Crystallography News

British Crystallographic Association

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Crystallography News September 2006

Contents

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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 **December 2006** issue are sent to the Editor to arrive before **25th October 2006**.

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This month's cover:
ECM 23 was in Leuven in August; reports on this great meeting will appear in the next issue.
Inset is the much loved Uli Arndt.

From the President

AS I write this column the Summer conference and holiday season is rapidly approaching. I am sure that we are all looking forward to both. I will be attending ECM23 in Leuven and I know that many of you will be going to the ACA Meeting in Honolulu. Of course by the time you read this the Autumn will be with us, so I hope that you all had a relaxing and enjoyable Summer.

Talking of conferences, you will be pleased to know that the planning for the BCA 25th Anniversary Spring Meeting to be held at the University of Kent at Canterbury between 17-19 April, 2007, is well underway. **Lindsay Sawyer**, the Chair of the Programme Committee, and his team already have a very exciting and wide ranging programme mapped out, details of which are given in this issue of Crystallography News. We are particularly pleased to welcome back the X-ray fluorescence community and the British Association of Crystal Growth this year. I am also delighted to see that the Young Crystallographers are running a satellite meeting again in 2007 after the great success of their meetings in 2004 and 2006.

As Canterbury will be the 25th Anniversary of the BCA the general theme will to look forward to the next 25 years of developments in crystallography, in all its aspects. At the meeting we are delighted to be able to welcome the extremely eminent mathematician, **Professor Sir Roger Penrose**, who will give the Bragg Lecture. The Hodgkin Lecturer is chosen by the BCA Officers from nominations put forward by the BCA Membership, and I am most grateful to all those who responded to my e-mail request for nominations earlier in the year. The officers were presented with a very strong list of candidates and we are very pleased to announce that the **Dorothy Hodgkin** Lecturer for 2007 will be **Professor Judith Howard FRS**. Judith was chosen because of the outstanding quality of her science and because of her long association with Dorothy both as a student and colleague.

You may also notice a few administrative changes relating to the Spring Meeting as it approaches. The BCA website is being upgraded and a specific conference link included that will allow for on-line registration and payment. We hope that this will make the registration process easier, and I am most grateful to **Elaine Fulton**, from Northern Networking Events, and **Jeremy Karl Cockcroft**, the BCA webmaster, and their colleagues for making this possible.

I have recently discovered that another very pleasant duty of the BCA President is to organise the Call for Nominations for Honorary Members of the BCA. This is our highest membership accolade, and is awarded to a small and select group of colleagues who have contributed significantly to crystallographic science and to the work of the BCA. In recent years we have elected **Paul Barnes**, **Chris Gilmore**, **Mike Glazer**, **Peter Main** and **George Sheldrick**. In the coming year we anticipate electing one or two new Honorary Members. Therefore, it gives me great pleasure to issue the Call for 2007. Please send your nominations, together with a short supporting case to me at president@crystallography.org.uk by the **31st October 2006**.

Finally, I am most grateful to all those who have contacted me since reading my column in the June issue of *Crystallography News* offering support and ideas with regard to promoting crystallography in education at undergraduate and school levels. I will be moving this process forward over the Summer and will have more news in the Autumn.

Paul Raithby

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www.crystallography.org.uk

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

BCA Corporate Membership

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

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

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

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

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From the Editor

AS the President mentions, this issue seems to fall between things. Although both the ACA and the ECM will seem quite a while ago to readers, the mechanism of publication means that we have to go to press just after the ACA and actually before the ECM. The cover picture will have to be a promise of reporting on Leuven in the December issue!

This year, a preliminary account of plans for the Spring Meeting in Canterbury is ready for this issue, and **Lindsay Sawyer** has produced a summary of the general situation. Not all groups are at the same state of preparation, and praise should be given to the joint Industrial Group – XRF programme which is almost complete, and is given on page 7.

We am particularly indebted to **Stephen Wallwork** for letting us publish an abbreviated form of the prehistory of the BCA which he and **David Blow** originally wrote for the Royal Society. For many of our members, the BCA will seem to have been going on forever, and this report from way back in the twentieth century may come as something of a surprise!

Stephen's article is intended to form part of an issue of the IUCr Newsletter on Crystallography in Great Britain and Ireland. Progress on this has been very slow; understandably, people don't these days jump at the chance to write yet another report on what they are doing. We have, however, received some very good offerings, and hope to encourage more writing by publishing some of the articles here first!

Everyone knows the highly successful CCP4, but how many other CCPs can you name or remember? A few minutes on Google © is very instructive! For crystallographers, by far the most lively other is CCP14, and we are very glad to be able to publish something about their work in this issue.

Puzzle Corner does not appear this time. I apologise, but am running a little low on inspiration. My last effort produced no replies whatever, but I promise that the December issue will once again contain something. Ideas for anything interesting with a crystallographic flavour are very welcome.

Bob Gould

Letters to Ed.

From Professor Bill Duax

Dear Bob,

Excellent issue of the BCA Newsletter. Espcially the very well- written, lively and humorous student reports that included among other things useful ideas for future meetings. I still find there are British words that I don't understand such as "bowfed" in the letter from Lindsay Sawyer. (I'm not exactly sure about Lindsay's reference to me either?)

Having judged posters at crystallographic meetings in several countries I was pleased to read David Watkin's article on the subject. I agree fully with points 2,3,4,5,6, and 8. I would leave it to the author to decide how much detail to add after they follow David's organizational recommendations. With respect to point seven, I would recommend the authors find innovative ways to turn tables into graphs or diagrams that do a more effective job of conveying the table's content.

Best regards,
Bill

Ed. **Dear Bill,**

Very many thanks for your kind letter! I'm glad you like the student reports. I have rather good fun cutting and pasting bits together to get reasonable coverage – and as they have to put in reports anyway it works out advantageously all round!

As far as Lindsay is concerned, I think that his vocabulary is considered just as eccentric in the UK as in the USA - or in Canada, where I am currently writing this! I think that "bowfed" is a sort of combination of "barked" and "woofed", but I'm not entirely sure. The reference to you is truly mystic. He (and others) frequently accuse me of using you as a role model, though...

And yes - David's article on winning a poster prize gets three cheers from me too, and from other readers who have asked for permission to reproduce it! My spirits sink when I see acres of beautiful unreadability at meetings! The main trouble almost always is, as you point out - too many words! Plus, of course, the unhelpful printing of black gothic on dark purple. In fact, I'm turning my ire more to those who design ludicrously fussy powerpoints on the same basis.

Bob

BCA 2007 Spring Meeting

University of Kent at Canterbury

THE 2007 Spring Meeting will take place at the University of Kent from 16-18 April. The overall theme is "New Methods and Innovation". Full details will be given in the December issue, but mark these dates in your diary now!

Young Crystallographers

This hugely successful event will be held again – this time at Canterbury, organised by **Alex Griffin** and her team. Further information from a.griffin@bristol.ac.uk. It will be held on Monday afternoon and Tuesday morning, 15-16 April.

The full meeting will run from Tuesday to Thursday, 16-18 April. We are very happy to be joined again by the X-Ray Fluorescence group, whose programme is given on page 7.

Named Lectures

This year, the full set of three will be given:

Lonsdale Lecture

Professor Bill David *(ISIS/RAL)*

Hodgkin Lecture

Professor Judith Howard *(Durham)*

Bragg Lecture

Professor Sir Roger Penrose *(Oxford)*

View of Canterbury Cathedral from the Campus. (With thanks to Jim Higham, University of Kent)

Keynote Lectures so far arranged:

Chemical

Professor Chick Wilson (Glasgow)
"Beans, sausages and pancakes: a recipe for understanding thermal motion in crystals."

Industrial

Professor R.L. Snyder (Georgia Institute of Technology)
There will also be keynote lectures sponsored by the **PCG** and the **BSG**.

Scientific Sessions

These are developing rapidly at present, but suggested contributions are most welcome. Anyone wishing to be considered for a contributed oral presentation should submit an abstract by **October 16 2006** to **abstractbca@glasconf.demon.co.uk**, giving the session desired.

Parallel Sessions already fixed:

Joint **PCG** and **CCG session** on "New Science from Big Facilities", chaired by **Jon Wright** from ERSF.

CCG sessions on *"Transport and Reactivity in Crystals"* and *"Dynamics in Crystals"*

PCG Sessions on *"Disordered Materials and Glasses"* and *"Computational Methods in Crystallography".*

IG sessions on *"Co-crystals of Pharmaceutical Materials", "Diffraction from Surfaces and Two-dimensional Crystallography", "101 Ways to Prepare an XPRD Sample.",* and *"A Standardless Future for Quantitative XRPD?".*

BSG sessions to be announced.

Motherwell Event

A special event will be held to mark the retirement of **Sam Motherwell** – known to most of us as Mr Pluto! See the notes on page 8 from **Frank Allan**.

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

X-Ray Fluorescence at the BCA 2007 Spring Meeting

WE plan a comprehensive XRF programme over the three days and also encourage dedicated XRF posters at this meeting. There is a £50 cash prize and champagne for the best poster! Details of submitting posters will appear here nearer to the meeting but now is the time to start planning your poster! We particularly welcome offers of talks from users in any of these sessions, please contact the appropriate session organiser to offer a presentation. For further details, see the IG website: www.crystallography.org.uk/ig

XRF Session Details
Tuesday 17th April 2007

MORNING:

Tutorial / Workshop Session

"XRF: WHERE ARE WE NOW?"
Mark Ingham is organiser and chair. We hope to secure two speakers of international renown to present the following sessions.

10:00 XRF: What instruments have we got, or are likely to get soon.
1 hour + 15 minutes for questions.

11:15 Coffee

11:45 XRF: What can we do with it?
1 hour + 15 minutes for questions.

AFTERNOON:

14:00 Semi-quantitative
Ros Schwarz is organiser and chair.
If you have ever been asked 'What on earth is it?', this session is here to help. Talks on any application of semi-quantitative ("standardless") analysis, such as sorting unknowns for the most suitable quantitative technique, trouble-shooting production problems and identifying contamination and corrosion are most welcome.

15:30 Calibration Samples
Ros Schwarz is organiser and chair.
Because good quantitative calibrations are critically dependent on the quality of the samples used, this session is designed to consider some of the options available from setting-up samples through to fully certified reference materials. Talks on the issues involved, such as validation, are invited and experiences of the preparation of calibration samples in-house in cases where suitable materials are not affordable or available, are particularly welcomed.

17:00 -18:30 XRF Exhibitors' Forum.
Dave Taylor is organiser and chair.
Exhibitors will be allowed to give commercial talks aimed at encouraging delegates to visit their exhibition stand for further information. Exhibitors will be required to register in advance to give a presentation and the available time of 90 minutes will be divided equally to fit in all the talks.

EVENING:

Posters and Exhibition with buffet and wine.

Wednesday 18th April 2007

MORNING:

10:15 - 12:00 XRF / XRD Joint session on thin films.
Dave Taylor & Chris Staddon are the organisers.
This joint session is designed to give delegates an insight into what can be achieved by using XRF and XRD to investigate thin films and coatings. We are planning to start the session with an overview of what can be achieved and follow with presentations on specific applications of the techniques.

AFTERNOON:

13:30 - 15:00 and 15:30 - 17:00 XRF Applications - including Cultural Heritage
David Beveridge is organiser and chair.
If you have an interesting XRF application, come and tell us about it! Both short and long talks will be welcome; and both wavelength-dispersive and energy-dispersive techniques will be included. We would particularly like to have a number of talks relating to cultural matters.

Thursday 19th April 2007

MORNING:

10:00 XRF Keynote Lecture "Environmental Issues"

11:00 - 12:30
Presentations on Environmental issues.
Margaret West is organiser and chair.
If you have an environmental application we'd like to hear from you. This session will cover sampling strategy and the analysis of liquids, solids, powders and particulates in air by portable, bench top or floor mounted systems. Talks on analysis to satisfy legislation, environmental surveys and workplace monitoring are especially welcome.

XRF sessions close at lunch to allow delegates to attend an afternoon XRD session.

Motherwell Symposium
BCA Canterbury

SAM MOTHERWELL will retire from his position as CCDC Research Manager on 31 December 2006. Sam obtained a BSc (chemistry) and a PhD (crystallography - with John Iball) from Dundee/St Andrews and joined the embryo CCDC in 1968. Sam's scientific interests have been wide ranging. He was one of the pioneers of molecular graphics software through the Pluto program, was involved in the early development of direct methods, and played a major role the very first releases of the Cambridge Structural Database. For the CSD, he wrote the original 2D substructure search code (CONNSER) and extended this to 3D substructure searching and data analysis in the GEOM program. Many of these fundamantal ideas (and even some code) have contributed to the more recent CSD programs QUEST and ConQuest.

In 1978, Sam moved to the University Library in Cambridge as Head of Automation, rejoining the CCDC in January 1992. Since that time, his research career has moved towards applications of CSD information in crystal engineering and pharmaceutical materials development, including work in crystal structure prediction, where he has organised three well-known 'blind tests' of developing CSP methodologies. Since 2002, he has been an Associate Director of the Cambridge-based Pfizer Institute for Pharmaceutical Materials Science, and has worked closely with scientists from the University Departments of Chemistry and Materials Science, and with Pfizer scientists worldwide.

Sam has published more than 110 papers (and rising), and has been responsible for originating software and ideas that have been used by generations of crystallographers and chemists. The speakers at the Symposium will reflect the scientific range of Sam's unique contribution.

Frank Allen

Fifteenth Slovenian - Croatian Crystallographic Meeting

THE 15th Slovenian-Croatian Crystallographic Meeting was held from 14-18 June in Jezersko, a small village, lying some 900 m above the sea level and surrounded with Alpine peaks up to 2560 m high, still covered with snow during the meeting. The Meeting passed very smoothly, not to say successfully, scientifically and socially, and offered a friendly and domestic atmosphere. There were 68 active participants and 15 accompanying persons from eight countries.

There were four plenary lectures, describing modern approaches in crystallography: **William Duax** (Buffalo, USA): The genes, amino acid sequences and crystal structures of short chain oxidoreductase enzymes; **Robert Dinnebier** (Stuttgart, Germany): Powder diffraction at non-ambient conditions using 2D-detectors; **Marija Kosec** (Ljubljana, Slovenia): Ferroelectrics-from bulk to nano; and **Goran Stefanic** (Zagreb, Croatia): The formation of high-temperature ZrO_2 polymorphs at room temperature.

Forty four short oral contributions were presented with different but contemporary topics in crystallography: e.g. macromolecules, organic, organometallic and inorganic compounds, crystal architecture, mineralogy, archaeology, ceramics, zeolites, metals and alloys, thin films, solid solutions, ill-crystallized materials, structure and properties, microstructure, small-angle scattering. In my opinion, some of the talks need special mentioning and I choose my top five: crystal structure of a glucansucrase, glycine zinc chloride compounds, peculiar properties of cholic acid as a host molecule, stereisomers of platinum coordination compounds, and SAS and the "dead leaves" model.

The next meeting will be held in Croatia in June 2007, in a tourist resort on the Adriatic Coast. We would like to welcome again all participants of previous meetings as well as all others who would like to experience a gathering of crystallographers in a very friendly atmosphere. For more information please contact **S.Popovic**, Zagreb, spopovic@phy.hr, or **I.Leban**, Ljubljana, ivan.leban@fkkt.uni-lj.si . Please send us an e-mail address if you would like to be on our mailing list.

Ivan Leban
Slovenian Crystallographic Society

CCP14

A Time for Change: The Next Generation?

AS we approach the end of the current CCP14 grant, we are presented with an opportunity to reflect upon the achievements of the project since its inception in 1994. Although the original aim of developing "linking" software never took off, the creation of the initial ftp site where crystallographic software for powder diffraction was collected and distributed formed the early beginnings of a very successful web site. The latter mushroomed organically during the second phase of CCP14 funding without much regard to web site organization. Subsequently, all of the other CCP projects followed the lead set by CCP14 in web site provision for their user communities.

During the current 3rd phase of funding, we have been attempting to overhaul the web site to give it more structure (a behind-the-scenes job). The aim is for a newer, cleaner, less cluttered look, with improvements to the hardware and software environments to ensure a reliable 'always on' service. As ever, new software continues to be added to the suite. The strength of the in-depth approach continues, with multiple programs available with multiple solutions for whatever problem you might be attacking: if you cannot find what you need we are always happy to try to point you in the right direction.

We are now the sole holders of **Robin Shirley's** Crysfire 2004 suite, which Robin completed just before his tragic death in 2005. This version is available alongside the previous stable release, and contains many enhancements over older versions. Crysfire 2000 users will find that the front-end interface largely remains familiar, but that the new Crysfire is now a close-coupled system, faster, more robust, and easier to use. Nothing has been lost and there are several powerful new facilities. The source code for the command module of Crysfire 2004 is actually four times as large as its equivalent in Crysfire 2000. Along with the program release, the source code will be made available for anyone interested in further development and future applications.

In addition, the project has also provided manpower to organize software "fayres" at various international crystallographic meetings during the last decade, the last being at IUCr XXI Florence in 2005. These fairs have provided the opportunity for authors to demonstrate the features of the various software packages that they have created. While some of the demos have provided huge interest, attendance at others has been, quite frankly, disappointing.

Since we are a user-driven service and in order to optimize the direction of the project for the coming years we would like you, the users to contact us with your ideas and suggestions. These could be requests for content on the site, ideas or suggestions for the web layout, even workshops for specific software suites. However, change for changes sake is neither useful nor productive, so your feedback really is essential. We look forward to hearing from you!

Richard Stephenson, Jeremy Karl Cockcroft, David Watkin, & Bob Cernik.

CCP14 web site and contact details:
www.ccp14.ac.uk
www.ccp14.ac.uk/people/people.htm
r.stephenson@mail.cryst.bbk.ac.uk

Richard Stephenson at work.

BCA IG/RSC XRF Meeting

May 2006, BGS, Keyworth

MORNING SESSION

Welcome
Dave Taylor, BCA Industrial Group

Dave provided the welcome for the day from the Industrial Group of the BCA for this first joint XRF meeting with the RSC Atomic Spectroscopy Group. He thanked all the sponsors for their kind contributions. Dave then commented that the aim of bringing together an independent UK forum for XRF appeared to be bearing fruit with 70 delegates registered for the meeting.

Introduction & tour of BGS
Charles Gowling, British Geological Survey.

Owing to Mark Ingham having lost his voice, Charles Gowing kindly stepped in to the breach by providing the introduction. He ran through the usual formalities of safety and continued with a review of the day's agenda.

The whole group then split into two for a tour of the British Geological Survey XRF facilities. The laboratory itself was well equipped with PANalytical XRF instrumentation. In daily use are 3 WDXRF instruments - a PW2400, a MagixPro and a new Axios. On the EDXRF side was an Epsilon 5, used when Rh excitation becomes limited e.g. for Sb analysis etc. Outside in the sunshine we were given a tour round the BGS's newly converted mobile laboratory. It is equipped with both a bench top and handheld EDXRF systems. So far the lab has been successfully trialled locally but has not been put to full use in the field. We all returned to the meeting room for the remainder of the day.

Chair, Morning Session
Andy Scothern, RSC.

Andy took the opportunity to inform the delegates of the 13th Biennial National Atomic Spectroscopy Symposium being held at Glasgow Caledonian University from 10th to 12th July organised by the Atomic Spectroscopy Group of the RSC. He then introduced the keynote speaker Dany Doyen.

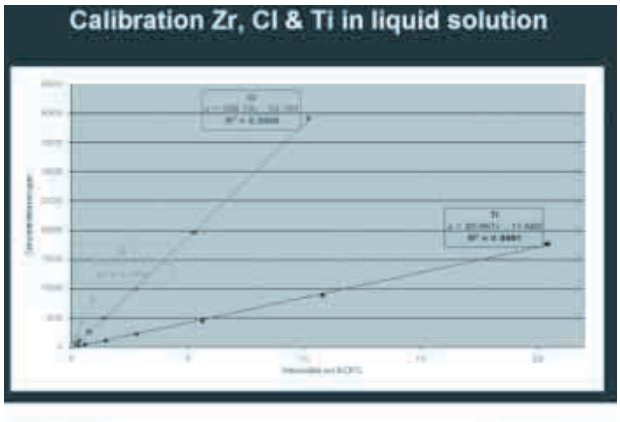
Keynote Lecture - From Catalyst to Final Product: An overview of XRF analytical and sample preparation techniques in a leading European R&D polymer laboratory.
Dany Doyen, INEOS Polyolefins, Belgium.

E-mail: dany.doyen@innovene.com

Dany began his talk with a brief history of INEOS Polyolefins plus an overview of the company as it is today.
INEOS have a range of analytical techniques that are available in the business so why choose XRF. It is a robust and reliable technique with pros and cons.

A wide range of sample types are analysed at INEOS. These include catalysts, additives, polymers, deposits and defaults (problems). As the majority of the samples are polymeric a 1kW Bruker system with a He atmosphere is used otherwise both standards and samples would be destroyed by the beam. Difficulties arise for the analysis of P, S, Cl and Si, which migrate to the surface of hot pressed films. INEOS get around this by cutting away the surface prior to measurement in their XRF.

A range of sample preparation techniques are employed. Catalysts are measured in solution. Additives such as TiO_2 are analysed for their Ti content as pressed pellets and sometimes, especially for pure TiO_2, fused beads are used with $Li_2B_4O_7$ as flux. Dany then covered a range of INEOS specific applications and solutions.



Validation of their XRF is carried out twice weekly and monitored using a control chart. Using these data decisions are taken as to when drift correction is required. Also, every quarter, these data are shared between the different control labs around the INEOS facilities to monitor the company agreement.

Dany concluded that WDXRF provides a rapid analysis for a competitive price.

A Discussion on the Estimation of Uncertainties in XRF Measurements

Ros Schwarz, London & Scandinavian Metallurgical Co Ltd.

Ros introduced her talk by explaining that she is not an expert in statistics but believes it is important for the analytical community to have an understanding and apply it as appropriate.

At London & Scandinavian Metallurgical Co Ltd (LSM) the range of sample types is vast and Ros would like to be able to estimate the uncertainty associated with an XRF measurement so that she can optimise her analysis parameters without spending a vast amount of time running through repeatability/ reproducibility exercises. Her aim is to find a simple way to calculate an uncertainty estimate of any element in any matrix.

Documentation Ros has referred to has been the Eurachem/ Citac guide and BS EN ISO 12677:2003. "Chemical analysis of refractory products by XRF - fused cast bead method".

For her initial work Ros has assumed that instrument uncertainty and sample preparation uncertainty are not correlated. The factors she is concentrating on are instrumental variance, the detector and counting error/statistics. She is then using this for modelling for changing counting rates. Ros then asked for feedback on her ideas to date and any suggestions on how to apply this idea to matrix corrections which led to useful discussion.

Alison Burke
Huntsman Pigments

AFTERNOON SESSION

Chair, Afternoon Session

Margaret West

How Corus Group Share Best Practice

Ann Townend, Corus plc. Scunthorpe

Corus is an international metals company which provides steel and aluminium products to customers worldwide. Ann gave a revealing account of what happened when analysts from the four Corus sites (Scunthorpe, Teesside, Stocksbridge and IJmuiden in the Nederlands) were gathered to pool their knowledge in an exchange of best practices. The XRF analytical group found that completely different techniques had been adopted in site laboratories; sometimes fusion techniques were being used and sometimes pressed pellets for the same analysis. Even when the same techniques had been used, the conditions used were different. To complicate matters, all were using different sample preparation equipment and different XRF instrumentation.

Two years on now, consistency of methods is being achieved. The same fusion equipment is now used at all four sites. Round Robin exercises in the analysis of test samples are showing convergence of the results obtained for the different sites. There have been some spin-offs: for instance, by adopting one site's method, using 8g rather than 10g of flux as used at other sites, £3200 per annum is potentially saved by the company. However, the main gain has been in the exchange of ideas between the analysts of the company's laboratories. Future co-operative plans include joint development of wide range calibrations and the pooling of resources in producing calibration standards.

XRF and Coating Processes at Cranfield University

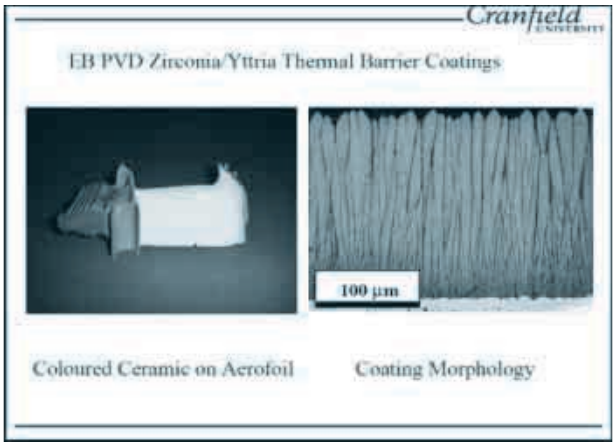
K. J. Lawson

E mail: K.J.Lawson@Cranfield.ac.uk

Ken summarised some of the major coatings activity in the National High Temperature and Surface Engineering Centre at Cranfield University. He demonstrated the value of XRF in analysing and monitoring the application of surface coatings, using spectra obtained from a Bruker S2 Ranger multisample XRFS system. He illustrated his talk with applications relating to coatings used on aerospace gas turbine components. Such coatings are applied to give either heat, oxidation or abrasion resistance using specialist processes such as electron beam physical vapour deposition, plasma spraying, metal sputtering and multilayer deposition. They included, amongst others, zirconia-based ceramics used for thermal barrier coatings, superalloys and bond coats. Particular emphasis was placed on the analysis

Speakers, Chairs and Guides. From left to right: Front row - *Sharon Fraser, Heather Harrison (tour guide), Ann Townend, Ros Schwarz, Margaret West (PM chair).* **Back row -** *Andy Smith, Daniel Capon, David Beveridge, Dany Doyen, Andy Scothern (AM chair) Charles Gowing (tour guide).*

of trace elements in the materials, the concentrations of rare earth oxide dopants and their importance in thermal barrier coating technology.



Silver Determination in Photographic Emulsion by EDXRF

David Beveridge, Harman Technology Ltd - IlfordPHOTO

E-mail: david.beveridge@harmantechnology.com

David described his frustrating quest to provide a simple XRF determination of silver in photographic emulsions (suspensions of silver chloride, bromide and iodide in gelatin solutions) as an alternative to the traditional determination -titration with thioacetamide - a relatively toxic reagent.

Since the emulsions tend slowly to settle out, direct determination in a liquid cell was not an option. So he attempted to obtain a clear solution by dissolution of the silver halides. His first thought was to start with a reagent similar to photographic fixers, solutions of ammonium thiosulphate and acetic acid. He added strontium nitrate as an inert heavy absorber, to nullify changes in X-ray ray absorption coefficient of the sample solution due to the variable composition of the emulsions and to decrease critical depth to less than that of the liquid cells. Unfortunately, this resulted in a cloudy suspension solution. He believes this must have been due to the formation of strontium sulphite by reaction with sulphite impurities in the ammonium thiosulphate supply. When he substituted sodium thiosulphate, which could be obtained in a purer form, the required clear solution was obtained. Now, he became concerned that the combination of the strontium nitrate with thiosulphate could potentially prove explosive if it dried out. So he substituted strontium acetate for the nitrate. As final flourish he added a little acetic acid to the solution to the "strontium fix" to lower the pH and to assist in the dissolution of the gelatin of the emulsions.

He now had an XRF method, which he was able to demonstrate gives the same result (±1%) as the titration method as shown in the table below. However, his company has yet to approve a change.

Comparison of ED and WD XRF Emulsion Silvers

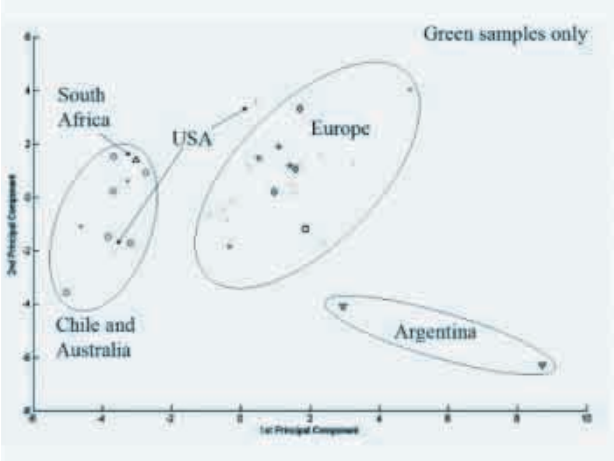
WDXRF	EDXRF	ED/WD
121.3	120.4	99.3 %
120.1	118.3	98.5 %
158.3	155.4	98.1 %
146.9	144.7	98.5 %
165.4	161.0	97.4 %
73.9	73.9	100 %
87.8	87.4	99.5 %
37.9	38.8	102.4 %
	Average	99.2 %

Archaeology of the present?

Sharon Fraser[1], Dave Polya[1], Paul Lythgoe[1] and Tim Insoll[2]

1. School of Earth, Atmospheric and Environmental Sciences, The University of Manchester
2. School of Arts, Histories and Cultures, The University of Manchester

Sharon explained that as a prelude to carrying out a project into the feasibility of provenancing ancient glassware finds on the basis of their XRF analysis of trace elements, she wanted to establish the best XRF analytical methods using less precious artifacts i.e. wine bottles from the local bottle bank. The technique she used was to finely grind the glass before analysing it as a powder. Using a PANalytical Axios WDXRF spectrometer with Protrace software, she was able

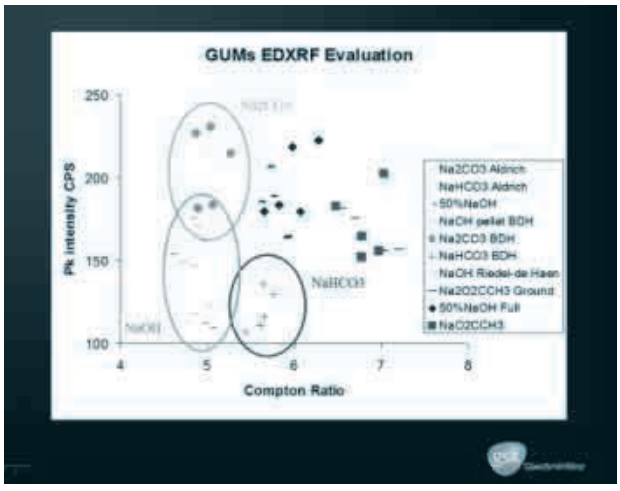


to determine 44 elements from Cl to U of concentrations down to 2 ppm. Using Principal Component Analysis - a statistical three dimensional breakdown of patterns of elemental concentration - she attempted to identify clusters of data corresponding to different provenances for the glass bottle. She was able to show that it was possible to distinguish between green glass of bottles of European and South American or of Australian origin. However, it was not possible to distinguish a similar pattern of clusters corresponding to different origins for wine bottles made of clear glass. Nevertheless, having proved the potential value of the technique, she now proposes to advance her project attempting to establish the provenance of glass artifacts of Islamic art found in Bahrain and Syria.

A different use for ED-XRF within the Pharmaceutical Industry"

Andy Smith, GlaxoSmithKline R&D. (Stevenage) and Martin Teasdale, GlaxoSmithKline R&D.(Tonbridge)

Andy described his attempts to use XRF as a rapid technique to confirm the identity of inorganic compounds used as starting materials in manufacture of pharmaceuticals in pilot plants. Identification of such "General Use Materials" (GUMs) is required by "Good Manufacturing Practice" (GMP) procedures even on small scale production of clinical grade "Active Pharmaceutical Ingredients" (APIs). These inorganic compounds are currently identified using relatively complicated and time-consuming tests involving techniques such as titration and ion chromatography. He used a PANalytical Minipal4 EDXRF spectrometer. This instrument is simple, low cost and small enough to fit on a standard laboratory bench top. The XRF technique - basically loose filling liquid cells with the powders - is simple and quick. In many cases, a simple matching of XRF spectra with library spectra could be used. However, to distinguish some anion salts of metals, it was necessary to take into account the relative ratios of elemental peaks and Rayleigh and Compton scattering peaks. Using principal component analysis, compounds as similar as sodium carbonate and sodium bicarbonate could then be distinguished.



The work is very promising. GSK propose working with PANalytical towards putting together a suitable software package for general use in the pharmaceutical industry. This method should be suitable for relatively inexperienced operators with very little need to interpret the spectra.

"XRF in the glass industry"

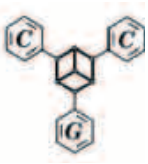
Daniel Capon and M Marshall, Glass Technology Services
9 Churchill Way, Chapeltown, Sheffield S35 2PY

Daniel gave a rapid overview of the tricks used by the glass industry to obtain the required colours of glasses. These were interesting, not especially for an account of the metals which produce the different colours, cobalt-blue etc, but for the different additives which could be used to make the glass appear colourless. These included oxidising agents, added to change the valency state of ferrous iron - the main contaminant giving glass a green colouration - to the ferric state, giving it a less noticeable yellowish tint. Another trick is to introduce a metal salt giving a complementary colour to that due to the contaminants, so cancelling it out, though this tended to produce glass with a greyish tint. With greater use of recycled glass these techniques were coming more into play and depended heavily on the rapid analysis of the glass melts to determine corrective actions. XRF was an ideal technique for this purpose. Andy said that GTS was developing methods for analysing the majority of trace colouring elements commonly found in glass in order to help customers solve problems. Allied with this is the development of specialist drift correction glasses containing detectable quantities of multiple elements, for use with XRF spectrometers.

Margaret West closed the meeting by thanking all the speakers for the work that went into their presentations. She also thanked the staff at the venue for helping to make the meeting a success and for an excellent lunch. She closed the meeting by thanking the delegates for sparing valuable time to attend and gave a reminder of the next meeting in Canterbury in April 2007.

Rob Foster
Health and Safety Laboratory

Groups



CCG AGM held at the BCA Spring Meeting at Lancaster University

12noon 5th April 2006

THERE were 47 members present at the AGM

1) **Apologies for absence:** No apologies for absence

2) **The minutes of the previous meeting:** The minutes of the AGM held at UMIST in 2004 were accepted by **Paul Raithby** and **Andy Parkin**. There were no matters arising from those minutes.

3 **Chairman's Report**

The Chairman, **Dr. Simon Parsons**, said that the CCDC prize, awarded this year to **Graeme Day** who gave an excellent lecture yesterday, had been raised to £600 by the CCDC. More thanks to chemical program overseen by **Richard Cooper** thanks for his hard work and thanks to chairs and especially to **Andy Parkin** for organising the Young Crystallographers part of this meeting.

He thanked Oxford Diffraction and CCLRC who sponsored the last Autumn meeting. The next autumn meeting will be sponsored by Rigaku. For some years we have had free registration for autumn meetings provided by Pfizer.

Two poster prizes will be presented at this meeting, one is our own CCG prize and the new one is sponsored by CrystEngComm. The winners will be announced at the conference dinner tonight.

Autumn meeting will be on 15 November 2006, in Glasgow; the local organiser will be **Andy Parkin** and the topic will be Crystal Engineering.

Simon Parsons thanked the committee for their hard work and support, particularly **Mary Mahon** who is retiring from the CCG committee. We welcome **Hazel Sparkes** as the new member of the committee. There was one nomination and so she comes straight onto the committee.

The UK contribution to IUCr newsletter is overseen by **Bob Gould** and the Chemical group part of this by **Andrew Bond**. He thanked them for their work on this and encouraged members to contribute if they are approached.

The CCG Durham School next year will be held from 24 March to 2 April 2007. He reminded members that there will be an election for BCA president and that **Paul Raithby** had made a significant and valued contribution to Chemical crystallography over the years, such as overseeing the program for this spring meeting. He encouraged all members to vote at the AGM this afternoon.

4) **Secretary/Treasurer's report**

Georgina Rosair presented the Group's financial statement for 2005. The group's finances are in a healthy position. 82 people at Autumn meeting which has a surplus of £1000, as membership fees paid to the BCA were processed in 2006 . We had many computational chemists who were non members and their registration fee includes BCA membership funds so the CCG pay their BCA membership. She thanked local organisers **Jane Whittington** and **John Warren** who were vital for the smooth operation of the meeting.

A payment of £500 was made to the Charge Density Sagamore meeting agreed by the committee, the treasurer agreed because accounts were in a healthy position.

She asked those present to support attendance at the Durham School with a sum of £700 (or its equivalent) as had been agreed at the 2004 AGM.
There were no queries of the accounts.

Mike Glazer queried our running large surplus of £7000 and said that we could do more to run down this surplus in the service of the aims of the BCA although he realises we are keeping money for a rainy day. He suggested waiving a conference attendance fees.

The Treasurer replied that the CCLRC sponsorship provided the surplus for the autumn meeting.

Sandy Blake added that the CCG had no insurance against a meeting going under so we have to be able to cover the costs of a meeting. **Paul Raithby** said that a £5000 buffer was good and that we had the second smallest reserve out of all the interest groups.

Simon Parsons said that this issue will be raised at the committee meeting.

7) **Autumn Meeting**

No further details to be added as this item was contained in the Chairman's report

8) **AOCB** None

9) **Next AGM**

The next CCG AGM will be held during the BCA Spring Meeting at Kent University (date and precise venue to be arranged)
The meeting closed at 12.20pm.

Georgina Rosair

CCG Autumn Meeting - Crystal Engineering: The Secrets Revealed!

THE Autumn Meeting of the CCG will be at Glasgow University on Wednesday 15th November 2006, and will be sponsored by Rigaku Ltd and Pfizer. An application form may be downloaded from the website: www.crystallography.org.uk/ccg

Cheques should be made payable to "Chemical Crystallography Group" and sent with the completed registration form to the CCG Secretary/Treasurer, **Georgina Rosair** (e-mail: G.M.Rosair@hw.ac.uk):

Richard Cooper

Current CCG Committee

Simon Parsons (Chairman) (2005 – 2007)
Richard Cooper (Deputy Chairman) (2005 – 2007)
Georgina Rosair (Secretary Treasurer) (2004 – 2008)

Ordinary members of the committee:
Charlie Broder (2005 – 2008)
Andrew Bond (2004 – 2007)
Alexandra Griffin (2005 – 2008)
Li-Ling Ooi (2005 – 2008)
Andrew Parkin (2004 – 2007)
Hazel Sparkes (2006-2009)
John Warren (2005 – 2008)

Hazel Sparkes joins us and we thank **Mary Mahon** for her service to the committee.

Left to right: *Hazel Sparkes, Georgina Rosair, Simon Parsons, Alex Griffin, John Warren, Charlie Broder, Andy Parkin, Richard Cooper*

IG Committee

Chairman: Jeremy Cockcroft
Vice-Chairman: Richard Morris
Secretary/Treasurer: David Beveridge
Ordinary Committee Members: Roy Copley, Martin Gill, Anne Kavanagh, Judith Shackleton, Chris Staddon
Co-opted: Mark Farnworth, Steve Norval
ICDD Representative: Dave Taylor

IG Committee, left to right: *Jeremy Cockcroft, Dave Taylor, Judith Shackleton, Chris Staddon, Richard Morris, Anne Kavanagh, Martin Gill, David Beveridge, Steve Norval, Mark Farnworth, Roy Copley.*

BACG and BCA Joint session on Crystal Engineering 06/04/06 at BCA Spring Meeting, Lancaster UK.

AS part of the joint BACG/ BCA meeting, this session, focused on Crystal Engineering, was organised by Dr Nick Blagden (Chair), University of Bradford and Prof Kevin Roberts (co-Chair), University of Leeds. The program was varied, covering both experimental and computational aspects of crystal engineering, with the link to crystal growth being very evident.

Christer Aakeröy, Constructing co-crystals with molecular sense and supramolecular sensibility.
Prof Aakeröy's presentation focused on the production of heteromeric crystalline material, and the elucidation of a robust synthetic approach to achieve this in a reproducible fashion. Success to date is based upon using the supramolecular synthon approach pioneered by Etter. Aakeröy outlined the different co-crystalline material his group has recently synthesed; by focusing on the competition between hydrogen bond donor and acceptors to form differing and competing synthons for both binary

and tertiary component systems. There was also a dramatic video example of solvent drop grinding as a technique for systems which change colour as the co-crystal was formed. The delivery was crisp, to the point and amusing, all you could ask for from a speaker.

Dario Braga, Making crystals by reacting and transforming crystals. Prof. Braga also dealt with the subject of co-crystallisation. However he also touched upon both organic and inorganic materials, in particular co-ordination systems that form diverging polymeric type networks. Braga discussed mechanical synthesis, reiterating the usefulness of the solvent drop grinding technique for co-crystal synthesis and the use of this approach to generate seed for further crystallisations. The talk also touched upon the use of solid state NMR to track the role of the hydrogen bonding in solids, and the importance of polymorphism in crystal engineering. The talk was well delivered and ended with a request for help from someone able to solve structures from powder data, which from a student's perspective was refreshing.

Jonathan Stead, Anion binding, Venus's flytraps and tweezers, Dr Stead's talk differed slightly from the abstract submitted, a fact that the speaker apologised for before admitting to his excitement over his new findings. Dealing mainly with anion binding in supramolecular gels, he described how the hydrogen bonding of the test system was altered by increasing steric hindrance, thus changing the usual tape structure. This led to an alteration in physical properties and some interesting rheology. A theme throughout was that these gels can be made to crystallise, and the resulting crystal structures are derived from the molecular interaction present in the gel phases. Another very interesting and well-delivered talk.

Chris Gilmore, dSNAP: A new way of analysing the results of the CSD searches and a new tool for crystal engineering and structure prediction. Prof. Gilmore presented a talk on the dSNAP software and the application of this software to gain a better understanding of the hierarchy present in packing of crystals. The examples given were thought-provoking as to how we view the contribution of strong and weak interactions. Gilmore emphasised the power of this data mining tool, and highlighted further developments to the dSNAP program. A well delivered talk that threw much light on the potential of this approach. The software can be downloaded form: www.chem.gla.ac.uk/snap.

Chris Sumby Crystal engineering with derivatives of the molecular host cyclotriveratrylene (CTV). Sumby was the only student who gave a talk in this session He provided the audience with details of his work on CTV, with particular focus on a comprehensive study of a number of derivative families, highlighting their ability to form coordination polymers with interlayer packing. The unusual geometric constraints of the molecule allow exploitation of the host-guest behaviour and allow multiple inclusion compounds to be formed. The talk was well delivered to a steadfast and undiminished crowd.

Joshua McKinnon, Extensions of Hirshfield surface-based tools: decomposing fingerprint plots. Dr McKinnon gave the last talk of the session, and offered the audience the chance to see a new method of interpreting Hirshfield surface plots. Instead of a molecule being modelled as a whole, specific interaction types and short contacts are examined. This allows superior modelling of larger molecules and better quantitative comparisons - in particular how the van der Waals and electrostatic surfaces map to the specific type of intermolecular interaction. The fingerprint plots are employed to point to specific interactions across the molecular surface, which can be used to reveal the detail of subtle changes in particular of the weaker interactions within crystals for a class of molecules.

A very fitting and interesting end to a very well organised afternoon and conference - many thanks to all who made it happen. Prof. Dario Braga presented **Guillermo Minguez** with the crystal engineering poster prize, sponsored by Cryst. Eng. Comm.

David Berry, Colin Seaton, Toni Brook, and Hafsa Javed, Pharmaceutical Materials Group, School of Pharmacy, University of Bradford

Left to right *Joshua McKinnon, Chris Sumby, Kevin Roberts, Chris Gilmore and Jonathan Stead.*

PCG Rietveld Refinement School 2007

THE PCG/SCMP (Physical Crystallography Group of the British Crystallographic Association/Structural Condensed Matter Physics group of the Institute of Physics) will be holding a 3 day Rietveld refinement school at the University of Durham from 7/1/07 to 10/1/07.

The course will be run along similar lines to the 2004 course with a combination of lectures covering the theoretical aspects of Rietveld refinement supported by extensive hands

on practical sessions using a variety of modern software packages. You'll have ample opportunity to interact with expert lecturers and tutors!

Topics to be covered will include:

- Data collection strategies for X-ray and neutron diffraction
- Constant wavelength and time of flight diffraction
- Indexing powder patterns
- Rietveld, Le Bail and Pawley fitting methods
- X-ray and neutron combined Rietveld refinement
- Extended solids and molecular systems
- Restrained refinements
- Rigid body refinements

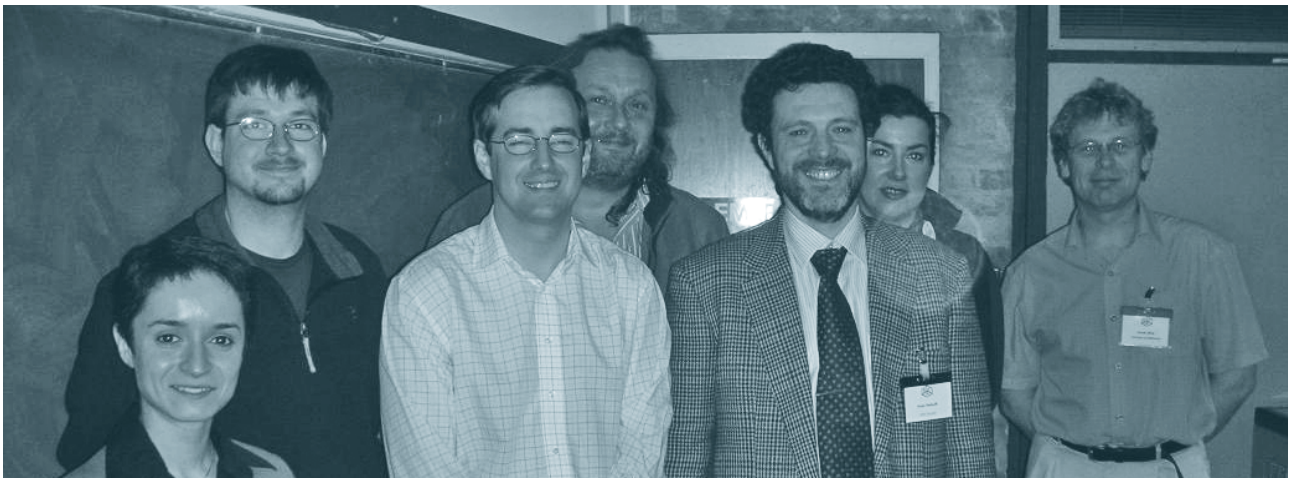
The PCG run a separate bi-annual school on magnetic refinements.

Accommodation will be at Trevelyan College and lectures/workshops will be held in the Chemistry Department. We hope to attract sponsorship to keep registration costs to a minimum. Registration forms will be available in autumn 2006. If you want to be placed on a mailing list to receive information about the school please email **john.evans@durham.ac.uk** or see the school webpage at **www.dur.ac.uk/john.evans/webpages/pcg_rietveld_school_2007.htm**

John Evans

PCG AGM

12:15 Tuesday 4th April 2006, Lancaster



The 2006 PCG committee members at the AGM in Lancaster. Unfortunately Andrew Wills and Serena Margadonna could not attend.
Left to right: *Mina Golshon, Jonathan Wright, Matt Tucker, John Loveday, Paolo Radaelli, Ivana Evans and Dave Allan*

There were 16 members present. Committee members present: Paolo Radaelli, Dave Allan, John Evans, John Loveday, Jon Wright, Mina Golshan.

1. Formal apologies for absence were received from **Andrew Wills** and **Pam Thomas**.
2. Minutes of the 62nd AGM held at Loughborough were circulated and accepted as an accurate record of the meeting.
3. There were no matters arising from minutes
4. **Paolo Radaelli** reported on another active year for the PCG/SCMP. Specific topics discussed were:
   a. A successful school on magnetic Rietveld refinement was held at Cosener's house in November 2005; thanks to **Juan Rodriguez Carvajal** – LLB, **Paolo G. Radaelli** – ISIS, **Andrew Wills** – UCL, **Laurent Chapon** – ISIS, **Aziz Daoud-Aladine** – ISIS for teaching and local organisation.
   b. The PCG/SCMP prize (£1000) attracted strong applications. To prevent conflicts of interest it was judged by an external committee who were thanked for their efforts. The prize was announced and a lecture given later in the meeting by **Dr Matt Tucker** (ISIS) for work on total scattering of framework inorganic materials to probe their structure and dynamics.
   c. The second Panalytical Thesis prize (£500) again attracted strong applications. The prize was announced/awarded to **Dr Andrew Goodwin** (Cambridge University, supervisor **Prof. Martin Dove**) for a thesis entitled "Dynamics from Powder Diffraction" later in the meeting at the conference dinner. Dr Goodwin will be invited to present his work at a future PCG/SCMP meeting.
   d. Sessions on high pressure, topology and a TOPAS training workshop have been organised by the PCG/SCMP for the BCA meeting.
   e. Sessions on "orbital ordering" and "magnetism" have been organised in collaboration with the neutron scattering and magnetism groups for CMMP06.
   f. The committee apologised for the lack of a winter meeting in 2005.

g. The 2006 winter meeting will be held on 25/10/06 in Edinburgh and will be entitled "A Snapshot of UK Physical Crystallography". JL/DA are local organisers.

h. A structural Rietveld refinement school will be held in Durham in early January 2007; **John** and **Ivana Evans** will be local organisers. The structural and magnetic schools will continue to alternate so that each generation of graduate students have the opportunity of attending.

i. The PCG/SCMP will support a meeting on protein crystallography by powder diffraction to be held in 2007 in Grenoble. JW is local organiser.

j. Comments were invited from the meeting about the possibility of methods by which the current PCG/SCMP teaching activities could be formalised and possibly "accredited" as part of postgraduate student training requirements. The meeting was broadly supportive of this activity. **Paul Fewster** offered to discuss the issue with the IOP accreditation committee on which he serves. The PCG/SCMP committee agreed to think further on this topic.

5. IOP matters were discussed under the Secretary/Treasurer's report.
6. There were no BCA matters raised.
7. Honorary Secretary/Treasurer's report:
   a. The secretary/treasurer presented the annual IOP activity report to the meeting and the financial summary appended. Minor financial discrepancies reported to the 2005 AGM due to double payment of a cheque by the IOP have been corrected.
   b. Issues regarding proposed changes to the IOP funding model were described. In brief it appears that current group funds will be zeroed at the end of this year and that the group will have to bid in advance for funds in the future. A plan for forward spend to support activities to the end of 2006 was presented to the meeting and agreed. Future committees will need to ensure that funding applications are submitted at the appropriate time. More details will become available during meetings for group officers to be held in May at the IOP. Action: group representatives to attend forthcoming IOP meetings.
   c. A PCG "annual diary" (appended) was presented for discussion to help future committees.
8. Committee posts for Honorary Secretary/Treasurer and ordinary members (retirement of **John Evans** after 3+1 years, **Jon Loveday** at the end of a three year term; resignation of **Jacqui Cole/Dave Laundy** after 1 year) were available. Nominations for posts are detailed below. All were elected unopposed.
   a. Honorary Secretary: **Matt Tucker**. Proposed: **John Evans**; Seconded: **Dave Allan**.
   b. Ordinary Member: **Jon Loveday** (re-election). Proposed **Paolo Radaelli**; Seconded: **Dave Allan**.
   c. Ordinary Member: **Ivana Evans**. Proposed: **Judith Howard**; Seconded: **Chick Wilson**.
   d. Ordinary Member: **Serena Margadonna**. Proposed: **Paolo Radaelli**; Seconded: **Jon Wright**.
9. Future meetings are detailed in the Chair's report above. **John Helliwell** asked the committee to consider the topic of single molecule diffraction for either an Autumn meeting or as a strand to a future spring meeting. **ACTION:** Group representative to raise at BCA planning meeting.

Financial Summary 2005

Balance as of 31.12.2004	£3,537.96
Group income for 2005	£1,728.00
Group expenditure in 2005	-£124.90
Balance as of 31.12.2005	**£5,390.86**
DETAILS OF SPENDING IN 2005 ACCOUNTS	
Miscellaneous	
Postage/printing	£58.00
Total misc	£58.00
BURSARIES IN 2005	
Sarah Lister	£150.00
Shu Yan Zhange	£250.00
Total Bursaries	£400.00
SPEAKER SPEND IN 2005	
Malcolm McMahon plenary at bca	£89.00
committee travel	£0.00
Total speaker spend	£89.00
2004 WINTER MEETING	
2004 winter meeting registration (income)	-£1,259.00
Winter meeting support cheque repaid	-£1,000.00
BCA fees for attendees	£52.50
Total winter meeting expenses in 2005 accounts	-£2,206.50

2005 RIETVELD SCHOOL	
Teacher expenses (travel, accommodation, food)	£548.60
Room hire/refreshments	£986.00
Total Rietveld School	£1,534.60
PROJECTED SPEND IN 2006	
Sagamore conference support	£1,000.00
PCG prize support	£1,000.00
Bursary application - Andrew Goodwin	£250.00
CMMP speaker expenses	£500.00
Winter meeting underwrite	£1,000.00
Rietveld school support/bursaries	£1,000.00
German Sastre travel	£133.33
Total General spend 2006 by 21st February	£4,883.33
Effective Balance on 21st Feb (estimated by jsoe)	**£507.53**

Notes:

Issues regarding IOP accounting at 2005 AGM have been resolved. IOP budget model will change from 2007 to a bidding system; total amount of group funding unchanged. Amount bid for should not normally change dramatically from the group's spending profile.

PCG Yearly Activity Diary

WHEN	WHAT	WHO
January	Finalise BCA spring meeting scientific programme	Sec
	Crystallography News Deadline (AGM+prize announcements)	Sec
	Email reminders about pcg prizes	Sec
	Instruct IOP to send hard copy information re AGM	Sec
February	Deadline for Thesis Prize	Chair
	Deadline for Physical Crystallography Prize (biannual)	Chair
	Ensure new committee members lined up for AGM	Chair
	Check end/start of year finances/grant correctly handled by IOP	Sec
March	Ensure all speakers for BCA organised	Sec/OM
April	BCA spring meeting activity	All
	Committee meeting before AGM	All
	Agenda/finances for AGM	Sec
	AGM during BCA spring meeting	All
	Ensure new committee members/officers in place	Chair
	PCG prize lecture	Chair
	Crystallography News Deadline	Sec
	Finalise winter meeting theme/chair/location	Chair
	BCA council meetings at spring meeting	Sec
	BCA Durham teaching school	some
May	IOP Annual representatives meetings	Chair/Sec
	BCA Spring meeting planning meeting	Sec
June	Structural Rietveld workshop (~biannual)	OM
July	Ensure final plans for winter meeting in place	Chair
	Crystallography News deadline (Announce winter meeting + workshops)	Sec
August	Mini committee meeting during e.g. IUCr or ECM as appropriate	Chair
September	Initial adverts for Winter meeting	Sec
	BCA Council meeting Birkbeck	Sec
October	Crystallography News deadline (reports on summer meetings)	Sec
November	Re-advertise winter meeting	Sec
	Announce pcg prize nominations as appropriate for year	Chair/Sec
	IOP group/divisional officers forum	Chair
	IOP annual report submission	Sec
	IOP funding applications submission?	Sec
	Magnetic Rietveld school (~biannual)	some
December	Winter meeting	OM
	Annual committee meeting	All
	Discuss BCA Honorary members and nominate	All
Ongoing	Other conferences (CMMP)	All
	Involvement in central facility workshops	OM
	Contact BCA/IOP members as required	Sec
	Webpages	??
	Bursary application/processing	Sec
	Newsletter for IOP members	??
	Liaison with RSC solid state group, neutron scattering group, magnetism group	OM's
	Lobby central facilities as appropriate	All
	Provide "seed funding/support" for e.g. future beamline applications	
	Articles/activity reports for Crystallography News and/or newsletter	All

John Evans

Prehistory of the BCA

ALTHOUGH X-ray diffraction was founded in physics, it rapidly became an interdisciplinary subject. Its potential for discovering the arrangement of atoms in crystals was recognized by the British physicists William Henry Bragg and his son William Lawrence Bragg. Structural research was thus providing information that was fundamentally chemical. It was appropriate that W. H. Bragg's appointment to the Royal Institution in 1923 was not only as Director of the Davy Faraday Laboratory but also as Fullerian Professor of Chemistry.

The Royal Institution was able to play a key role in the interdisciplinary development of X-ray crystallography because it was not a university. In the 1920s, departmental divisions in universities between physics and chemistry were usually rigid. The crossing of subject boundaries at the Royal Institution was facilitated by a family atmosphere within the research team, attracting not only physics-trained graduates such as **Kathleen Yardley** (later **Lonsdale**) and **Gordon Cox**, but also chemists such as **J. Monteath Robertson**. These three all went on to head departments of chemistry in universities where they introduced crystallography as the main line of research. As a result, crystallography was broadened to include molecular geometry, intermolecular interactions, and the possibilities for chemical changes in the solid state, alongside the physical interactions between atoms and ions, and the physical characteristics of crystalline matter. Meanwhile, **W. L. Bragg** founded research schools in the physics departments at Manchester and Cambridge universities whose specialities included crystal structure determination of chemical materials alongside physical crystallography. He was also conscious of the important applications of crystallography in industry, and in 1942 he held a large conference in Cambridge on relevant topics. He then founded, in 1943, an X-ray Analysis Group (XRAG) within the Institute of Physics.

One of the first international X-ray diffraction meetings was organized by **W. H. Bragg** at the Faraday Society in 1929, and this laid the foundation of a more formal international collaboration between crystallographers. Committees were set up to introduce a coordinated abstract scheme, to standardize crystallographic nomenclature, and to prepare and standardize space group tables. Publication of the first edition of the International Tables for Crystallography in 1935 was a major achievement, in which **Kathleen Lonsdale** played a particularly important part. The war severely hindered international cooperation in Europe, although in 1943, **W. L. Bragg** made a hazardous journey to Sweden to re-establish contact with Swedish scientists!

In postwar years, interdisciplinary collaboration in UK crystallography ran into some difficulty. In those years it was considered essential for a professional academic scientist to be a member of an appropriate society. The relevant societies for physics and chemistry were the Institute of Physics (IoP) and the Chemical Society (CS). In the 1950s, the IoP, having merged with the Physical Society, was not only a learned society, organizing and sponsoring scientific meetings: it was also a professional association, accrediting members at various levels, providing career advice and professional insurance, and publishing journals that were offered to members at a reduced price. The overhead costs of examinations, accreditation, publication, advisory services and insurance enforced a large annual subscription, equivalent to one or two weeks' salary for a young lecturer. The CS was the learned society predominantly serving academic chemists, accreditation functions being carried out by the then separate Royal Institute of Chemistry, and they did not merge until 1980. In universities, membership of the IoP or the CS conformed closely, in most cases, to departmental boundaries between physics and chemistry.

Originally, XRAG provided a valued meeting point. Because chemical crystallographers had no corresponding group, many chemists joined the IoP at the cheapest grade of Subscriber and could take part in XRAG with no additional payment. XRAG meetings catered for the interests of physical, chemical and biological crystallographers, and to some extent those of mineralogists, geologists and metallurgists.

This amicable state of affairs continued until 1966. By that time the volume of research in chemical crystallography had grown to such an extent that it was felt there should be a Chemical Crystallography Group (CCG) of the CS. Under the chairmanship of **Monteath Robertson**, the new Group encouraged more activity among chemists in using the techniques and results of structure determination. Though this was a useful development, it caused some ill feeling, because it created a separation between physical and chemical crystallographers, when a single group had been so successful in the past. Some chemists continued to belong also to XRAG, which in 1969 became the Crystallography Group of the IoP (here called PCG to avoid ambiguity!). Without anybody wishing it, the barely significant difference between physical crystallographers and chemical crystallographers had been set in stone because of the rigid walls between physics and chemistry departments in many universities.

On the initiative of the PCG committee, under the chairmanship of **Ted Steward**, a United Kingdom Crystallographic Council (UKCC) was set up in 1969 which tried to prevent overlaps between crystallographic meetings, both of dates and topics, and to encourage occasional joint meetings. It catered not only for the chemists and physicists but also for other crystallographers. It fulfilled a useful function, but because it had to avoid challenging the roles of the PCG and the CCG it proved too weak and ineffective to become a unifying British crystallographic society. It was the establishment of the European Crystallography Meeting (now the ECA) in 1970, and discussions

At the historic meeting in Durham, 1982, left to right: *Brian Isherwood, Arthur Wilson, Andrzej Skapski, Charles Taylor, David Blow and David Phillips*

about how the UK should be represented on it, that brought the groups together, with a joint members' meeting in 1971.

Meantime, the Royal Society had set up the British National Committee for Crystallography (BNCC) to represent it on the IUCr and to distribute its block grant for scientists attending the meetings of the IUCr. This job was complicated by the division in British Crystallography, and in 1978, **Arthur Wilson**, then chairman of the BNCC, proposed that it should provide an umbrella organisation for the PCG, the CCG and the UKCC. An ad hoc group was established, and it prepared a proposal for the 'Formation of a British Crystallographic Association' which was presented by **Andrzej Skapski** to the BNCC in May, 1979. However, there were two main difficulties – financial andorganisational. The report said: 'A reserve fund of £4000-5000 would be invaluable in aiding the BCA to start its activities.' And was it right to attract membership from crystallographers loyal to the existing Groups?

In the summer of 1980, **John Robertson**, in an article published jointly in the PCG and CCG newsletters, said that 'the crystallographic community of this country is divided into two major portions; there is consequent loss of much of the richness of our subject, and consequent frustration for our committees.' This alerted the two Groups to the seriousness of the division but it was **Stephen Wallwork** who suggested how it might be overcome. His idea was that the PCG and CCG members should automatically belong to the new organisation and these Groups should continue unchanged, as joint groups linked both to their own society and to the new organisation.

Important steps were taken at the J. M. Robertson Symposium held in Glasgow in September 1980, a landmark meeting because it included the two Groups. Wallwork's proposals were favourably discussed and it was decided to arrange a special meeting of the two Groups to consider them in more detail and, if they were accepted, to set up a Working Party to plan the formation of the new body. The initial proposals were put to the Councils of the RSC and the IoP, who were both very supportive. The Working Party rapidly agreed the name 'British Crystallographic Association' (BCA) and began work on a draft constitution. Wilson, who had much experience of this kind of drafting, was the mastermind in this activity. In comparison with the UKCC, the new organization would be much more powerfully placed to be the national representative of UK crystallography. The Working Party also set a target date for inauguration of the BCA at a crystallographic meeting in Durham, already planned for April 1982, a target that maintained a sense of urgency.

A proposal made in May 1979 to amalgamate the two Newsletters was finally implemented, and in March 1981 the first joint issue of a Newsletter, edited by **Moreton Moore**, was published by the PCG and the CCG. The second issue (June 1981) was entitled Crystallography News, and it is still published under this name.

After considerable delay, approval of the charitable status of the new organisation was obtained only three weeks before the inauguration date. **David Blow** had solved the problem of initial financial resources by suggesting that crystallographers should be invited to become Founder Members. By the inauguration date, 23 of these had guaranteed £100 each (as a ten-year membership subscription) and there were also five Founder Sponsors at this stage, offering £1850. The Inaugural Meeting, on 6 April, 1982, was attended by 127 people, and the recommendations of the Working Party were accepted unanimously, including the election of **Sir David Phillips** as President, and **Dorothy Hodgkin** as Vice President. Hodgkin and **Henry Lipson** spoke at the inauguration. At the end of the Inaugural Meeting, **Brian Isherwood** proposed the establishment of an Industrial Group of the BCA, and **David Blow** proposed the establishment of a Biological Structures Group. This structure of four specialist Groups within the BCA still survives, the Crystallography Group of the IoP having become the Physical Crystallography Group.

At the end of this historic meeting there was a great sense of euphoria. At the same time, members of the Working Party were well aware that the financial resources of BCA were inadequate. Indeed, some even doubted whether it could survive. The financial position soon improved, however, helped by the Founder schemes. These were held open until the end of 1982, after which there were 52 Founder Members, and also 31 Founder Sponsors who donated over £12,000 between them. Most importantly of all, the BCA succeeded beyond all expectations as a scientific organization, with its active groups, its exciting annual meetings and, crucially, its large and enthusiastic membership. It has become one of the biggest crystallographic societies in the world.

David Blow and Stephen Wallwork

[a fuller account is published in Notes Rec. R. Soc. Lond. 58(2), 177-186(2004)]

Obituary

Ulrich Wolfgang Arndt (1924-2006)

ULRICH WOLFGANG ARNDT was born in Berlin in 1924, to parents with mixed German-Russian-Dutch origins. His family moved to London in 1936 to escape the increasingly repressive atmosphere in Germany, and Uli went to school at Dulwich College. After initially specialising in Classics, he switched to science, in spite of the fact that this was held in low esteem by many at the time. Following another family move, he finished his schooling at King Edward's School in Birmingham and spent a year at Birmingham University before going to Emmanuel College, Cambridge to read Natural Sciences in 1942. While still at Birmingham, Uli had met **Max Perutz** briefly following an introduction by family friends. Uli greatly enjoyed his time in Cambridge, and took full advantage of the many College and University societies, being particularly active in the Emmanuel Debating Society. Because of war-time restrictions, he was allowed to spend only two years at Cambridge, and after obtaining a first at the end of his freshman year opted to complete the Tripos in two years rather than the usual three. Despite recording the best Physics Tripos of his year, his final degree was only a II-2, but this did not prevent him from enrolling as a PhD student in the Crystallography Department of the Cavendish Laboratory, then run by **Henry Lipson**. His work involved characterising iron-copper-nickel alloys using a Debye-Scherrer powder camera. Uli quickly decided that the photographic methods in use at the time were too tedious and inaccurate, and decided to build a diffractometer equipped with a Geiger counter to do the job. Making extensive use of Government surplus supplies, he succeeded in his task by the time he left Cambridge in 1948, but unfortunately had not recorded sufficient experimental data to write up his thesis. He then joined **Wally Hall** at Birmingham University as a Research Fellow, and drew on his experiences at Cambridge to design and build one of the very first precision diffractometers. This finally yielded sufficient material for his thesis, although all the writing had to be done in his spare time.

In 1949, he moved to London to join **Dennis Riley** at the Royal Institution. Here he developed a compact rotating anode generator and several automatic diffractometers for low angle diffraction, again making extensive use of Government surplus equipment. Realising the limitations of Geiger counters, he developed some of the first proportional counters, making use of equipment from the vaults of the RI left over from Dewar's work on liquefaction of gases. Following Pauling's publication of the alpha-helical model for proteins in 1951, Uli and Dennis were able to determine the radial distribution function of bovine serum albumin and found excellent agreement with that predicted by Pauling's model. This provided some of the first experimental support for the alpha-helix, although subsequent work showed that the agreement was largely fortuitous! **Lawrence Bragg**'s arrival as Director at the RI led to a change in focus towards single crystal diffractometry, and a very fruitful collaboration began with **David Phillips** in 1955. This led to the development of the linear diffractometer, controlled by an analogue computer, which was used to collect some of the data for **Kendrew**'s 5Å resolution structure of myoglobin.

A collaboration with **Terry Willis** at Harwell resulted in a greatly improved version of the diffractometer for neutron work, and an X-ray version of this instrument was subsequently commercialised very successfully by Hilger and Watts. Uli and Terry's collaboration also led to the publication a few years later of the classic monograph "Single Crystal Diffractometry".

Uli's pioneering work in instrumentation and automation had not gone unnoticed, and in 1962 **Max Perutz** invited him to join the newly founded MRC Laboratory of Molecular Biology in Cambridge. Uli took up the invitation the following year. The challenge of measuring the many thousands of reflections required for protein work led him to re-examine the possibility of using the only two-dimensional detector available at the time, namely X-ray film. This in turn led to the development of automatic densitometers to speed up the measurement of film data recorded with precession cameras. Uli soon realised that the availability of scanning densitometers eliminated the requirement for the spots to lie on straight lines, opening up the possibility of using screenless oscillation photography. In the late 1960's Uli's PhD student, **Paul Phizackerley**, investigated the potential of this method, and this led to the development, with **Alan Wonacott**, of the Arndt-Wonacott oscillation camera, marketed by Enraf Nonius. This device revolutionised data collection methods, and cameras were soon to be found in almost all the protein crystallography laboratories throughout the world. Indeed, although film has since been replaced by electronic area detectors, the rotation method remains the standard procedure for macromolecular data collection. An international meeting on the use of the rotation method was organised by **David Blow** in 1975, and the proceedings were published in a monograph edited by **Uli Arndt** and **Alan Wonacott** (who jointly contributed 11 of the 17 chapters), which rapidly became a standard work. In fact, the oscillation camera was only intended to be a short-term solution, as Uli's real ambition lay in developing a fully electronic area detector based on TV cameras. In the event, it was many years before this detector, the FAST, became commercially available, and the oscillation camera remained the workhorse in many laboratories until the late 1980s. By this time the FAST faced stiff competition from multiwire chambers, and subsequently from image plate detectors, and it never achieved the same level of popularity as its more humble predecessor. Despite the shortcomings of a relatively small active area, technical improvements to the original design (a double buffer) allowed it to collect oscillation data in

a “shutterless” mode, a highly desirable feature that is still not possible with modern CCD detectors.

Although never attracted to working at large scale facilities such as synchrotrons (he was always much happier working with the LMB electronic and mechanical workshops), Uli was inevitably drawn into committees involved with the design of instrumentation for the new generation of X-ray sources. This led him to take a fresh look at focussing optics for use with laboratory sources. A literature search revealed a source of toroidal mirrors designed originally for X-ray astronomy, and theoretical calculations suggested that if these were combined with a very small focal spot size then it would be possible to obtain a brightness comparable with rotating anode generators from a sealed tube running at a fraction of the power. By this time Uli had reached retirement age, but the microfocus system was his idea of an ideal retirement project. Together with **Peter Duncumb** and **Jim Long**, both experts in electron optics, and supported by grants from the Royal Society, Uli spent the next ten years bringing the project to fruition. The tube/mirror system was marketed by Bede Scientific Instruments, and performed remarkably well. It seems likely that his work in this area strongly influenced the development of microfocus sources by the much larger commercial X-ray equipment manufacturers, which have effectively replaced the more conventional designs that had remained almost unchanged for twenty years. Uli was not one to rest on his laurels, and was actively engaged on designing and fabricating improved mirror optics until a few weeks before his death.

Uli was very much a feature of life at LMB. With his trademark bow tie and, until smoking was finally banned, his pipe, he was often to be seen in the canteen explaining his latest ideas on improving his designs, often with the aid of a picture scribbled on a paper napkin or an envelope. He was also an excellent story-teller, with a host of amusing anecdotes to hand. His autobiography entitled “Personal X-ray Reflections”, soon to be published, is sure to provide entertaining insights into the life of one of the most influential figures in X-ray instrumentation.

Biographical Outline

Ulrich Wolfgang Arndt; born Berlin 23rd April 1924
Graduated Cambridge University 1944
PhD Cambridge University 1948
Staff, Metallurgy Department, Birmingham University 1948-9
Staff, Davy-Faraday Laboratory, Royal Institution 1950-63,
Dewar Fellow 1957-61.
Staff, University of Wisconsin, Madison 1956
Staff, Medical Research Council
Laboratory of Molecular Biology, Cambridge 1963-89.
Staff, Institut Laue-Langevin, Grenoble, 1972-3.
FRS 1982.
Married Valerie Hilton-Sergeant 1958 (three daughters).
Died Cambridge 24 March 2006.

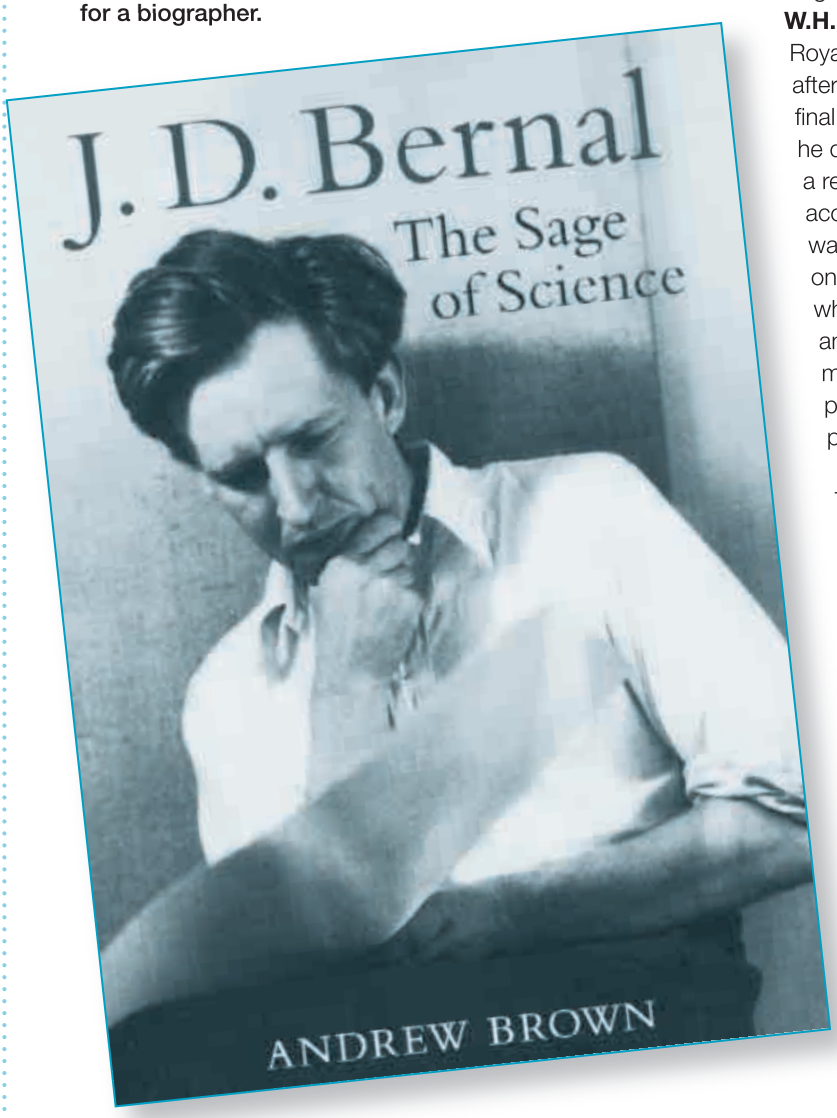
Andrew Leslie, September 2006
See also obituary in The Independent, Saturday 8 April.

Books

J.D.Bernal
The Sage of Science

Andrew Brown
Oxford University Press, 2005
Price: £25 (hardback)
ISBN 0-19-851544-8, 576 pages, 27 photographs

JOHN DESMOND BERNAL was a remarkable man; born in Ireland in 1901 he spent most of his life in England where he died in 1971. He had an attractive personality and an insatiable curiosity; unlike most people he could recall information and talk knowledgeably on many topics, which caused his colleagues to refer to him as "Sage" since his undergraduate days. His wide interests in science, politics and the arts make him a very difficult subject for a biographer.



Dorothy Hodgkin took ten years to write his 'Biographical memoir' (see Ref 1 below) for the Royal Society. A contemporary of his, the novelist **C.P.Snow**, wrote a novel, "The Search" in 1934, where one of the main characters is an X-Ray crystallographer with many resemblances to Bernal. **Brenda Swann** and **Francis Aprahamian** edited a collection of essays mainly on his life in politics published in 1999 (see Ref 2 below).

Andrew Brown, an English radiation oncologist practising in New Hampshire, has been working on this biography for the last five years and has interviewed many eminent scientists and others who knew Bernal. The result is this massive work, weighing 1 Kg, where he describes both the political activities in Europe and the science being carried out at the time to set the scene in which Bernal found himself. For example, the work of the Braggs leading to their Nobel Prize in 1915 is described because **W.H.Bragg** was about to become the Director of the Royal Institution just before Bernal went to work there after graduation in 1923. He spent a lot of time in his final undergraduate year working on a paper in which he derived the analytical theory of point systems, as a result he failed to get a first and so could not be accepted as a doctorate student at Cambridge. This was one of his characteristics, getting sidetracked on other projects rather than concentrate on the one which others may have thought most important, and also in those projects deriving things written up more thoroughly later by others. Later he suggested problems for his students, five of whom won Nobel prizes.

The book is ordered chronologically, divided into 22 chapters and a Postscript, each with extensive footnotes, on average about 70 per chapter. The footnotes might have been better printed at the end of each chapter instead of all being collected together at the end of the book. The chapters themselves have names and numbers but the footnotes sections only numbers which makes them hard to find when one finger is keeping your place in the chapter, the other fingers are trying to hold several hundred pages together while with the other hand you are trying to find which section of Notes to read.

There is only one diagram which seems strange when crystallographers think in three dimensions and descriptions of biological molecules in words take longer to understand. I have not met 'Bernal Charts' and would have liked to see a diagram of one.

Other things lacking are a complete bibliography of all his works, though you can probably construct one from the Notes, and a brief summary of the important events in his life.

There are 27 photographs, which appear to be an afterthought as I could not find any reference to them in the body of the text. They cover a period of time between about 1900, photographs of his parents, to 1962, Bernal listening to Krushchev addressing a World Congress on Disarmament on Peace in Moscow.

There is much new detail in this book, for example, about his mother, 'Bessie' Bernal. He was her first child and she taught him to talk in French and English, answered his endless questions and encouraged his interest in travel by taking him across the Atlantic by sea and on across the continent by train to visit his American relatives as a child of 3.

Bessie was the daughter of the **Reverend William Young Miller**, a Presbyterian Minister from New England, who had married her mother Elizabeth in Illinois. When he retired in 1883 he moved to San Jose, California not far from Stanford University which Bessie attended to study languages. Her influence may explain why Bernal was willing to give women a chance to work on crystallography in his Birkbeck laboratory, an unusual occurrence in those days just after World War II.

In his youth he was a devout Catholic and when he lost his faith almost immediately he found Communism which he treated with religious fervour being reluctant to see evil in any Soviet actions, In chapter 6, 'Soviet Pilgrims', we learn he went to Leningrad on a lecture tour with **Margaret Gardiner** at the time of Kirov's assassination but dismissed the rumour that Stalin had ordered the killing as 'malicious gossip'.
Bernal lived through most of the turmoil of the 20th century. He travelled from Ireland to school in England at the time of the Easter rebellion in 1916, survived influenza in the pandemic of 1918, lived through the Depression of the 1930s, lived a Bohemian life style between the Wars in an unconventional marriage where both partners took lovers; his 4 children had 3 different mothers. He worked with **Lord Mountbatten** during World War II on the planning for the D-Day landings and worked tirelessly for peace. **Andrew Brown** gives extensive background information on all of these events but there is not space to summarise them here.

Buy the book for yourself and read the chapters on the early history of molecular biology, the Physics of Life and the difficulties of doing crystallography without access to modern computers so your calculations have to be done using 7-figure log tables.

Kate Crennell, July 2006

REFERENCES

1. **John Desmond Bernal** 1901-1971 Biographical Memoirs of the Royal Society, 26, 17-84 pub 1980 Dorothy Hogkin

2. **J.D.Bernal A LIfe in Science and Politics.** Editors Brenda Swann and Francis Aprahamian pub 1999 by Verso ISBN 1-85984-854-0

This contains two useful appendices:

a) A list of his non-scientific works and a summary of his scientific ones

b) A Calendar of Events, a 'time-line' of the important dates and events in his life

3. **Articles in 'Crystallography News'**

- no 68 March 1999 page 14 report on the Meeting to celebrate the 50th anniversary of the opening of the Biomolecular Structure laboratory at Birkbeck College by W.H.Bragg

- no 74 September 2000 page 38 Review of reference 2, above by K.M.Crennell

- another review of Reference 2 above by Alan McKay (not printed in the paper newsletter, only stored on the BCA website with the other review)

Membership Subscriptions

THE AGM of the BCA passed a motion to raise the membership subscription rate w.e.f. 1st January 2007 by £5.00 per annum, from £15.00 to £20.00, with the other rates increasing proportionately. Thus, from 1st January 2007 the membership subscription rates for the BCA are

£20.00 per annum Full membership

£10.00 per annum Student, retired and unemployed

£7.00 per annum IOP CMMP members

£27.50 3 yr term Students only

£100.00 5 yr term Overseas members only

We will be getting in touch with everyone on our membership database to let them know of these changes, and to ask for new standing order mandates etc., but in the meantime you can sit back and enjoy all the exciting programmes and informative issues of Crystallography News coming your way!

Sheila Gould, Treasurer, BCA

Fellowships at Oak Ridge National Laboratory (USA)

THE Clifford G. Shull Fellowship Program is aimed at attracting new scientific talent to the Oak Ridge National Laboratory (ORNL) and its neutron science programs, making it possible for these outstanding new scientists to continue on the path to excellence while substantially contributing to ORNL and U.S. Department of Energy missions and goals. The Shull Fellowship is open to fields of science and engineering that further advances in neutron science. Shull Fellows are expected to provide valuable stimuli to the research efforts of the Laboratory, make available the most recent developments of university science and engineering departments, and represent the Laboratory to its sponsors and collaborators in the scientific community.

The Shull Fellowship Program is directed to recent doctoral degree recipients of exceptional ability who show clear and definite promise of becoming outstanding leaders in scientific research and development. The Program will provide them with the opportunity to:

- **develop neutron science programs in areas of national importance**
- **pursue research programs within their areas of interest and expertise**
- **collaborate with Laboratory R&D staff and distinguished scientists**
- **have access to Laboratory expertise, facilities, and programs**

Shull Fellows carry out and develop research programs to enhance the knowledge of the structure or dynamical behavior of advanced materials using neutron scattering as a primary tool; work with scientists in ORNL and other research institutions on collaborative research programs using neutron scattering experiments; educate and promote the use of neutron scattering to new user communities; publish research results in scientific journals; and assist Spallation Neutron Source and High Flux Isotope Reactor instrument scientists and design teams in the development of new instrumentation to meet research program goals.

Each applicant must be the recipient of an earned doctorate and must be no more than three years beyond the doctorate. Applicants should not have previously served more than one postdoctoral appointment. Current ORNL postdoctoral appointees and staff members cannot be considered as valid applicants. A Ph.D. in materials science, materials engineering, chemistry, physics, biology or a related field is required. Candidates with expertise in nano materials are particularly welcome, and those with strong processing or characterization skills are also encouraged to apply. Previous experience in neutron or X-ray scattering techniques is a plus. Strong written and oral communication skills and the desire to work in a team environment on scientifically challenging problems are required.

ORNL is an equal opportunity employer and is committed to workforce diversity; women and minorities are strongly encouraged to apply. Applicants need not be U.S. citizens.

For more information and to apply online:
www.sns.gov/shullfellowship.
Applications will be accepted until September 30 2006.

Bob Martin
Oak Ridge National Laboratory

Newsletter of the IUCr Teaching Commission

THE first edition of the IUCr Teaching Commission newsletter is available on-line as an Adobe Acrobat PDF file via: www.iucr.org/iucr-top/comm/cteach/newsletters/june2006/

The theme of this edition is "Teaching Crystallographic Fundamentals"
The table of contents follow:

- Siena 2006 : IUCr School on Basic Crystallography
- Einstein's tongue for teaching crystallography to biologists - Philippe Dumas, Julien Vanwinsberghe and Vincent Cura
- Crystallography Education and Training in the United States - Katherine A. Kantardjieff
- Crystallographic Teaching in Pakistan - Zia Khan
- A Guided Tour in Fourier Space - Fokke Tuinstra
- The British Crystallographic Association Intensive Courses in X-ray Structural Analysis - David Watkin
- Teaching of the Fundamentals of Crystallography - Dieter Schwarzenbach
- Teaching Crystallography and Related Subjects at Novosibirsk State University, Russia - Elena Boldyreva
- Crystallographic Teaching at the Laboratory of Inorganic Crystal Chemistry at Moscow State University, Russia - Evgeny Antipov
- M.Sc. Crystallography at Birkbeck College, University of London, UK - Alan L. Mackay
  - Addendum 1: reprint of webpages containing the (now defunct) Birkbeck College M.Sc. Crystallography Course Syllabus in its final form (taken from Jeremy Cockcroft's website)
  - Addendum 2: mid 1950's (rejected) submission on crystallography by J.D. Bernal et al to the Encyclopaedia Britannica. The article was rejected as too long but it embodied the syllabus and intention of the Birkbeck College M.Sc. course in crystallography.
- Calls for contributions to Newsletter No. 2

Lachlan Cranswick

Ludo Frevel Crystallography Scholarships 2007

TO encourage promising graduate students to pursue crystallographically-oriented research, the International Centre for Diffraction Data (ICDD) has established a crystallography scholarship fund, now known as the Ludo Frevel Crystallography Scholarship Fund. Its new name was recently adopted to honour the founder of the fund, Dr. Ludo Frevel.

While the Ewald Prize is awarded by the American Crystallographic Association every three years to an internationally recognized crystallographer, little effort has been made by science Departments to cultivate aspiring crystallographers. Convinced of the beneficial, scientific impact of the proposed scholarships for crystallographically-oriented research, the ICDD has solicited funds from private and industrial sectors to support this program. The ICDD has awarded 71 scholarships since 1991. In the year 2006, Scholarship Awards were to the amount of $2,500 each. Applications for the year 2007 awards must be received by the ICDD no later than 31 October 2006. Over $154,000 has been awarded in Scholarships since 1991.

Applicant Qualifications

Applicants should be enrolled in a graduate degree program during the 2007 calendar year with major interest in crystallography e.g., crystal structure analysis, crystal morphology, modulated structures, correlation of atomic structure with physical properties, systematic classification of crystal structures, phase identification and materials characterization.

There are no restrictions on country, race, age or sex. The term of the scholarship is one year. The recipient may make application for one renewal at the end of the first year. Because a limited number of scholarships are awarded, renewal applications will be considered on a competitive basis in conjunction with all applications that have been submitted up to the closing date.

Application should consist of:

1. Letter of recommendation (limit 1 page) from the student's primary research advisor. Letters which provide specifics on the student's distinguishing qualities and accomplishments as a researcher are helpful in evaluating the applications.
2. A description of the candidate's proposed research (limit 2 pages) including: purpose and rationale for the research, proposed methodology to be used in the study, references and/or descriptions of the scientific background for the proposed research
3. A C.V. which includes: educational preparation (institutions, dates, degrees obtained and in progress, and particularly pertinent coursework), awards, honours received, any research publications and/or presentations given, any work experience (dates, employers, positions), professional activities, memberships

For further information, including previous recipients and their research proposals, please visit the web page: http://www.icdd.com/resources/awards/frevel.htm.

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Phone: +1 610 325 9814
Fax: +1 610 325 9823
Internet: information@icdd.com
Web Site: www.icdd.com

Meetings of interest

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

1 September 2006
EPDIC 'Under the Bonnet'
Powder diffraction Workshop:
University of Geneva, Geneva, Switzerland.
www.pa.msu.edu/cmp/billinge-group/Geneva2006Software

1-4 September 2006
EPDIC 10, European Powder Diffraction Conference, Geneva
www.sgk-sscr.ch/EPDIC10/EPDIC10.html

3-8 September 2006
13th BCA Summer School in Protein Crystallography, Biochemstry Department, Oxford University

4-8 September 2006
44th European High Pressure Research Group meeting, Prague, Czech Republic.
http://kfes-80.karlov.mff.cuni.cz/EHPRG/

7-14 September 2006
SHELX/MAXINF Workshop - Workshop on Experimental Phasing of Macromolecules.
Göttingen, Germany
http://shelx.uni-ac.gwdg.de/workshop2006/

10-12 September 2006
BACG Annual Meeting,
Heriot Watt University, Edinburgh.
www.bacg.org.uk

10-15 Septembre 2006
Summer School - Ecole thematique:
Analyse structurale par diffraction des rayons X, cristallographie sous perturbation.
Nancy, France.
www.lcm3b.uhp-nancy.fr/nancy2006/

11-13 September 2006
National Crystallography Service Advanced Skills Workshop, Southampton.
www.ncs.chem.soton.ac.uk/events.htm

11-16 September 2006
XX Conference on Applied Crystallography and Summer School on Polycrystalline Structure Determination,
Wisla, Poland.
http://crystallography.us.edu.pl/satel.php

12-15 September 2006
TRTR 2006: Test, Research and Training Reactors Conference, Austin TX, USA
www.engr.utexas.edu/trtr/

13-15 September 2006
ECRS 7 - The 7th European Conference on Residual Stresses. Berlin, Germany.
www.ECRS7.de

13-15 September 2006
13th CCP4 Protein Structure Workshop, Galashiels
www.ccp4.ac.uk

15-16 September 2006
5th International NCCR Symposium on New Trends in Structural Biology, Zürich Switzerland
www.structuralbiology.unizh.chsymposium06.asp

17-22 September 2006
ISRP-10 - 10th International Symposium on Radiation Physics.
University of Coimbra, Portugal.
http://pollux.fis.uc.pt/isrp10/

19-22 September 2006
PNCMI: Polarised neutron scattering techniques and their applications to small-angle scattering, reflectometry, diffraction and inelastic scattering, Berlin, Germany.
www.hmi.de/bensc/pncmi2006/school.html

19-22 September 2006
XTOP 2006 8th Biennial Conference on High Resolution X-Ray Diffraction and Imaging,
Baden-Baden, Germany,
http://xtop2006.fzk.de

25-28 September 2006
PNCMI 2006 - The sixth International Workshop on Polarised Neutrons in Condensed Matter Investigations,
Berlin, Germany.
www.hmi.de/bensc/pncmi2006/

25 September - 6 October 2006
VIII International School of Neutron Scattering "FRANCESCO PAOLO RICCI", Neutron scattering from magnetic systems,
Santa Margherita di Pula, Italy.
www.fis.uniroma3.it/sns_fpr

27-29 September 2006
Rietveld Refinement and Indexing Workshop, West Chester PA, USA.
www.icdd.com/education/rietveld-workshop.htm

28 September - 1 October 2006
Crystallography at High Pressures 2006, Dubna, Russia.
http://nfdfn.jinr.ru/~denk/crhp06

29-30 September 2006
WINS2006 - 3rd Workshop on Inelastic Neutron Spectrometers. Hahn-Meitner Institute,
Berlin, Germany.
www.hmi.de/bensc/wins2006

2-4 October 2006
International Workshop on Applications of Advanced Monte Carlo Simulations in Neutron Scattering.
Paul Scherrer Institut,
Villigen, Switzerland
http://lns00.psi.ch/mcworkshop

2-5 October 2006
Polymorph Screening: Techniques and Applications.
Stamford, CT, US.
www.assainternational.com

4-6 October 2006
German Conference for Research with Synchrotron Radiation, Neutrons and Ion Beams 2006,
Hamburg, Germany.
www.sni2006.de

16-17 October 2006
17th Annual International Light Scattering Colloquium,
Santa Barbara CA, USA
www.wyatt.com/events/colloquium/

16-19 October 2006
Polymorph Screening: Techniques and Applications.
Ettlingen, Germany,
www.assainternational.com

22-26 October 2006
4th International Conference on Structural Genomics,
Beijing, China
www.sino-meetings.com/icsg2006

23-25 October 2006
Basic and Advanced X-Ray Powder Diffraction: Pharmaceutical Applications,Part I: Basic crystallography. Stamford, CT, USA
www.assainternational.com

23-26 October 2006
Polymorph Screening: Techniques and Applications
Mallorca, Spain
www.assainternational.com

23-30 October 2006
EMBO Practical course - Solution Scattering from Biological Macromolecules. EMBL, Hamburg, Germany
www.embl-hamburg.de/workshops/2006/embo

24-27 October 2006
First African Structural Biology (FASB) conference,
The Wilderness, South Africa.
http://sbio.uct.ac.za/conference

25 October 2006
PCG Autumn Meeting
"A Snapshot of Physical Crystallography"
Edinburgh.
www.crystallography.org.uk/pcg

25-27 October 2006
Specimen Preparation for X-ray Fluorescence Workshop,
West Chester, PA, USA
www.icdd.com/education/spec-xrf-workshop.htm

25-27 October 2006
Argentine Crystallographic Association - The second gathering of the Argentine Crystallographic Association (Asociacion Argentina de Cristalografia, AACr). Puerto Madryn, Chubut Argentina
www.tandar.cnea.gov.ar/~vega

26-27 October 2006
Basic and Advanced X-Ray Powder Diffraction: Pharmaceutical Applications, Part II: Basic and advanced structure-solving solutions from X-ray powder patterns.
Stamford, CT, US
www.assainternational.com

9 November 2006
IG Autumn Meeting, Impact of Crystallography in an Industrial Environment, Pilkington European Technical Centre, Lancashire.
www.crystallography.org/ig

15 November 2006
CCG Autumn Meeting, Crystal Engineering, the Secrets Revealed!,
Glasgow
www.crystallography.org.uk/ccg

18-19 November 2006
Theoretical Crystallography and Materials Science - Satellite Conference of the AsCA'06 / CrSJ meeting.
Tsukuba, Japan.
www.lcm3b.uhp-nancy.fr/mathcryst/asca2006.htm

7-10 January 2007
PCG Rietveld Refinement School, Durham,
www.dur.ac.uk/john.evans/webpages/pcg_rietveld_school_2007.htm

14-19 January 2007
International School on Mathematical and Theoretical Crystallography.
The University of Havana, Cuba.
www.lcm3b.uhp-nancy.fr/mathcryst/havana2007.htm

21-24 January 2007
5th European Conference on Computational Biology - ECCB '06,
Eilat, Israel
www.eccb06.org

19-22 February 2007
6th Pharmaceutical Powder X-ray Diffraction Symposium, sponsored by ICDD,
Barcelona, Spain
www.icdd.com/ppxrd

2-6 April 2007
Latin American Workshop on Applications of Powder Diffraction and Satellite Workshop - Methods of Powder Diffraction,
Campinas, SP, Brazil
www.iucr.org/cww-top/mtg.anc4.pdf

17-19 April, 2007
BCA Spring Meeting,
University of Kent, Canterbury.
www.crystallography.org

23-25 May 2007
14th BENSC Users' Meeting, Hahn-Meitner-Institute, Berlin, Germany
www.hmi.de/bensc

7-17 June 2007
Engineering of Crystalline Materials Properties: the 39th crystallographic course at the Ettore Majorana Centre, Erice, Italy,
http://www.crystalerice.org/futuremeet.htm

21-26 July 2007
ACA Annual Meeting -
Salt Lake City, UT, USA.
www.hwi.buffalo.edu/ACA

13-17 August 2007
BSR2007 - Ninth International Conference on Biology and Synchrotron Radiation.
Manchester, UK
www.srs.ac.uk/bsr2007

22-27 August 2007
ECM-24, European Crystallographic Meeting, Marrakech, Morocco
www.ucam.ac.ma/fssm/ecm24

31 May – 5 June 2008
ACA Annual Meeting
Knoxville, TN, USA
www.hwi.buffalo.edu/ACA