional materials using such techniques as XRD.

Three stories were told to enlighten us;

*The Brownmillerite story.*

*The Zirconium Hydroxide Story and*

*The TEDDI story.*

#### **7. Building Your Own Furnace for HT-XRD – Gopinathan Sankar, Davy Faraday Research Laboratory, The Royal Institution.**

This paper described some of the *in situ* cells that have been developed for examining phase transformations in catalytic materials.

#### **8. Using High Temperature X-ray Diffraction with Steel / Aluminium Production: Look Where the Action is! – Stefan Melzer, Corus RD&T, Ceramics Research Centre, The Netherlands.**

This presentation described how production processes can be controlled and improved by following the melting and crystallisation of materials at high temperatures using X-ray diffraction.

#### **9. Inconstant Catalysts –**

**Steve Norval, ICI Measurements Science Group**

Amongst other processes, Steve described the importance of XRD in catalyst design noting amongst others the production of ethylene oxide (a major precursor of many surfactants) and the production of margarine from linoleic acid.

### **FRIDAY 14TH November am Industrial Group Award Lecture:**

#### **Adventures in Crystallography in the Gas Turbine Industry – Colin Small, Rolls Royce PLC, Derby.**

Following an introduction from Judith Shackleton in which Colin's' career in XRD at RR was described pictographically using “Haircuts Through the Ages” as its central theme, Judith presented Colin with his BCA IG award for outstanding contribution to X-ray Analysis which was a molecular model of Diopside ( $CaMgSiO_3$ ). She also presented him with a model of a Supermarine Spitfire and a pair of the most sought after Vulcan Appreciation Society socks!

After much applause, Colin thanked Judith and the audience and with his normal aplomb got stuck into his presentation. Oh dear, oh dear me. Colin was not up to his normal stratospheric presentational standards – no, this time he surpassed himself! His description and video footage of the Rolls Royce patented goose slicer (more of which later) will long be remembered by the traumatised audience (which included Colin's parents, wife and children). Colin went on to describe the Rolls Royce Trent 900 gas turbine engine, which will eventually be fitted onto the

Airbus A380 airliner, which will ferry us all about the planet during our summer holidays. (By-the-way, this engine has a by-pass ratio of 8.1:1 and develops 70,000 lbs of thrust).

As aeroplanes fly through the air they ingest any manner of debris; from hailstones through to the major constituent of your Christmas dinner. So, not surprisingly, the testing procedures that these engines have to endure are extremely rigorous. Some of these Colin described, including the hail gun, during which a zillion tons of ice per minute are “shot” at a running engine and the bird injection test, for which there are three standards – the small bird (2½lb chicken) the medium bird and the large bird, (the aforementioned goose) of about 8 lbs. Colin pointed out the importance of defrosting the feathery projectiles before shooting them into the engines!

Colin went on to describe the importance of determining the structural integrity of the turbine blades of the engine and how this is monitored using XRD. The turbine blade is also full of small holes, to allow the passage of 70 tons/min of air through the engine, and in dusty environments (e.g. deserts), these holes can clog up with dust which melts (to form Diopside which was identified using XRD). As the blades are operating at some temperature above their melting point this is not a good thing! Next was the problem of volcanoes – or more specifically the problems encountered when an aircraft flies through the dust plume of an eruption. The dust particles from an eruption are extremely abrasive, and it has been one of Colin’s major tasks over the last few years to understand exactly what goes on inside a gas turbine engine when it swallows umpteen tons of vaporised pumice. The fan blades of the engine – the ones at the front (which do the bird slicing) - are composed of three sheets of titanium and are hollow. The way in which the crystalline texture of these blades is effected during their manufacture is crucial. Colin went on to describe his use of pole figures, Euler space and orientation distribution functions in his quest for a numerical description of texture of the fan blades that engineers could understand.

Colin concluded his lecture by describing how the turbine rotor shaft is joined using an enormous inertia welding kit. The only way to examine the resulting joint is by neutron diffraction and this was carried out at the ISIS facility at RAL (must have been difficult getting the samples in and out of the hire car!). Another round of applause followed – Colin, X-ray diffraction lectures will never be the same again!

## **FRIDAY 14TH November pm** **Industrial Applications of XRD**

### **1. Microstructural Characteristics of Advanced Materials Using Electron Backscattered Diffraction (EBSD) – Philip Holdway (and H.S. Ubhi) QinetiQ Ltd. Cody Technology Park, Farnborough, Hampshire.**

Phil briefly described the theory of EBSD before moving on to some applications. First of all you need an SEM with the sample tilted to around 70°, and successful analysis relies

on having strain free surfaces and good Kikuchi patterns. These are produced from Bragg diffraction peaks of back scattered electrons from the sample which have an interaction depth on the sample of ~50 nm. Data collection is made by scanning over a grid and can be either manual or automatic. For example shape memory alloys – Ti/Ni – the SEM image is used to select a particle for analysis then EDS is used for elemental analysis and EBSD to determine the crystalline properties of the particle. In this way it is possible to obtain complete identification of small particles within an alloy with no need for TEM or XRD. Phil then went on to discuss the analysis of ZrH and ZrH<sub>2</sub> formation on the surface of Zircalloy, and the analysis of grain structure in laser deposited W, a process that enables the formation of complicated shapes that could not be manufactured using conventional machining techniques. (It is much less wasteful to build a structure up rather than start of with a large lump and end up with a pile of swarf). Phil went on to say that although EBSD is a powerful tool and can make up to 50 measurements a second, only a very small area is examined when compared with conventional XRD.

### **2. XRD and Reflectivity Measurements in the Glass Industry – Mark Farnworth, Pilkington plc.**

Mark described how the techniques of XRPD, GAXRD, pole figures and X-ray Reflectivity measurements can be used to examine samples from all stages of glass manufacture, from the crystalline raw materials to the amorphous final product. GAXRD is used to examine thin coatings on the glass surface for e.g. hydrophobic coatings, which disperse water. Refractory materials are examined to determine how much non-crystalline material is present and the amounts of quartz, cristobalite and tridymite. Also, multi-layer stack coatings are examined. e.g. Ti, ZrO<sub>2</sub>, Ag and Si. Texture maps can be produced which show the degree of texture in the silver layer of the coatings and the thickness, density, top and bottom roughness of each individual layer can be measured.

### **3. Applications of XRD in the Imaging Industry – David Beveridge, Ilford Ltd.**

With the advent of digital imaging technology the decline in sales of silver halide based film emulsions has been swift. So members of the imaging industry have had to adapt just as swiftly and this has had an effect of the type of samples that the X-ray crystallographer can now be expected to examine. David explained that, historically, most of his samples were silver halide film surfaces and included the identification of the composition of processing solutions. Now the majority of his samples are from printer-pigmented inks.

**Richard Morris**

## **FRIDAY 14TH November pm**

The final session of the forum was devoted to the theme of X-ray Diffraction: Past, Present, and Future. With the meeting being held in the Clore management centre in Torrington Square, Birkbeck College, it was highly

appropriate that Alan Mackay should open the session with a lecture on the past. The old buildings of the Crystallography Department as founded by J.D.Bernal used to stand on the adjacent site. Amongst the many photos of old equipment, he showed a picture of Bernal's X-ray rotation camera, and then contrasted it with the "big science" now done at the ESRF. Probably though the biggest changes have been in computing as shown by the photo of an early computer at Birkbeck college from the 1950s laboratory of Donald Booth. The second talk was by Judith Shackleton on present X-ray instrumentation, a difficult talk to give without advertising the advantages of one manufacturer over another. After working her way through the maze of primary and secondary optics, monochromators and mirrors, area and solid-state detectors, she arrived at the "Portable Stress Diffractometer", a most remarkable piece of kit capable of measuring stresses in very large objects indeed. One wondered what the response would be at Birkbeck College to its lack of radiation shielding! The Industrial Group committee decided, given the importance of future instrumentation for industrial crystallography, that the final talk of the forum should be an Alun Bowen lecture. The talk on the new UK synchrotron source was given appropriately by Alexander Korsunsky, who described the features of the beamline JEEP proposed for DIAMOND. The talk ended with an aerial photo of the DIAMOND site showing that construction was now seriously underway and the "future" lay just ahead.

Phil Holdway

### BCA IG Forum II 2003 : Pharmaceutical Parallel Sessions

**Over the course of two days three parallel sessions were held covering non-ambient PXRD applications, polymorphism case studies and the analysis of amorphous materials in a series of nine 30-minute lectures.**

The non-ambient session was started with an excellent introduction to RELATIVE HUMIDITY CONTROLLED X-RAY DIFFRACTION by Brett Cooper, (MSD), explaining what relative humidity is and how its variation can impact on pharmaceutical ingredients. He described the latest computer controlled system and how it is now possible to mimic the complementary technique of Dynamic Vapour Sorption (DVS). An example of one of these new computer controlled systems, the Bruker/Ansysos Hot Humidity Controlled system giving the ability to stress samples with combinations of high temperature and high relative humidity. Terry Threlfall (University of Southampton) spoke on STRUCTURAL SIMILARITY, DISSIMILARITY AND REPRESENTATION using alkali metal tartars, frusemide and sulphonamides as examples to reveal unexpected relationships between structures. The use of high pressure was described by Simon Parsons (University of Edinburgh), POLYMORPHISM INDUCED BY HIGH PRESSURE, pushing out the boundaries of polymorph hunting. He described the

experimental conditions using a diamond anvil cell, CCD diffractometer and 'fairly modest' pressures (1-15kbar) to search for new forms of formamide, pyridine and glycine. The high-pressure system was also used to study the formation of co-crystals. Chris Frampton, (Bruker-Nonius) POLYMORPHIC DRUGS SCIENCE, FASHION OR VALUABLE PRODUCTS gave a highly interesting and entertaining talk on the importance of establishing the most stable form of a compound and acquiring the intellectual property rights. He used the examples of Ranitidine, Ritonavir and Paroxetine to illustrate his talk. The importance of finding the most stable form was emphasised by Dan Cowell, (Pharmorphix Ltd.), POLYMORPHISM STUDIES IN THE PHARMACEUTICAL INDUSTRY. Dan stressed that high throughput screening was only part of the answer and that better focused screening at medium and low throughput could lead to the most stable form with greater understanding. THERMAL TRANSFORMATIONS-CASE STUDIES by Ron Roberts (AstraZeneca) showed examples of structural changes during heating and cooling using hot-stage X-ray diffraction. Examples of lattice expansion and calculation of thermal expansion coefficients were also shown. Stephan Watts, STRUCTURAL CHARACTERISATICS OF THE AMORPHOUS PHASE: A COMPUTER MODELLING APPROACH, (Pfizer Institute for Materials Sciences, University of Cambridge) talked about a new approach to the understanding of amorphous materials using molecular dynamic simulation techniques. The final two lectures concentrated on novel techniques for the quantification of the amount of the amorphous phase in materials. Paul Royall, (Kings College, London), APPLICATION OF DYNAMIC MECHANICAL ANALYSIS (DMA) IN THE CHARACTERISATION OF AMORPHOUS POWDER spoke of the application of DMA to powders as opposed to solid samples. Mixtures of amorphous and crystalline lactose were used to establish a linear relationship between the amorphous content and the DMA relaxation strength. The results from a sample of micronised crystalline lactose were more complex and further work is ongoing to understand these results. Susan Barker, (University of East Anglia), THE USE OF THERMALLY STIMULATED CURRENT SPECTROSCOPY (TSC) IN THE STUDY OF AMORPHOUS AND POLYMORPHIC MATERIALS, described TSC as an electrical technique whereby dipolar movement and relaxation are measured under the influence of varying thermal and electrical stresses. The various modes of operation of TSC were described in relationship to caffeine and indomethacin.

In all, a very interesting session for all those interested in the characterisation of pharmaceutical solids.

Phil Holdway



## Industrial Group AGM

The 21st ANNUAL GENERAL MEETING of the Industrial Group will be held at UMIST at 12:00 on 7th April 2004.

Nominations are sought for CHAIR, VICE-CHAIR and TWO committee members to serve for three years from April 2004. Nominations, which shall be proposed by not less than two members of the Group and shall be accompanied by the written consent of the nominee, shall be sent to reach the Honorary Secretary of the Group not later than seven days before the Annual General Meeting.

Contact the Secretary/Treasurer:

**MS J SHACKLETON**

Manchester Materials Science Centre,  
Grosvenor Street,  
Manchester M1 7HS

Tel: 0161 200 3581 Fax: 0161 200 3586 e-mail [judith.shackleton@man.ac.uk](mailto:judith.shackleton@man.ac.uk)

## Forthcoming BCA Industrial Group Meetings

**10th June 2004**

**Introduction to Powder Diffraction,  
Manchester.**

This is a training session for those new to the technique and in need of a grounding in what can be achieved with powder diffraction.

Contact: Ms J. Shackleton,  
Manchester Materials Science Centre,  
Grosvenor Street, Manchester M1 7HS.  
Tel: 0161 200 358,  
Fax: 0161 200 3586  
Email:

**24th June 2004**

**Pharmaceutical Special Interest  
Group, Venue to be confirmed.**

This follows the same format of previous SIG's with a mix of topical presentations at the forefront of the technique.

**Please consult the Industrial Group  
Website for further details of this meeting.**



**4th November 2004**

**Autumn Meeting "DIY  
Crystallography",  
Birkbeck College, London.**

The morning theme will be "Heath Robinson Hardware" and the afternoon devoted to public domain software.

Contact: Dr J K Cockcroft,  
Birkbeck College, Department of  
Crystallography, Malet Street,  
London, WC1E 7HX.

Tel: 020 7631 6849 Fax: 020 7631 6803  
Email: [cockcroft@img.cryst.bbk.ac.uk](mailto:cockcroft@img.cryst.bbk.ac.uk)

Further details of all these meetings and on-line registration, will shortly be available on the BCA Industrial Group Website.



## Winter Meeting PCG December 2003: Report



**THE** Winter Meeting of the Physical Crystallography Group was held at the Cosener's House, Abingdon on December 8 and 9, 2003. The meeting commenced with lunch on the Monday and ended with lunch the following day. The theme of the meeting was that of disorder in materials, with a provocative title of "Structure at the nanoscale: fact, fiction or hype?" This meeting was well attended by approximately 45 scientists who listened to 6 invited and 3 contributed talks. Excellent posters were also displayed.

The first talk was given by **Daniel Bowron** of the Rutherford Appleton Laboratory (RAL) focussing on liquid disorder. Daniel's talk progressed from the short-range to the long-range order. Complementarity was a major theme and Daniel presented experimental research using the Extended X-ray Absorption Fine Structure (EXFAS) as well as employing the technique of isotopic substitution in neutron diffraction to elucidate liquid structures. One example was the use of the relatively new technique of applying the method of Empirical Potential Structural refinement (EPSR) to obtain detailed information in 2D and 3D of the correlations between atoms in solution- probing the hydrophobic interactions! Moreover, Daniel left us with the thought of probing structure on the mesoscale.

**Simon Billinge** of Michigan University, USA, then took to the stage by stating that knowing the structure is fundamental to understanding the properties of material. Simon presented work concerning the advancement of pdf techniques to solve quantitatively the structure of complex materials on nanometre lengthscales. In particular the work concentrated on investigating the diffuse scattering component in total scattering experiments. Examples included studies made upon determining the Jahn-Teller distortion in "manganites". Other recent developments included high  $r$ -space resolution experiments using X-rays, the study of nanocrystallography and rapid data acquisition studies. For the latter, counting times can be reduced from 8 hours to 1 second, enabling studies to be made of phase transitions and redox reactions.

**Alex Hannon** (RAL) presented a new insight into the structure of Group II cyanides, structures that have eluded scientists for the past few decades. The structure factors for AgCN, AuCN and CuCN were measured by using the GEM instrument at ISIS, showed a distinctive saw-tooth diffuse scattering component. The structures were determined with the Reverse Monte Carlo method (RMC) using a random-chain displacement model.

**Jens Kreisel** of the EPSNG, Grenoble gave an insight into diffuse X-ray and Raman scattering studies of nano-structured  $\text{ABO}_3$  perovskite oxides. The study concerned ultrahigh strain and piezoelectric behaviour in relaxor based ferroelectric single crystals. Ultrahigh strain was determined by high-pressure Raman spectroscopy whilst X-ray diffuse scattering gave an insight into chemical (substitutional) or structural disorder.

**Bill David** (RAL) ended the scientific proceedings of the first day by presenting recent work concerned with the single crystal diffuse scattering of flexible molecules. Particular focus was made on the diffuse scattering from benzil, and the development of Monte Carlo simulations. Bill's presentation emphasised the power of modern day computer simulations to predict structures of complex materials.

Our appetites were fuelled with the thought of a traditional Christmas evening meal at Cosener's House to end the day.

**Trevor Rayment** (Cambridge) opened proceedings on the Tuesday by challenging us with the question "Why should you use X-ray Absorption Spectroscopy (XAS)?" Trevor replied to this question by describing the use of absorption spectroscopy techniques to investigate the electrochemical interface. XAS can identify oxidation states, bond distances, coordination numbers and identify the local surrounding atoms. Trevor presented 3 examples of electrochemical applications: electrode structure; electrochemical surface science; and electroanalytical chemistry. Importantly, Trevor stressed the need for 3rd generation detectors, if one is to use 3rd generation sources!

**Martin Dove** (Cambridge) presented work using complementary experimental and theoretical techniques to study the different polymorphs of silica. What is the nature of the Si-O bond in cristobalite? Using GEM total scattering measurements have been conducted on cristobalite to answer this question. The diffuse component provided information on the local structure and the Bragg scattering yielding both short- and long-range structural information. Martin detailed the use of Monte Carlo methods to obtain real-space structural information from the measured structure factor by building an atomic model based on the experimental data. The test of this approach was its ability to predict both the short-range and long-range structural ordering.

**Robert McGreevy** (RAL) entertained us with Magnetic Disorder in Crystalline Materials, "to the nanoscale and beyond..." In a study on Fe-Zr metallic glasses, Robert showed how complementary techniques could be exploited to determine the structure of condensed materials. In this instance, neutron scattering gives magnetic structure (remember the need for a model for magnetic disorder!), X-ray scattering determines the Fe structure, and Zr edge anomalous scattering determines the Zr structure. Further examples given by Robert included the La-Sr- $\text{MnO}_3$  system in which the coupling between the local atomic and local



magnetic structure was accessed through total scattering neutron experiments.

**John Dore** (Kent) ended proceedings before lunch with an insight into the structures of nanotubes and nanohorns. John detailed both historical and future perspectives of these technologically important compounds. Are Single Walled Nanotubes (SWNT) truly single walled? With a view to potential petrochemical industrial applications, can water be intercalated into nanohorns?

The organisers would like to thank the attendees for choosing this meeting, and the support of everybody that made this enjoyable meeting feasible. I would like to single out the staff at Cosener's House, a location that remains an excellent place to conduct scientific meetings.

Finally, it was encouraging that the presentations were stirred by the title "...fact, fiction or hype", and most of the talks entered into the spirit by giving examples of the above. In light of this, I'll sign off with the thoughts of Robert McGreevy. Maybe this alternative is apt, "Structure at the nanoscale: based on a true story..."

**Jonathan Wasse, PCG, Jan 2004**

#### Current PCG Committee

Title	Name	Grade	Since
Dr	Pam Thomas	Chairman	2002
Prof	Paolo Radaelli	Vice Chairman	2002
Dr	John Evans	Honorary Secretary/Treasurer	2002
Dr	Jon Goff	Ordinary Member	2001
Dr	Jeremy Cockcroft	Ordinary Member	1999
Dr	David Allan	Ordinary Member	1997
Dr	Steve Collins	Ordinary Member	1998
Dr	Jon Wasse	Ordinary Member	2002
Dr	Jon Loveday	Ordinary Member	2003
Dr	Tom Lyford	Ordinary Member	2003

(Ordinary members are permitted to serve two three year consecutive terms)



## The 61st Annual General Meeting of the Physical Crystallography Group of the British Crystallographic Association and Structural Condensed Matter Group of the Institute of Physics

**14:30 Wednesday 7th April 2004, UMIST**

1. Apologies for absence
2. Minutes from the 60th AGM held at Nottingham, 16th April 2003 (to be distributed)
3. Matters arising from minutes
4. Chairman's report
5. IOP matters
  - a. Nominations to IOP Conference Committee
  - b. Financial issues/budget capping
  - c. Appointment of representative to CMMP division of the IOP – propose that the vice chairman take this role during their 3rd year of office
  - d. Possibility of increasing interactions with the neutron scattering group of the IOP
  - e. Other IOP business
6. BCA matters
  - a. BCA subscription mechanism/rate for IOP SCMP member
  - b. Honorary members of BCA
  - c. Matters arising from BCA council/other BCA business
7. Secretary/Treasurer's report
  - a. Presentation of accounts (to be distributed)
8. Elections to PCG/SCMP committee
9. Future Meetings
  - a. PCG/CMSD co-sponsored workshop on Rietveld refinement to be held April 16th at Birkbeck
  - b. Autumn/Winter meeting 2004 proposed topic: proteins/neutrons/biophysics
  - c. BCA 2005 theme
10. New Activities
  - a. PCG/SCMP thesis prize for structural science
  - b. PCG/SCMP newsletter
  - c. Training workshops and educational activities
11. Any other business

#### Elections to Committee

There are vacancies arising for Ordinary Members of the committee owing to the retirements of Steve Collins, David Allan and Jon Goff. Nominations (with name of seconder and note of acceptance from the nominee) for these positions should be sent to the Honorary Secretary ([john.evans@durham.ac.uk](mailto:john.evans@durham.ac.uk)) by April 1st, or communicated to him in person at the 2004 BCA Spring Meeting.

#### Nominations received to date:

Mina Golshan

Proposed: Steve Collins; Seconded: Pam Thomas

## Minutes of the 60th Annual General Meeting of the Physical Crystallography Group of the British Crystallographic Association and Structural Condensed Matter Group of the Institute of Physics

12:00 Wednesday 16th April 2003, York

There were 27 members present. Committee members present: Pam Thomas, Paolo Radaelli, John Evans, Dave Allan, Jonathan Wasse, Steve Collins.

1. Apologies for absence were received from Sue Kilcoyne.
2. Minutes from the 59th AGM held at Nottingham, 27 March 2002 were received and accepted.
3. There were no matters arising.
4. Chairperson's report/discussion
  - a. Autumn meeting was organised by Dave Allan/Pam Thomas and was held on December 11th 2002 in Edinburgh. The meeting was well attended and a report has appeared in Crystallography News.
  - b. ISIS/PCG co-sponsored a workshop on Magnetic Rietveld refinement held at Cosener's house on 12/13th December 2002. All places were taken within 24 hours of the course announcement. Meeting organised by Paolo Radaelli with teaching by PGR, Andrew Wills and Juan Rodriguez-Carvajal. A report has appeared in Crystallography News.
  - c. Paolo Radaelli reported on the successful PCG/SCMP session on charge/orbital ordering during the CMMP meeting. Both talks and the ensuing discussions were of a high standard. General attendance at the meeting was low.
  - d. The future structure of CMMP meetings was described. These will be biannual.
  - e. General future activities of the group were discussed. The general consensus of the meeting was that training/tutorial sessions are an important role of the group, and should be emphasised. Suggestions for workshops on Rietveld refinement, diffraction methods and diffuse scattering were made. The teaching of symmetry should be raised at BCA council. **Action:** JSOE.
  - f. Bursary applications from members were encouraged.
  - g. The proposal of Mike Hart and Mike Glazer as honorary members of the BCA was agreed. This will be raised at council. **Action:** JSOE.
  - h. Sue Kilcoyne was thanked for her work as a committee member over the past 3 years.
5. Secretary/Treasurer's report
  - a. The accounts were presented and accepted by the meeting.
6. Elections to Committee
  - a. John Loveday was elected as an ordinary member of the committee.

- b. Thomas Lyford was elected as an ordinary member of the committee.
7. Pam Thomas was reappointed as representative to CMMP division of the IOP
8. Future Meetings/activities discussed were:
  - a. A structural Rietveld workshop to be held in Autumn/Winter 2003/4. Birkbeck/Jeremy Cockroft were suggested as venue/coordinator.
  - b. A workshop on physical diffraction methods. Tom Lyford/PANalytical have agreed to investigate this possibility.
  - c. A second magnetic Rietveld workshop to be held in Autumn/Winter 2004/5.
  - d. A teaching session on diffuse scatter was suggested – possibly for spring meeting 2004.
  - e. "Disordered Materials" was suggested as a possible theme for the Autumn Meeting. Jonathon Wasse/Paolo Radaelli to coordinate. Cosner's House as a possible venue.
  - f. "Synchrotron Radiation"/"In-situ Studies" suggested as possible sessions for 2004 spring meeting to be held in UMIST. These will be raised at the planning meeting. **Action:** JSOE.
9. Any other business
  - a. The issue of the lack of crystallography in school/undergraduate curricula was raised. The PCG/SCMP should raise this issue with IOP. **Action:** PT.



*Cosener's House: Venue for the PCG Winter Meeting*

# Meetings of interest

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

11-14 March 2004

Hands-on Crystallization Course,  
Jena Germany  
[www.conventus.de/kristalle/](http://www.conventus.de/kristalle/)

15 March 2004

2nd Annual Biomaterials Workshop,  
Cranfield University, Shrivenham  
[www.cranfield-biomaterials.com](http://www.cranfield-biomaterials.com)

15-19 March 2004

DGK/DGKK Conference (German  
Crystallographic Meeting, Jena,  
Germany  
[www.conventus.de/kristalle/](http://www.conventus.de/kristalle/)

17-20 March 2004

International Workshop on Structural  
Analysis of Supramolecular  
Assemblies by Hybrid Methods,  
Granlibakken Conference Center,  
Lake Tahoe CA USA  
[www.embl-heidelberg.de/%7Eemhybrid/](http://www.embl-heidelberg.de/%7Eemhybrid/)

22-26 March 2004

APAC2004 - The Third Asian Particle  
Accelerator Conference. Gyeongju,  
Korea.  
[www.apac04.postech.ac.kr/index.htm](http://www.apac04.postech.ac.kr/index.htm)

29-31 March 2004

ELSPEC: 1ère conférence  
francophone sur les spectroscopies  
d'électrons SACLAY France  
[www.vide.org/elspec2004/](http://www.vide.org/elspec2004/)

30 March-1 April 2004

Neutron Scattering in Materials, at  
the IOM3 Congress in Carlton House  
Terrace, London  
[www.iom3.org/congress2004](http://www.iom3.org/congress2004)

6-8 April 2004

BCA Annual Meeting, UMIST,  
Manchester.  
[www.isis.rl.ac.uk/BCA2004](http://www.isis.rl.ac.uk/BCA2004)

26-30 April 2004

Practical X-ray Fluorescence  
Spectrometry, ICDD, Newtown  
Square PA, USA  
[www.icdd.com/education](http://www.icdd.com/education)

3-6 May 2004

11th Beam Instrumentation  
Workshop, Knoxville TN USA  
[www.sns.gov/biw04/](http://www.sns.gov/biw04/)

10-14 May 2004

The Second Moroccan School of  
Crystallography, EMC2, El Jadida,  
Morocco  
[www.ucd.ac.ma/fs/emc2](http://www.ucd.ac.ma/fs/emc2)

12-14 May 2004

CANSAS-IV Rutherford Appleton  
Laboratory, Didcot  
[www.isis.rl.ac.uk/LargeScale/LOQ/canSAS/canSAS4/canSAS4.htm](http://www.isis.rl.ac.uk/LargeScale/LOQ/canSAS/canSAS4/canSAS4.htm)

13-16 May 2004

High Resolution Drug Design,  
Bischoffberg, France.  
[www-igbmc.u-strasbg.fr/HRDDM.html](http://www-igbmc.u-strasbg.fr/HRDDM.html)

24-27 May 2004

Medsi 2004 - Workshop on  
Mechanical Engineering Design of  
Synchrotron Radiation Equipment  
and Instrumentation. Grenoble,  
France.  
[www.esrf.fr/Conferences/Medsi2004](http://www.esrf.fr/Conferences/Medsi2004)

28-29 May 2004

Fifth Canadian Powder Diffraction  
Workshop, Waterloo ON Canada.  
[www.cins.ca/cpdw/](http://www.cins.ca/cpdw/)

June 1-4 2004

PNCMI, The fifth international  
workshop on Polarized Neutrons in  
Condensed Matter Investigations  
Washington DC USA.  
[www.sns.gov/pncmi2004/](http://www.sns.gov/pncmi2004/)

2-4 June 2004

13th Annual CCP13/Fibre Diffraction  
& Non Crystalline Diffraction  
Workshop, ILL/ESRF, Grenoble,  
France.  
[www.ccp13.ac.uk](http://www.ccp13.ac.uk)

6-10 June 2004

American Conference on Neutron  
Scattering, College Park MD, USA  
[www.ncnr.nist.gov/acns](http://www.ncnr.nist.gov/acns)

7-11 June 2004

Fundamentals of X-ray Powder  
Diffraction, ICDD, Newtown Square  
PA, USA  
[www.icdd.com/education](http://www.icdd.com/education)

9-20 June 2004

Electron Crystallography: Novel  
Approaches to Structure  
Determination of Nanosized  
Materials, Erice, Italy.  
[www.crystalerice.org/2004/EICryst2004.htm](http://www.crystalerice.org/2004/EICryst2004.htm)

9-20 June 2004

Polymorphism : Solvates and Phase  
Relationships. Erice, Italy  
[www.geomin.unibo.it/orgv/erice/bernstei.html](http://www.geomin.unibo.it/orgv/erice/bernstei.html)

14-18 June 2004

Advanced Methods in X-ray Powder  
Diffraction, ICDD, Newtown Square  
PA, USA  
[www.icdd.com/education](http://www.icdd.com/education)

1-10 July 2004

XVI International School on the  
Physics and Chemistry of Condensed  
Matter: Structural Aspects of Solids,  
Bialowieza, Poland  
[www.alpha.uwb.edu.pl/schoolXVI/](http://www.alpha.uwb.edu.pl/schoolXVI/)

5-9 July 2004

EPAC'04 - 9th European Particle  
Accelerator Conference. Lucerne,  
Switzerland.  
[www.epac04.ch/](http://www.epac04.ch/)

11-17 July 2004

LAM12: Twelfth International  
Conference on Liquid and  
Amorphous Metals, Metz,  
France.  
[www.lam12.sciences.univ-metz.fr/](http://www.lam12.sciences.univ-metz.fr/)

17-22 July 2004

American Crystallographic  
Association Meeting, Chicago, IL.  
[www.hwi.buffalo.edu/ACA/index.html](http://www.hwi.buffalo.edu/ACA/index.html)