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**NEXT ISSUE OF  
CRYSTALLOGRAPHY NEWS**

**CRYSTALLOGRAPHY NEWS** is published quarterly (March, June, September and December) by the British Crystallographic Association. MSword97 documents (or earlier versions) may be sent on a PC disk or electronically, (only small files < 500K please, image formats JPEG, GIF). 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 **March 2002** issue are sent to the Editor to arrive before **26th January 2002**.

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*President's Remarks*

*The October Council meeting was the usual lively affair with a great deal to discuss, but the most important issue was the Spring Meeting in Nottingham. Arrangements are now in place and it has a lot going for it: we have put together a cheap package for students; there is an excellent scientific programme, and the Nottingham University campus is a very pleasant environment for a conference. Some of the scientific programme is interdisciplinary - we have a two sessions on 'Phasing Methods', for example, where overlapping problems in macromolecular crystallography, powders and electron diffraction are covered with plenary lecturers who are international figures. In addition the nature of the programme means that anyone will find sessions of interest running right through the three days of the meeting. Hopefully also, the funding of students will address the concerns expressed at the last BCA AGM. Full details of the Nottingham arrangements can be found within this newsletter.*

*We will also have a new Newsletter Editor in 2002. Jo Jutson has done a great job in transforming the newsletter to a new style and format without losing the information content of the piece. She has done a year of this and did have intentions to do*

*a further two, but circumstances change, and she now finds that others need her help in a way that was not anticipated. The BCA is very grateful to her for all her hard work - and it is very hard work!*

*However, we have a new editor in Bob Gould at the University of Edinburgh. Bob retired recently, but seems busier than ever. So, working on the principle of asking busy people to help, he seems an obvious choice, and his huge experience of crystallography and its practitioners will be a great asset. His first issue will be in March 2002 and we wish him all the best.*

*Other issues: Chick Wilson has designed a BCA poster which should be available soon. Part of its purpose is to encourage new members to join even if they are only on the periphery of crystallography. At the last count we had 999 members; we need more for our voice to be heard more strongly.*

*See you in Nottingham.*

**Chris Gilmore**  
August 2001

**Cover pictures left to right:**

Children discovering what 3D shapes can be built from 2D hexagon

'Improbabubbles', from Beevers Miniature Models

The 250,000th crystal structure archived to the Cambridge Structural Database (CSD)

Structure of Earth's interior

CCDC Prize presentation to L. Dobrzycki (Warsaw University, Poland)

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<http://bca.cryst.bbk.ac.uk/BCA/>

### *The fourth issue*



*This issue of the newsletter contains eight pages with information about the 2002 BCA Spring Meeting in Nottingham. There you will find details of all the sessions, information about the meeting venue and how to register. Also included in this issue, is news of the 250,000th crystal structure to be archived to the Cambridge Structural Database (CSD), articles on "Education in Crystallography" and news about the Arnold Beevers Bursary Fund. This is the fourth newsletter in the new format and the last issue I shall*

*edit. I agreed to take on the editorship of Crystallography News initially for one year. I have found editing the newsletter interesting and challenging but in the past year my family commitments have increased to the extent that I am finding it difficult to set aside the time required. Bob Gould has agreed to take on the editorship and I would like to wish him every success as editor.*

**Jo Jutson**  
**December 2001**

### *People in the News*

#### **Professor Julia Goodfellow - New BBSRC Chief Executive**

Professor Julia Goodfellow from Birkbeck College, University of London, will become one of the first women to head one of the government's seven scientific Research Councils. Professor Goodfellow is currently Vice-Master and Head of the School of Crystallography at Birkbeck College, University of London. She will take up the position of Chief Executive in January 2002. Professor Goodfellow has been on the BBSRC Council since 1997. Her research interests include the use of computer simulation techniques to study the structure and function of large molecules. Professor Goodfellow's highly regarded research group is studying the properties of proteins implicated in the onset of disease.

#### **Professor Sir Graeme Davies - New Chair for CCLRC**

Professor Sir Graeme Davies has succeeded Dr Brian Eyre as Chair of the Council for the Central Laboratory of the Research Councils (CCLRC).

Sir Graeme is currently Principal and Vice-Chancellor of the University of Glasgow. He is the academic and executive head of the University and is responsible to the University Court for the running of the University. Prior to this, he has been Chief Executive of the Higher Education Funding Council for England; the Universities Funding Council; and the Polytechnics and Colleges Funding Council and vice-chancellor of Liverpool University. He trained as a material scientist and was Professor of Metallurgy at the University of Sheffield. He is a Fellow of the Royal Academy of Engineering and of the Royal Society of Edinburgh.

**The Institute of Physics has launched a new web site [www.physics.org](http://www.physics.org) - a simple one stop shop for any question on physics!**

[www.physics.org](http://www.physics.org) uses a powerful natural language programme to give an accurate and relevant answer to your question using a database of refereed resources that are recommended by the Institute. Providing more information for the search such as your name and your knowledge of physics, focuses the answers to your level.

Please visit [www.physics.org](http://www.physics.org) and help us test the site and the database of resources.

**Dr Jason Wilde**  
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## *Arnold Beavers Bursaries in 2002*

The bursary fund was renamed the Arnold Beavers Bursary Fund in April 2001 and endowed with £20,000 from the funds received from Crystal Congress Glasgow. BCA Council gratefully acknowledges several generous donations to the fund in its first few months of operation and welcomes further contributions to this worthwhile cause.

**GIFT AID:** The funds have also been boosted by a council decision to allocate Gift Aid refunds to the Arnold Beavers Bursary Fund. The 2001 Gift Aid refund of £668.32 has added to the fund and council thanks the 183 members who have signed a gift aid declaration and contributed to the claim. Members who haven't already done so and are eligible for the scheme are encouraged to sign a Gift Aid declaration. Your membership renewal documents for 2002 will advise you if you have already signed a form.

### **Applying for Bursaries in 2002**

#### **Bursaries for Nottingham Spring Meeting (25- 28 March 2002):**

A limited number of bursaries are available from the Arnold Beavers Bursary Fund to cover the £165 three day accommodation package and £15 student conference dinner at Nottingham (Student Registration is Free). The bursary will not cover travel expenses

and recipients will be expected to present a poster. Council is seeking commercial sponsors of Spring Meeting Bursaries and it is hoped to offer some Named Bursaries at this meeting.

The closing date for all applications is **25th January 2002**, applicants should ask for an Arnold Beavers bursary application form from the BCA Administrative Office (details below).

#### **Bursaries for other BCA Meetings and Schools:**

These are administered directly by the organisers of the Meeting or Teaching School. They will publicise the procedure for their bursary applications, whether funded by the BCA itself or a constituent group.

#### **General Bursaries:**

Arnold Beavers Bursaries are available to members, (see point (a) below) who wish to attend relevant scientific meetings in the UK or abroad which are not organised by the BCA.

All applications are considered by the BCA Bursary Committee, comprising the President, Vice President, Treasurer and Secretary and are guided by the following considerations:

(a) The bursaries are primarily intended to support bona fide research students and postdoctoral workers who are BCA members. Applications from those with more senior non-tenured positions, and from those in junior permanent positions where university or

industrial funds are unavailable, may be supported at the discretion of the BCA Bursary Committee if BCA funds are available.

(b) Applicants must normally have been a BCA member for 6 months before applying.

(c) Applicants will not normally be considered if they have been awarded a general bursary in the previous two years.

(d) Preference will be given to applicants who have attended a BCA meeting. Applications must be received at least 6 weeks before the date of the meeting/visit. No retrospective applications are possible.

Successful applicants are expected to submit a word-processed short scientific report on the meeting/visit soon after their return; this should include details of the sessions attended and of the applicant's presentation. The reports may be submitted via electronic mail to the BCA Administrative Office and may be published later in 'Crystallography News'.

**Applicants should ask for an Arnold Beavers bursary application form from the BCA Administrative Office.**

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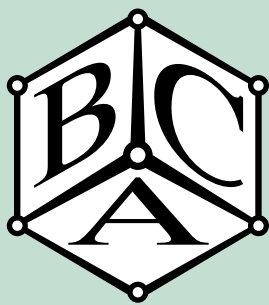


## *Minutes of the BCA Annual General Meeting 2001*

*Held on Monday 9 April in the Palmer Building, Reading University at 4.00 p.m. with the President, Professor Chris Gilmore, in the Chair.*

A short silence was observed in memory of Arnold Beevers.

1. The **agenda** was approved.
2. There were **apologies for absence** from Michael Woolfson and Chick Wilson.
3. The **minutes** of the previous AGM (held at Heriot-Watt University, Edinburgh on 5 April 2000) had been published in the December



### *Acknowledgements BCA Sponsors*

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

2000 issue of Crystallography News. They were approved and signed by the President. There were no **matters arising** from them.

4. The **Secretary's Report to Council**, which had been published in the March 2001 issue of *Crystallography News*, was accepted.
5. The proposed amendments to the Statutes and By-Laws had been published in the December, 2000 issue of *Crystallography News*. Frank Allen explained that this was a tidying up process which would a) recognise that Joint Membership with the Royal Society of Chemistry is no longer appropriate, b) change the name of Sponsors to Corporate Members, c) clarify the status of the original Founder Members and d) formalise the category of Honorary Members. The acceptance of the amendments was proposed by Anne Bloomer, seconded by Paul Raithby and carried unanimously.
6. Gill Houston of Northern Networking reported on their activities since they had been appointed to run the administrative side of the BCA. There were 909 members and the membership database has been transferred. There were 8 Corporate Members. In collaboration with the new Newsletter Editor the Newsletter was now in an A4 format. Northern networking had played a major role in the organisation of the current Spring Meeting. The number of delegates was 266 which was a little low and members should encourage colleagues and students to register next year.
7. **The Treasurer Reported** that the 2000 accounts showed major changes to the BCA funds. The BCA had received a donation of £75,000 from IUCr99 and the fixed interest investments start to mature over the next few years. Council would be considering the best way to invest our surplus funds. Financial administration of the Physics Crystallography Group has been transferred to the Institute of Physics. The administration of the Bursary Fund has been overhauled. The Heriot-Watt Spring Meeting made a loss of £5248. The Newsletter made a profit of £2714, which helped to defray some of the £5625 cost of the additional IUCr Colour Supplement. Charges for nine months from Northern Networking are included as well as the costs of the handover from Stephanie Harris to Northern Networking. A Bad Debt of £540 from X-ray Associates has been written off. The Treasurer encouraged members to sign a Gift Aid Declaration. He proposed that in future a summary of the accounts would be printed in *Crystallography News* and full copies would be available on request. The accounts were prepared by R. A. Young of The Young Company, Huntingdon.

The Treasurer for IUCr99 (Sheila Gould) handed the President a cheque for £31,000 payable to the BCA as a final payment from the profits of the Congress.

8. **The Acceptance of Accounts** was proposed by Harry Powell and seconded by Michael Glazer. The accounts were accepted *nem con*.

9. **Election of Officers and Ordinary Members of Council**

*For Vice-President* - Professor Bill Clegg had been proposed by Mrs Kate Crennell and seconded by Dr Frank Allen. Professor Paul Fewster had been proposed by Dr Chick Wilson and seconded by Professor John Finney and Dr Pam Thomas. After a secret ballot (tellers Jeremy Cockcroft and Harry Powell) Paul Fewster was declared duly elected.

*For Secretary* - Dr Christine Cardin had been proposed by Dr Hilary Muirhead and seconded by Mr David Taylor. As hers was the only nomination, she was declared duly elected.

*There were no Vacancies for Ordinary Members of Council.*

The President thanked Frank Allen (retiring Vice-President), Hilary Muirhead (retiring Secretary) and Kate Crennell (retiring Newsletter Editor) for their work on behalf of the BCA.

10. **Appointment of Examining Accountant for 1999.** Mr R. A. Young of The Young Company, Huntingdon was

appointed as Examining Accountant. He was proposed by Mike Glazer, seconded by Paul Fewster.

11. **Any Other Business**

The President reminded members that that some information was sent out by e-mail. If they were not receiving these e-mail messages and wished to do so they should check with the registration desk.

Judith Howard said that one reason for low attendance at this meeting was the high registration fee and the low level of student bursaries. Elspeth Garman also made the point that in order to boost attendance bursaries must be increased. The Treasurer replied that the bursary level of £50 per student was tried as an experiment this year. Only 50 students had applied for bursaries.

The meeting closed at 4.50 p.m.

**Hilary Muirhead  
April, 2001**

## Nominations for the BCA Prize Lecture

Nominations are sought for the BCA Prize Lecture. The system is a little unusual but works as follows:

1. It is called the 'BCA Prize Lecture' and can be awarded to any crystallographer in the world, but is named in honour of a prominent British crystallographer; this name would change with each award. So we would have, for example, 'The BCA Prize Lecture in honour of XXX'.
2. The crystallographer in whose honour it is given would attend the BCA Meeting and present the prize. Their expenses would be paid for by the BCA. There should be some link between the work of the two people involved.
3. The recipient would receive full travel costs, and would give a lecture at the BCA Meeting.
4. Nominations for this award, to be presented at the Nottingham BCA Spring Meeting are now sought. They should be sent to the Secretary, Dr Chris Cardin whose address can be found in the list of BCA officers. They should be received by February 1st 2001. Nominations should include a summary of the achievements of the two crystallographers involved.

**Chris Gilmore**

## The partitioning of strain during rock deformation

Article reprinted courtesy of ISIS

Deformation at the Earth's surface, such as occurs during major earthquakes, is ultimately driven by solid-state convection within the Earth's mantle. A detailed understanding requires knowledge of the structure of the Earth's interior and the way in which mantle rocks deform. Our knowledge of deformation derives largely from measurements of the seismic (elastic) properties of geological materials. These properties are affected by grain-scale variations in composition and microstructure influences; experiments on ENGIN are exploring this, providing unique information on deformation

accommodation within rocks with a wide range of compositions and microstructures.

The rocks that make up the Earth's crust and mantle (Fig.1) generally comprise two or more minerals, each with different mechanical properties. During the deformation of such materials, the different minerals experience different strains. The key to understanding what controls the resulting whole rock mechanical properties is to measure the extent of this strain partitioning and how it varies with rock composition and microstructure. In normal deformation experiments, such information is not obtainable because only whole rock properties can be measured and not the contribution that each mineral phase makes to those

properties. However, the penetrating power of neutrons circumvents this problem. By conducting the deformation experiment in the neutron beam, the change in the crystal lattice dimensions of the component minerals may be monitored as a function of applied load, and from this information it is straightforward to calculate the average elastic deformation experienced by each individual mineral as a function of load.

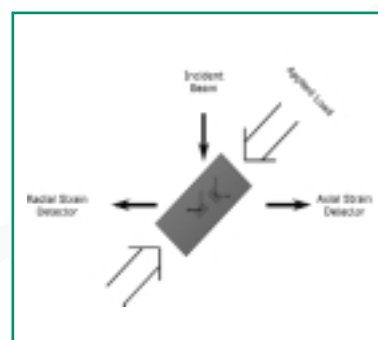


Figure 2. A schematic representation of the specimen, incident beam, detector geometry and applied load. Lattice planes oriented to represent the radial and axial directions are indicated.

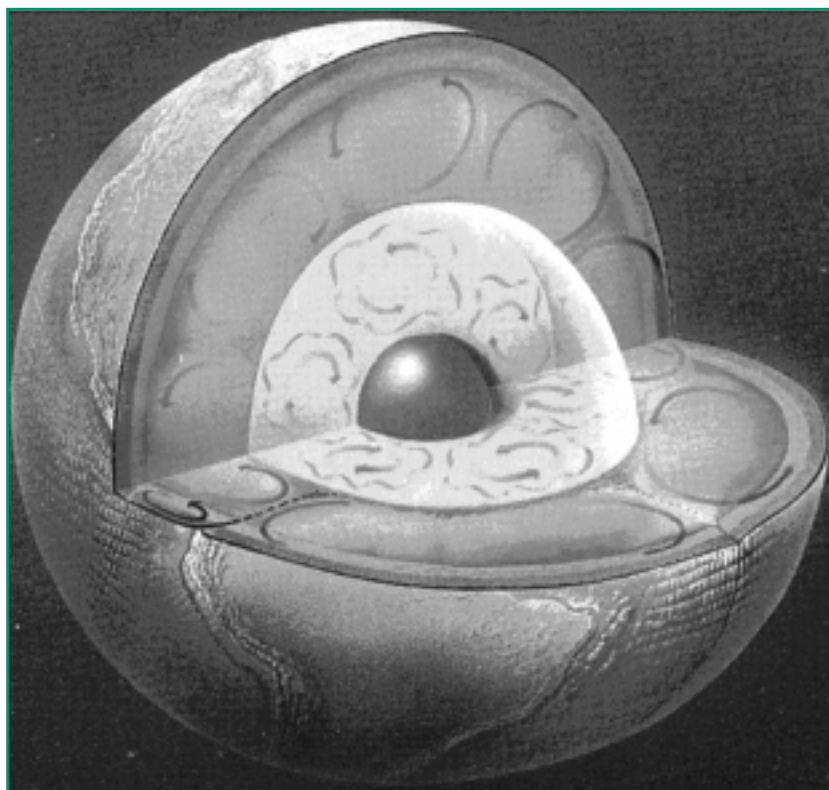


Figure 1. Structure of Earth's interior

On the ENGIN beamline, entire diffraction patterns are collected simultaneously by two fixed-angle detector banks located, one on either side of the specimen, at 90° to the incident beam. With the sample oriented at 45° to the beam, one of the detector banks only detects neutrons with scattering vectors from lattice planes oriented parallel to the loading direction, and the other only detects neutrons with scattering vectors from lattice planes oriented perpendicular to the loading direction (Fig.2). Consequently, both the axial and the radial strains in each mineral present in the rock may be measured simultaneously at each applied load (Fig.3).



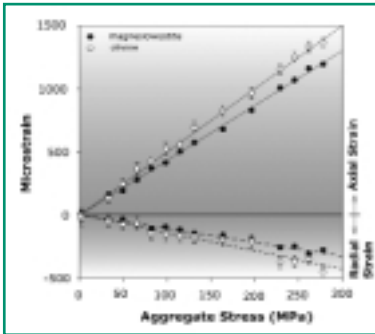


Figure 3. The axial and radial microstrains of both phases in the aggregate are measured simultaneously at incremental aggregate stresses.

We have performed experiments on several different rocks, both synthetic and natural. Typical results for an isotropic olivine+magnesiowüstite rock, two important minerals within the Earth's mantle, are shown in Fig.3. These particular results reveal that the measured strain partitioning falls within the bounds predicted by the widely used Hashin-Shtrikman variational method of calculating the elastic properties of isotropic composites from the properties of the component minerals. The Hashin-Shtrikman bounds are extremely close for this material and the fact that the experimental results fall within the bounds (Fig.4) provides strong confirmation of the experimental technique. Having demonstrated the technique for isotropic materials, we are currently using it to investigate how strain partitioning varies in samples, which are strongly textured, and where the mineral phases are non-randomly distributed through the rock. Encouraged by the success of the experiments, we have also used them to investigate how strain

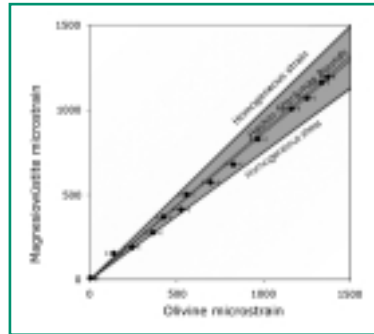


Figure 4. The Hashin-Shtrikman bounds are extremely close for this material (dark shaded region) and the fact that the experimental results fall within the bounds provides strong confirmation of the experimental technique.

partitioning changes between the phases when one or more phases starts to deform permanently by intracrystalline plasticity. The principle behind this is that if we know the elastic strain in a phase, we can calculate the stress in that phase, and then if we know the stress/plastic strain curve for that phase, we can obtain information about the plastic strain. Knowledge of this gives us the second key ingredient referred to above for understanding mantle convection, that is, information for establishing the way in which mantle rocks deform. So far our experiments have been on synthetic calcite+halite (Fig.5) and garnet+halite samples. We find that within uncertainty the elastic strain partitioning between the two phases is unaffected by the plastic yielding of the weak phase (halite at 350  $\mu$ strain in Fig.5) but that when the second phase starts to yield (calcite at 550  $\mu$ strain) there is a major change in the strain partitioning behaviour which reflects the onset of load transfer between the phases. The application of neutron diffraction to the measurement

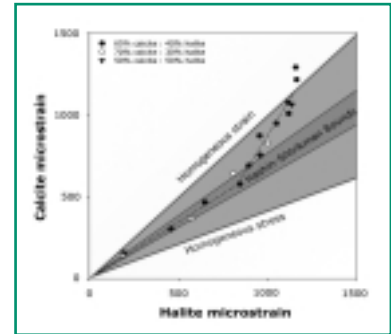


Figure 5. Divergence of strain partitioning behaviour from the Hashin-Shtrikman bounds as the calcite undergoes plastic deformation, reflecting the onset of load transfer.

of strain partitioning in polymineralic rocks is providing clear insights into the mechanical properties of deforming rocks. The implementation of ENGIN-X will greatly enhance this work by providing much tighter constraints on deformation induced textural changes as well as permitting work on common, but crystal chemically complex minerals.

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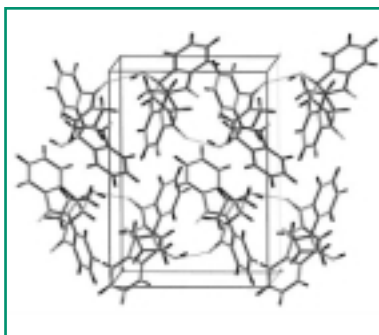
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## The Cambridge Structural Database: A quarter of a million crystal structures and rising...

On October 5th 2001, the 250,000th crystal structure was archived to the Cambridge Structural Database (CSD), marking another milestone in the ever-accelerating growth of the world's repository of small molecule organic and metal-organic crystal structures. The 250,000th CSD entry describes the structure of an organic compound, the product of a photocyclization reaction. It has been assigned the CSD reference code IBEZQA and was one of two structures published in *Angewandte Chemie (International Edition)*, 2001, **40**, 577-579. The paper's authors are A.G. Griesbeck, W. Kramer and J. Lex, of the University of Köln, Germany.



This landmark in the history of the Cambridge Crystallographic Data Centre (CCDC) comes almost exactly 36 years after the inception of the CSD project in the Department of Chemistry, University of Cambridge, UK. From small beginnings - just a few hundred structures per year

in the late 1960s - the CCDC archived data for more than 20,000 small-molecule crystal structures during the past year. In those early days, all data were re-keyboarded from original published papers, and the original database was held on magnetic tapes with a punched card backup. Nowadays, the CSD has direct deposition arrangements with 50 major international journals, and more than 80% of data now arrives in electronic form via the Internet.

Analyses of 25-year growth statistics predict that the CSD archive will contain 500,000 structures by 2010, assuming that existing methods of data generation, publication and data acquisition remain largely unaltered. Thus, the CCDC will process more information in the next decade than was processed in the previous 36 years of its existence.

Since 1989, the CCDC has been constituted as a self-supporting non-profit institution, and is responsible not only for the CSD archive, but also for a wide range of CSD-related software products. These include ConQuest for database access, Mercury for structure visualisation, and Vista for data display and analysis. Added to that, the distributed CSD System also includes IsoStar, a knowledge base of intermolecular interactions. A second knowledge base, Mogul, which contains intramolecular geometry information, is being developed. The CSD System is distributed to academic scientists in 58 countries, and to more than

100 industrial companies worldwide.

In line with a policy of making CSD data more accessible and more valuable to the scientific community, the CCDC is also involved in a number of in-house and collaborative software developments, all of which make use of CSD information in various forms: SuperStar for investigating protein - ligand interactions, GOLD for protein - ligand docking, the Relibase+ database derived from the PDB and structured for examining protein -ligand interactions, and DASH for structure solution from powder diffraction data.

The CSD System and other CCDC products provide methodologies that are widely used in scientific research, and have so far been employed in more than 800 published projects. Full references and brief summaries of these papers are collected in a small database, DBUse, maintained by the CCDC and made freely available via its website at <http://www.ccdc.ac.uk/dbuse>

The CCDC acknowledges and appreciates the co-operation and support received over many years from data depositors and journals, and from users of the CSD System and other products. We look forward to the future challenges of maintaining the CSD archive, and continuing to improve our services to the scientific community.

**Steve Maginn**  
CCDC

## *Education in Crystallography*

### **Crystallographic Education for All**

Very young children are intensely curious about their environment. Watch a toddler gazing intently at the different shaped stones on a gravel path and you will see an embryonic materials scientist wondering why stones are the shapes they are; why are they all different colours and shapes? We need to help children to retain this sense of enquiry. By playing 'crystallographic games' we can introduce them to many concepts which are essential to an understanding of the science we hope they will study later. These are ideas of symmetry, the lattice, shapes of polyhedra, including space filling ones and the packing of spheres.

Although children's building blocks in the UK are usually rectangular, other shapes can be made and used to show what other simple shapes can be fitted together to fill space, a concept which can later lead to the idea of crystal classes. I have designed several different polyhedral nets which can be cut out and constructed by older children to make their own 3D models. Alternatively, mothers (or elder siblings) might like to make a new baby a 'Crystal mobile of the Platonic Solids' to hang over the cot for the baby to look at. We might consider making a 'BCA Mobile' with one simple object for each Group which can be simply constructed and which is

an example of the science done by each group. With older children soap bubbles are fun to play with and can also be used to show how different shapes fit together in foams, which are important in modern materials.

Another important shape is the sphere. Children enjoy trying to pile up spheres to see what shapes can be made. Although special kits of spheres can be bought, it is probably better to use whatever is possible in your environment, such as spherical chocolate sweeties (especially in summer when the 'balls' melt and can be eaten), oranges, steel ball bearings, cannon balls etc.

History can be useful too. Why split knowledge into tight compartments? Pupils may remember how to pack spheres if it is approached historically. Which general offered a prize for the most efficient way to store his army's cannon balls? Who won the prize?

Special exhibits can be set up for local museums or taken round to schools to enrich their mathematics or 'design' classes. While taking exhibits of polyhedra to local shows I find many people who 'hate maths' and refuse to try to understand geometry yet are happy to construct polyhedral shapes to decorate their Christmas trees.

Crystal growing competitions for schools are popular in the UK; while waiting for the crystals to grow the children can be encouraged to make their own models and discover by experiment which can fill space.

Older children can use the Internet to learn how crystals are important in our everyday lives, by finding links to topics such as 'how a quartz watch works' or making better turbine blades for power stations.

I am trying to make a set of Web pages for the British Crystallographic Association incorporating these ideas and would be most grateful for suggestions of other ideas or links to educational web sites.

**Kate Crennell**  
[BCA@isise.rl.ac.uk](mailto:BCA@isise.rl.ac.uk)

### *New Journal of Physics*

New Journal of Physics (NJP) is a peer-reviewed, all electronic journal publishing original research in all areas of physics and is available free of charge via the Internet. It is a joint venture between Institute of Physics and Deutsche Physikalische Gesellschaft. NJP is financed by article charges that cover the cost of peer review and the publication process.

For further information visit the journal web site ([njp.org](http://njp.org))

## Mineral Detectives at the Museum - an educational half-term activity

The Oxford University Museum of Natural History decided to help parents to amuse their primary school age children at the half term break in February 2001 by arranging entertaining activities on 3 afternoons. I was asked to provide a 'crystallographic' activity to compliment the 'mineral' activities.



Figure 1.

Bright yellow plastic 'clip together' polygons that made up into truncated octahedra were made as part of a BCA 'design an interactive exhibit' competition in 1994. This picture (Fig.1) shows children discovering what 3D shapes can be built from 2D hexagons by allowing regular shaped polygonal holes.



Figure 2.

Another activity (Fig.2) showed how a crystal shape with flat sides could be built up from layers of spheres. The picture shows a small girl wrestling with the problem of how to assemble the rafts of spheres (Ping-Pong balls) stuck together with plastic model glue). This needs an adult supervisor otherwise the balls soon become unstuck.



Figure 3.

The last activity (Fig.3) used the 'Improbabubbles', from Beavers Miniature Models. These are wire frames in standard polyhedral shapes, which are used with dilute washing up liquid to explore minimal surfaces. These were popular with all ages especially some of the parents.

### Kate Crennell

**Acknowledgement for the images:** Helen Cowdy of the Museum staff took these photographs. They are copyright of the Oxford University Museum of Natural History, we are grateful for permission to publish them here. Admission to the Museum is free, details of opening hours and special activities can be found on their website at <http://www.ashmol.ox.ac.uk/oum/> (A full account of the activities will be found on the BCA website)

## Crystallography Beamlines on DIAMOND?

The planning for the design and building of the New DIAMOND synchrotron is well under way. The first seven beamlines (Day-1 beamlines) have been approved and bids for Day-2 beamlines are being considered. The crystallographic community is participating actively in this second round, and two bids have been submitted to the first stage of the process. The bids are for a high-resolution powder beamline and for a single crystal diffraction beamline. Both these bids are focused on the 'exciting' new science that will be possible using the enhanced intensity, the tuneability and the time-structure of the synchrotron. They will build upon the 'cutting-edge' science that is currently being carried out on the powder and single crystal stations at the CLRC Daresbury Laboratory, and at other synchrotrons worldwide. One of the main thrusts of the research to be carried out on the proposed powder station will involve the rapid collection of very high resolution data suitable for structure solution and Rietveld refinement of key inorganic and organic materials. The single crystal station has been designed to study the structures of molecules in their excited states, to probe *in situ* reactions, to carry out rapid and highly accurate charge density and anomalous dispersion studies, to investigate the relationship between molecular disorder and the physical properties of materials, and to develop mesomolecular crystallography.



The results of the initial bids will be known before the end of December 2001, and for those that are successful a more detailed proposal will be submitted by the end of January 2002. The powder bid is being co-ordinated by Jeremy Cockcroft (Birkbeck College, London) ([cockcroft@img.cryst.bbk.ac.uk](mailto:cockcroft@img.cryst.bbk.ac.uk)) and the single crystal bid by Paul Raithby (University of Bath) ([p.r.raithby@bath.ac.uk](mailto:p.r.raithby@bath.ac.uk)). They would both welcome suggestions of new experiments that could be carried out on DIAMOND, and seek the support of the crystallographic community for the beamlines that will keep British Crystallography at the forefront of research in the 21st century.

The first meeting of the DIAMOND Special Interest Group for crystallography will take place at the Nottingham BCA Spring Meeting.

**Jeremy Cockcroft**  
**Paul Raithby**

## The EPSRC National X-ray Crystallography Service is expanding!

Following a review by the EPSRC Chemistry Programme, two major grants have been awarded for continuation and further development of the service into exciting new areas.

One of these grants will support the continuation, for a five-year period, and expansion of the National Service at Southampton. A significant component of the funding is for an additional KappaCCD diffractometer at the

second window of the molybdenum rotating anode generator. This will be fitted with Osmic Confocal MaxFlux mirrors to give a significant increase in intensity levels: a factor of 3-4 is predicted. This will enhance work with small and weakly diffracting crystals and complement the existing services of handling twins and other difficult diffractors, high resolution studies and other non-conventional experiments. Delivery and installation of these facilities is expected in January 2002. Staffing levels will remain as before and funds have been provided to support more visits by users, who can then gain hands-on experience.

The second grant is to Prof. Bill Clegg at the University of Newcastle and adds a new component to the service, in the form of substantial access to synchrotron data collection facilities. Samples that are not amenable to study with standard diffraction equipment in local departments, or even with the advanced equipment in Southampton, can be investigated at the Synchrotron Radiation Source (SRS) at Daresbury Laboratory, where Bill holds a formal Joint Appointment. The synchrotron X-rays are considerably more intense and are used in the single-crystal diffraction station 9.8 that has been operating now for several years. A new detector system, to be installed soon, will further enhance the capabilities of this facility. The grant provides for regular allocations of beam time over the next five years. As with the Southampton service, we can provide either data collection or full structure determination. The two parts of the service are being

operated with a single integrated user interface at Southampton for approval of projects, receipt and administration of samples and screening of candidates to proceed onto the SRS, providing a seamless route between the two facilities.

We expect this extension of the national service will increase the size of the user base, and it will certainly provide rapid and easy access to the power of synchrotron crystallography without the need for cumbersome applications or expertise in the technique. There is, however, provision in the grant for some user involvement and training, which is encouraged by EPSRC. This will include some workshops as well as the possibility of direct involvement in the experimental work. Researchers with substantial requirements for access to station 9.8 are still expected to meet their needs through responsive mode grants, as the service uses only a fraction of the available days of beam time.

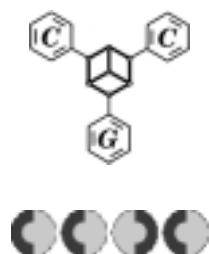
A call for applications will shortly be issued, via heads of UK University chemistry departments, for use of the service from 2002. All academics eligible for funding through the EPSRC Chemistry Programme may apply for an allocation.

See <http://www.soton.ac.uk/~xservice> and <http://www.ncl.ac.uk/xraycry> for further details.

**Mike Hursthouse and Simon Coles,**  
University of Southampton  
**Bill Clegg,** University of Newcastle upon Tyne and Daresbury Laboratory



## Chemical Crystallography Group News



### CCDC Chemical Crystallography Prize for Younger Scientists 2001

Nominations are invited for this award, to be made at the BCA Spring 2002 Meeting. The award is sponsored by the Cambridge Crystallographic Data Centre. The award is for: Original research in the field of chemical crystallography or the application of crystallographic information to structural chemistry. This definition shall include advances in instrumental, experimental, theoretical or computational techniques that contribute to this field.'

The CCG Committee will select the award winner on the basis of the published research papers of nominated candidates. Candidates should not have reached their 35th birthday by 1st January 2002, but candidates up to five years older may be considered under exceptional circumstances. The award winner will receive a commemorative item and a monetary prize, and will give a lecture on his/her research at the BCA Spring

Meeting which will be held at University of Nottingham in March 2002.

The winner of the award in 2001 was Dr Claire Wilson of the School of Chemistry, University of Nottingham.

Further details and a nomination form may be obtained from the Secretary of the Chemical Crystallography Group -

**Dr H.R. Powell,**  
MRC Laboratory of Molecular  
Biology, MRC Centre, Hills Road,  
Cambridge, CB2 2QH,  
e-mail: [hrp1000@cam.ac.uk](mailto:hrp1000@cam.ac.uk)  
fax 01223 213556).

Nominations must be received  
January 11th, 2002.

### Chemical Crystallography Group - Call for Nominations

Elections will be held at the CCG AGM in Nottingham for four (4) ordinary members of the Committee; the present incumbents will each have served a full term of three years and will not be eligible for re-election to the same posts (see rules 12 and 15 of the Constitution).

The deadline for nominations is seven days before the CCG AGM in Nottingham. The constitution of the Group can be viewed online at  
<http://bca.cryst.bbk.ac.uk/BCA/CCG/CNST.html>

**Harry Powell**  
CCG Secretary/Treasurer

### European Spallation Source (ESS) User Meeting, Bundeshaus Bonn, 15-17 May 2002

At the last ESS Council meeting in Abingdon (UK) it was decided to launch the ESS project at a European User Meeting in Spring 2002, i.e. to

- Present the ESS project to the public, science organisations and funding agencies
- Initiate the decision process for the ESS
- Initiate the process to find a site for the ESS

The presentation will be embedded in a European neutron users meeting and a symposium on neutron scattering - the scientific perspectives opened up by the ESS - to be held 15-17 May 2002 in "Bundeshaus Bonn" (The old German house of Parliament).

The preliminary agenda for the meeting is:

- 14 May Welcome and registration in the evening.
- 15 May National and European neutron users meetings (science with neutrons today).
- 16 May ESS presentation for the invited decision makers, press and users.
- 17 May European Symposium on Neutron Scattering (science with neutrons in the future).

## *British Crystallographic Association*

## *Spring Meeting 2002 - The University of Nottingham*

### **The BCA Spring Meeting**

The BCA Spring Meeting will take place at the University of Nottingham from Monday 25 March to Thursday 28 March 2002.

The Scientific Programme, including all Plenary Lectures, Symposia and Workshops will take place under one roof in the Pope Building, part of the University Park Campus, as will the Poster Sessions, the Commercial Exhibition, tea/coffee sessions and lunch.

Tea/Coffee will be served at 10:30 hrs and at 15:30 hrs in rooms A13 and A14 of the Pope Building, on each full day of the meeting.

The Commercial Exhibition will run from Monday 25 March to Wednesday 27 March. For more information on the Exhibition and Sponsorship opportunities, please contact The BCA Administrative Office at the address on page 16.

The Local Organisers for the Spring Meeting in 2002 are Dr Sandy Blake and Dr Claire Wilson.

The BCA Administrative Office will manage all administrative issues. Any queries should be directed to Euan Woodward, Project Manager at the address on page 16.

#### **REGISTRATION**

No registration fee will be charged to students and the unemployed, however student and unemployed delegates must cover the cost of their meals and accommodation.

<b>Early Registration Fee:</b>	<b>£135.00</b>
<b>Late Registration Fee:</b>	<b>£180.00</b>
<b>Retired Registration Fee:</b>	<b>£75.00</b>
<b>Exhibitor Registration Fee:</b>	<b>£135.00</b>
<b>Student/Unemployed:</b>	<b>FREE</b>

All delegates who do not wish to book accommodation at the University of Nottingham will be charged a non resident supplement of £55.00. This fee covers morning and afternoon refreshments and all lunches (25, 26 & 27 March). Non Residents can also buy a £30.00 Conference Dinner ticket, £15.00 for Students.

**Please note that the deadline for early registrations is 22 February 2002. ALL registrations received after this date will be charged £180.00.**

#### **ACCOMMODATION**

Please note that accommodation at the University of Nottingham can only be purchased on a full board basis in three day packages.

Each three day package entitles the delegate to accommodation on the nights of Monday 25, Tuesday 26 and Wednesday 27 March 2001. All meals apart from the conference dinner are included in this package (dinner on Monday 25 and Tuesday 26 March, and lunch on Monday 25 March, Tuesday 26 March and Wednesday 27 March). All dinners will be served in Hugh Stewart Hall.

Two packages are available.

**Accommodation with shared bathroom: £165.00**

**Accommodation with en-suite bathroom: £215.00**

*(Sole use of a shared bathroom)*

Please note: En-suite accommodation is limited and will be allocated on a first come basis, so early registration is recommended. An allocation of bedrooms has been reserved in Hugh Stewart Hall which is a short walk from the Pope Building. Once this allocation is filled, accommodation, if available, will be in outlying halls a 15 to 20 minute walk from the Pope Building. We would therefore recommend that you register early.

Please note that en-suite rooms have the sole use of a shared bathroom.

#### **MEALS**

On Monday 25 March, Tuesday 26 March and Wednesday 27 March, lunch will be served in rooms A13 and A14 of the Pope Building. Dinner (including the Conference Dinner) will be served in the Hugh Stewart Hall. All meals apart from the conference dinner are included in the three day accommodation packages.

A non resident supplement of £55.00 will be charged to those delegates who do not wish to book accommodation at the University of Nottingham. This will entitle the delegate to lunch on Monday 25 March, Tuesday 26 March and Wednesday 27 March, to dinner on Monday 25 and Tuesday 26 March and tea/coffee at all breaks. The Conference Dinner can be purchased at a cost of £30.00, £15.00 for Students.

## SOCIAL EVENTS

A free Delegate Reception will be held at 20.00 hrs on Monday 25 March 2002 in the Portland Building. This is included in the registration fee.

On Tuesday 26 March 2002, the Posters/Exhibitors Reception will be held in rooms A13 and A14 of the Pope Building from 19.30 hrs. Delegates will have the opportunity to chat with exhibitors and poster presenters in a relaxed, informal setting. Complimentary refreshment will be provided.

The Conference Dinner will be held on Wednesday 27 March at 19:30 hrs in Hugh Stewart Hall at a cost of £30.00 per person (£15.00 for students).

## FUN RUN

A fun run around the campus is being planned for the BCA Spring Meeting. It is being sponsored by Molecular Structure Corporation and will follow the general form of their popular event which has become a regular feature of the ACA Conference.

Further details will be available shortly before the meeting from Harry Powell ([hrp1000@cam.ac.uk](mailto:hrp1000@cam.ac.uk))

## CAR PARKING

The main visitor's car park is adjacent to Hugh Stewart Hall and currently all parking is free for conference delegates. There is also limited car parking available in the vicinity of the Pope Building which is also currently free of charge. We cannot however guarantee car parking spaces to all delegates.

## ABSTRACT SUBMISSION

Submission of Abstracts will be electronic. For instructions, please visit the website: <http://www.isis.rl.ac.uk/BCA2002>

If you have any queries regarding Abstract Submission, please email: [BCA2002@isisa.rl.ac.uk](mailto:BCA2002@isisa.rl.ac.uk)

**Please note that the deadline for receipt of Abstracts is 22 February 2002.**

## BCA BURSARIES FOR BCA SPRING MEETING

A limited number of bursaries are available from the Arnold Beavers Bursary Fund to cover the £165 three day accommodation package and £15 student conference dinner at Nottingham (Student Registration is Free). The bursary will not cover travel expenses and recipients will be expected to present a poster.

Council is seeking commercial sponsors of Spring Meeting Bursaries and it is hoped to offer some Named Bursaries at this meeting.

The **closing date** for all applications is **25 January 2002**, applicants should ask for an Arnold Beavers bursary application form from the BCA Administrative Office (details below).

For up to date information please visit the BCA website:

<http://bca.cryst.bbk.ac.uk/BCA/>

Further information can be obtained from the BCA Administrative Office:

Northern Networking  
1 Tennant Avenue  
College Milton South  
East Kilbride, Glasgow  
G74 5NA

Tel: ++44 (0) 1355 244966  
Fax: ++44 (0) 1355 249959  
Email: [bca@glasconf.demon.co.uk](mailto:bca@glasconf.demon.co.uk)



## THE UNIVERSITY OF NOTTINGHAM

The University of Nottingham started life in 1798, first as an adult school and then as a college in the centre of Nottingham before moving to its current site after World War 1.

This large estate, three miles west of the city centre, was provided by

one of Nottingham's most famous dignitaries, Sir Jesse Boot, later Lord Trent, founder of the Boots Company. It has gradually expanded into today's 330-acre University Park Campus. Set in an extensive belt of woodland, parks and playing fields, it is now the focus of life for more than 22,000 students. University Park is one of the largest and most attractive campuses in the UK, with modern teaching facilities, 12 halls of residence, a conference and

exhibition centre and an award-winning main library.

For further information on the University of Nottingham, including travel details and campus maps, please visit their website:

<http://www.Nottingham.ac.uk>



Nottingham University

#### THE SCIENTIFIC SESSIONS:

The format of the scientific programme at this BCA Meeting will differ from previous years. The sessions are based on current "hot-topics" in the field of crystallography and cross the boundaries of the various groups of the BCA. Most sessions are therefore organised by several groups. There are also many parallel sessions to try and ensure that there are interesting sessions (hopefully with no conflicts) for all delegates throughout the conference.

There is one plenary and one parallel session on "**New methods of structure solution and phasing**" covering single crystal and polycrystalline analyses. There are also sessions on "**Rietveld refinement**" and "**Polymorphism and structural changes**," these are areas of great activity in industry and academia. "Hot-topics" in the biological field include "**DNA recombination and repair**" and the more general area of "**Protein crystallography, drugs and disease**" and these both have three-hour sessions each. "**Detectors**" are of interest to us all and there is a session on this topic. "**Thin films**" is a diverse area of activity and a very important technology requiring challenging methods in analysis and three hours are devoted to this topic. In addition, throughout the meeting there will be a series of workshops including

**Thin film analysis, Amorphous materials, Powder diffraction, Macromolecular crystallisation, the CCP4 program suite** and the **CRYSTALS software**. Also there are **prize lectures** and special interests groups (SIGs) on **Educational matters** and on the status of the **DIAMOND** synchrotron project.

The posters are also a critical part of this meeting bringing a great opportunity to discuss the latest work over a glass of wine. All poster exhibitors will have the opportunity to give a brief oral presentation and a chance to win one of the poster prizes. We hope that you will find this meeting a very fruitful and enjoyable scientific experience.

#### SCIENTIFIC SESSIONS

**Plenary Session: New methods in structure solution and phasing:**

Monday 25 March, 14:00 - 15:30 & 16:00 - 17:30

*Coordinator: Paul Fewster*

The conference is opened with the plenary session and there are four speakers covering aspects of "New Methods in Structure Solution and Phasing." The lectures will cover the latest in solving molecular structures from single crystals to polycrystalline materials. There will be four speakers: Carmelo Giacovazzo (Bari)  
Bill David (RAL)  
Kevin Cowtan (York)  
Lynne B McCusker (ETH Zurich) - *Solving complex Zeolite structures from powder diffraction data*

**Polymorphism and Structural Changes:**

Tuesday 26 March, 09:00 - 10:30, 11:00 - 12:30 & 16:00 - 17:30

*Organisers: Sandy Blake, Chris Frampton & Chick Wilson*

The structural complexity of many molecular systems offers the possibility of many different crystal structures of a single compound. This property of polymorphism and the associated phenomenon of structural transformation means that the structural study of these compounds, and the understanding of the relationship between different forms, can be challenging. This session will reflect the importance of undertaking structural studies across multiple polymorphs or structural variants in providing a complete understanding of the behaviour of such materials. Comprehensive structural characterisation in this area also has significant benefits for



polymorph prediction and computer modelling which work best when an existing polymorph is already well characterised crystallographically. This area has important implications, for example, in developing new pharmaceutical compounds. The session will also reflect on the fact that in developing our understanding of structure-property relationships and phase transformations from one crystal form to another, a broad range of physical characterisation techniques are required in addition to crystallographic methods.

**Speakers (with provisional titles) will include:**

Chris Frampton (Southampton)

Stephen Tarling (Birkbeck) - *Crystallography for the Rich*

Colin Pulham (Edinburgh) - *Crystallographic and spectroscopic studies of new phases of simple molecular materials*

Mike Hursthouse (Southampton) - *New polymorphs and solvates of sulfathiazole, sulfapyridine and sulfanilamide: implications for structure prediction*

Andy Jephcoat (Oxford) - *High pressure Raman studies of structural changes*

**New Methods in Structure Solution and Phasing**

Wednesday 27 March, 09.00 - 10.30 & 11.00 - 12.30

*Organiser: Chris Gilmore*

New Methods in Structure Solution and Phasing will deal with proteins, powders and electron diffraction and look at the ways in which methods of structure solution can work together, and their common basis. Speakers include Kenneth Shankland (RAL) on powders; Helen Saibil (Birkbeck) on cryo EM; Randy Read (MRC) on the molecular replacement method; James Foadi (Glasgow/York) on ACORN; Gerard Bricogne (MRC/LURE) and Chris Gilmore (Glasgow) on electron diffraction.

**Rietveld Refinement**

Thursday 28 March, 09:00 - 10:30 & 11.00 - 12.30

*Organisers: Chick Wilson, Chris Frampton*

Following on from the PCG teaching workshop on Rietveld refinement of powder diffraction data, this session is aimed at discussing some of the recent developments and applications of the technique. The talks will concentrate on non-standard applications such as the development of Rietveld methods for larger structures, combining Rietveld techniques with computational methods, applications

to disordered structures, parametric Rietveld refinement and model-free methods. Along with a review of the state-of-the-art, the session will provide a snapshot of current trends and a view of the exciting applications to which this powerful method is being applied.

**Speakers (with provisional titles) will include:**

John Evans (Durham) - *Parametric Rietveld refinement*

Jon Wright (ESRF) - *Extending Rietveld methods to larger systems*

Steve Hull (ISIS) - *Rietveld refinements of disordered crystalline solids*

Jeremy Cockcroft (Birkbeck) - *Current status and forward look for Rietveld methods*

Karsten Knorr (Kiel) - *ODF/model-free methods*

**DNA Recombination and Repair**

Tuesday 26 March, 09.00 - 10.30 & 11.00 - 12.30

*Organiser: Peter Moody*

The session on "DNA Damage, Recombination and Repair" will feature talks by Titia Sixma (Netherlands Cancer Centre) on DNA mismatch repair, Dale Wigley (ICRF, Clare Hall) "Relating structure to mechanism in DNA helicases", Daniela Stock (MRC-LMB Cambridge) "Structure of reverse gyrase: DNA gymnastics at high temperatures", Tracey Barrett (Institute for Cancer Research) "The crystal structure of a eukaryotic resolvase", Malcolm White from St Andrews on "Archaeal DNA binding and repair proteins" and one or two talks selected from the submitted abstracts.

**Protein Crystallography of Drugs and Disease**

Wednesday 27 March, 09.00 - 10.30 & 11.00 - 12.30

*Organiser: Jonas Emsley*

Speakers from both academic and commercial backgrounds will present their data on protein structures of biomedical interest and strategies for drug design. The speakers include: William Hunter (Dundee University) "The Pteridine reductase of trypanosomatid parasites and anti-folate drug resistance."; Andrew Pannifer (Astrazeneca) "Structure of the anthrax lethal factor"; Harren Jhoti (Astell) "Structure based lead discovery" and Richard Pauptit (Astrazeneca) "Drug design trends and strategies"



**Thin Films**

Wednesday 27 March, 09:00 - 10:30 & 11:00 - 12:30

*Organiser: Jon Goff*

This session, organised by the PCG, will follow on naturally from the IG workshop in this area, and will offer talks on some of the recent research being undertaken in this topical area. Covering both non-magnetic and magnetic thin films and multilayers, the session will reflect the basic research interest and the high degree of applications-oriented work being undertaken.

Speakers to be announced.

**Detectors**

Tuesday 26 March, 16.00 - 17.30

*Organiser: Peter Moody*

This session will bring us up to date with the latest development in detectors, speakers include Wasi Faruqi of LMB "Recent developments in Semiconductor Detectors - possible benefits for crystallography", George Fraser from Dept. of Physics and Astronomy at Leicester on what is new from outer space. We will also have experts from several of the detector companies telling us about their latest developments, including Jules Hendrix (Marresearch) on solid state detectors, the experience of CCDs in the home lab. from Bruker-Nonius, and the latest from Oxford diffraction.

**IG Workshop: Introduction to Thin Films (Tutorial on Reflectometry)**

Tuesday 26 March, 9:00 - 10:30

The tutorial is designed to give a basic introduction to the analysis of thin films. This method is often referred to as "Glancing Incidence X-Ray Analysis (GIXA)" or reflectometry. It is used to determine the thickness, roughness, density etc of layers, which are less than (about) a micron in thickness. Typical examples are layers deposited to form electronic devices and also optical coatings on glass.

The tutorial will be divided into three sessions. Firstly, Paul Fewster, (Philips), will introduce some of the physics behind reflectometry. Next, the practical aspects of aligning the sample, collecting and analysing the data will be discussed by Christoph Schug (IBM SSD Mainz, Germany). Finally, we will describe some practical examples.

This workshop is designed for the beginner as well as those who have some experience of the technique. There will be time to ask questions and to discuss any problems which you have encountered.

The Physical Crystallography Group have a session on "Thin Film Analysis" on Wednesday morning, when you will be able to test your new skills.

**For further information, please contact**

Judith Shackleton  
Manchester Materials Science Centre  
0161 200 3581  
[Judith.Shackleton@man.ac.uk](mailto:Judith.Shackleton@man.ac.uk)

**IG Workshop: Powder Diffraction Surgery**

Tuesday 26 March, 11:00 - 12:30

*Panel Session chaired by J.K.Cockcroft*

Following on from the highly successful workshop on sample preparation organised by Steve Norval at the BCA 2000 meeting at Heriot-Watt University, the Industrial Group of the BCA plans to hold a "Powder Diffraction Surgery", for which active audience participation is sought. So bring along all your old powder diffraction problems that have been tucked away for years in drawers and fire them at experts on the panel who will try to suggest some ideas for solving them! Subjects up for discussion will include theoretical concerns versus practical realities, software issues, do thermal ellipsoids mean anything?, best quantitative practice, and many more.

**IG Workshop: An Introduction to Amorphous Materials**

Tuesday 26 March, 16:00 - 17:30

*A Tutorial session in two parts.*

Part 1 - J.M. Parker, University of Sheffield.  
For many purposes the diffuse X-ray scattering produced by a glassy phase is regarded as a nuisance when trying to obtain diffraction data from crystalline phases. However it does contain useful information about the structure and quantity of glassy phase present, although there are no diffraction pattern datafiles available to aid this process. In this tutorial session methods of measuring and interpreting the scattering from the glassy phase will be discussed and a number of case studies of applications of these techniques presented. Finally the application of neutron diffraction will be shown

to provide additional valuable information, complementing the results obtainable using X-rays.

The second part will cover other important aspects including quantification with the tutor and final details still to be confirmed.

For more information please keep an eye on the Industrial Group Web Pages or contact the session organiser:

Dave Taylor  
[djtaylor@lineone.net](mailto:djtaylor@lineone.net)  
Tel: 01744 893108

### **BSG Crystallisation Workshop**

Thursday 28 March, 09.00 - 10.30 & 11.00 - 12.30

*Organisers: Naomi Chayen and A. Marek Brzozowski*

The session will focus on the practical aspects of protein crystallogeneses. It will cover: tailoring proteins for crystallisation process, screening strategies, crystal growth optimisation, membrane protein handling. The progress and challenges of the high throughput crystallisation will be also addressed. An ad hoc discussion event covering the most important developments reported during the 9th International Conference of the Crystallisation of Biological Macromolecules is also planned.

### **CCP4 Workshop**

Wednesday 27 March, 14.00 - 15.30

*Organiser: Harry Powell*

Software demonstration including recent developments and overview of CCP4 software.

### **CRYSTALS Workshop**

Thursday 28 March, 09.00 - 10.30 & 11.00 - 12.30

The CRYSTALS Workshops attached to previous BCA (and other) meetings have proved astonishingly popular. A similar small workshop has been scheduled for the morning of Thursday 28 March. The format will be the same as at Reading - a brief presentation on new and changed features, followed by hands-on experience of the current release using the 20 PCs available to us.

We were a bit over-run with participants at Reading, leading to overcrowding at the workshop. This year there is a tick-box for the workshop on the meeting

registration form. It would be very helpful if we knew in advance how many people were planning to attend.

Richard Cooper and David Watkin will be available throughout the Spring Meeting to try to help new and experienced users who bring them particular problems.

For more information, contact us at:

[richard.cooper@chem.ox.ac.uk](mailto:richard.cooper@chem.ox.ac.uk),  
[david.watkin@chem.ox.ac.uk](mailto:david.watkin@chem.ox.ac.uk) For the latest version of CRYSTALS see <http://www.xtl.ox.ac.uk/>

### **Education SIG**

Monday 25 March, 17.30 - 18.15

I am planning another session on 'Education' for the BCA meeting in Nottingham, and wondering what form it should take. What do you think? Are there any burning educational issues which you think the BCA is neglecting? Would you like to tell your fellow members about them in a short talk lasting between 5 and 10 minutes? If so, please send me a brief abstract, just a sentence or two, preferably by email, so that I can select some for presentation. I would be delighted to see any new teaching aids you find useful, diagrams for teaching symmetry, software new or old which your students can use, new molecular or crystal models, etc so that I can update the BCA list of educational resources.

I can tell you about BCA plans for an improved 'educational website' aimed at showing children and the general public something of the excitement of crystallography or I can demonstrate the paper cut out 'molecular models of the crystal classes' which I hope to have available from the BCA Website soon.

It has been suggested that since education affects all BCA Groups, there might be a Special Interest Group (SIG) for those members interested in education. We might have a regular article in 'Crystallography News' on teaching topics, such as 'Designing a Winning Poster', 'How I teach the stereographic projection', 'Helping students to use the International Tables', 'Teaching crystallography to Toddlers'. Is this a good idea? Do you want a SIG?

Your ideas are welcome. Come along to the session on Monday 25 March 2002 at 17.30 or catch me at any time during the meeting to tell me about them. I plan to submit a Poster on Education with a few of my ideas, but leave lots of space, so come to the

Poster session with an A4 page of your ideas and help me make a better Poster. Should a section of the Posters be devoted to 'Education'?

Kate Crennell  
email: [BCA@isise.rl.ac.uk](mailto:BCA@isise.rl.ac.uk)

**Formation of DIAMOND SIG:**  
Tuesday 26 March, 17:30 - 18:15

*Organiser: Paul Fewster*

This is a forum to listen and discuss the new developments and future plans for the new UK synchrotron source due for commission in 2007. The exact format has yet to be finalised and the content of this session will probably be determined by the project status close to the Meeting. In recent months there have been many discussions concerning the requirements of the community, hopefully a clearer vision of what the scientific community should expect from this important facility will be made during this session.

**The BCA Prize Lecture:**  
Wednesday 27 March, 17:00 - 18:00

The topic of this lecture will not be known until closer to the date when the prize-winner is announced. This should be a very enjoyable event closing the sessions on Wednesday before the conference dinner.

## PRIZE LECTURES

**PCG/CCG Award Session**  
Wednesday 27 March, 14:00 - 15:30

*Chairs: John Finney, Paul Raithby*

This session sees the presentation of the 2002 PCG Philips Analytical Award and CCDC CCG Prize, both for outstanding young crystallographers. The award presentations are followed by the Prize lectures.

## POSTERS

**The main poster session will take place in rooms A13 and A14 from 19.30 - 22.30 on Tuesday 26 March. Please be present at your poster throughout this session.**

**BSG Oral Poster Session**  
Tuesday 26 March, 14:00 - 15:30

All potential registrants are reminded about the

annual BSG poster competition. A prize of £100 plus a Blue John trophy is awarded to the best BSG poster presented at the spring meeting.

**CCG/IG/PCG Oral Poster Session**  
Tuesday 26 March, 14:00 - 15:30

*Chairs: Bob Gould, Chick Wilson*

Presenters of posters in the Physical, Chemical and Industrial Group poster sessions have the opportunity to publicise their poster in this session. Each presenting author is expected to speak for 2-minutes in order to sum up the important points of their poster and encourage people along to view it during the formal poster session in the evening. Always a fun and enjoyable session, but with a serious point.

**BCA AGM**  
Wednesday 27 March, 16.00 - 16.45

**CCG AGM**  
Tuesday 26 March, 12.30 - 13.00

**PCG AGM**  
Wednesday 27 March, 12.30 - 13.00

**BSG AGM**  
Wednesday 27 March, 12.30 - 13.00

**IG AGM**  
Thursday 28 March, 12.30 - 13.00

**BCA Council Meetings**  
Monday 25 March, 11.00 - 12.00 & Thursday 28 March, 13.30 - 16.00

**PCG Workshop - Introduction to the Principles and Practice of Rietveld Refinement**

## Satellite meeting to BCA 2002 Spring Meeting

The workshop will take place immediately prior to the Nottingham BCA meeting, on Sunday 24 and Monday 25 March, 2002, in Room A63a, Economics & Geography Building.

This meeting is intended to begin a series of tutorial workshops organised by the PCG on powder diffraction profile refinement methods. This technique, much used and a vital component of much of physical crystallography, is very powerful but if improperly used can lead to problems both in the refinement process itself and in the resulting structural models. The aim of these workshops is to

provide a general introduction to the method and its applications. They are aimed both at those new to the technique, particularly research students and post-docs, and those who feel the need for a refresher.

The first of these workshops will introduce the basics of profile refinement using the Rietveld method. The workshop will include introductory lectures, demonstrations and hands-on examples. Topics will include:

- principles of Rietveld refinement, including minimisation;
- crystal structure refinement and what it achieves, including the use of constraints and restraints;
- data collection strategies, including angle- and energy-dispersive techniques with both X-ray and neutrons;

- basic refinement strategies - how to give yourself the best chance to get the right result;
- an introduction to some of the software suites available.

Speakers will include Bill David (ISIS/UCL), Jeremy Cockcroft (Birkbeck) and Kevin Knight (ISIS). Further details will be announced on the meeting Web sites -

<http://www.isis.rl.ac.uk/Crystallography/RietveldWorkshop.htm>

<http://bca.cryst.bbk.ac.uk/BCA/pcg/Riet2002.htm>

or contact the organiser Chick Wilson ([C.C.Wilson@rl.ac.uk](mailto:C.C.Wilson@rl.ac.uk)) for more details.

## BCA Spring meeting Nottingham 2001 Outline draft timetable

	Monday 25 March	Tuesday 26 March			Wednesday 27 March			Thursday 28 March		
	Room A2	C16	C14	C17	C16	C14	C17	C16	C14	Terminal room
09.00 hrs		DNA Recombination and Repair	Polymorphism and structural changes	IG Workshop Introduction to Thin Films	New methods in Structure solution and phasing	Protein Crystallography of Drugs and Disease	Thin Films	Rietveld refinement	BSG Crystallisation workshop	CRYSTALS workshop (Dave Watkin)
10.30 hrs	Coffee	Coffee			Coffee			Coffee		
11.00 hrs	BCA Council Meeting 11.00 hrs - 12.00 hrs (A2)	DNA Recombination and Repair (Continued)	Polymorphism and structural changes (Continued)	IG Workshop: Powder Diffraction Surgery	New methods in Structure solution and phasing (Continued)	Protein Crystallography of Drugs and Disease (Continued)	Thin Films (Continued)	Rietveld refinement (Continued)	BSG Crystallisation workshop (Continued)	CRYSTALS workshop (Dave Watkin) (Continued)
12.30 hrs	Registration (A13)		CCG AGM 12.30 hrs - 13.00 hrs		PCG AGM 12.30 hrs - 13.00 hrs	BSG AGM 12.30 hrs - 13.00 hrs		IG AGM 12.30 hrs - 13.00 hrs		
	Lunch C16	Lunch/Exhibition C16	Lunch/Exhibition C14	Lunch/Exhibition C17	Lunch/Exhibition C16	Lunch/Exhibition C14	Lunch/Exhibition Terminal Room	Lunch Room A2		
14.00 hrs	Plenary Session 'New methods in Structure Solution and Phasing' Carmelo Giacovazzo, Bill David, Kevin Cowtan, Lynne B McCusker	BSG Oral posters	CCG, IG & PCG Oral posters		Prize lectures PCG & CCG Awards		CCP4 workshop	BCA Council Meeting 13.30 hrs - 16.00 hrs (A2)		
15.30 hrs	Coffee			Coffee						
16.00 hrs	Plenary Session (continued)	Detectors	Polymorphism and structural changes	IG Workshop: Introduction to Amorphous Materials	C16 BCA AGM 16.00 hrs - 16.45 hrs 17.00 hrs - 18.00 hrs BCA Prize Lecture					
17.30 hrs	Education SIG Kate Crennell	Formation of DIAMOND SIG								
18.15 hrs	Dinner 20.00 hrs Reception Portland Building	Dinner 19.30 hrs Poster/Exhibitors Wine Reception Rooms A13 & A14			19.30 hrs Conference Dinner Hugh Stewart Hall					

Unless otherwise stated, morning sessions run from 09:00 hrs - 10:30 hrs and from 11:00 hrs - 12:30 hrs  
Unless otherwise stated, afternoon sessions run from 14:00 hrs - 15:30 hrs and from 16:00 hrs - 17:30 hrs

## Physical Crystallography Group News

### 2002 Philips Physical Crystallography Award Call for Nominations



# PHILIPS

The Philips Analytical Physical Crystallography Award is presented annually for the best recently published work (say 2-3 papers) by a relatively young person (usually 35 years of age or younger) working in the field of Physical Crystallography. It is to be expected that his or her research has or is expected to make a significant impact in this field. The 2002 award will be made during the Annual British Crystallographic Association Spring Meeting at the University of Nottingham and the recipient will be expected to give an oral presentation of his or her work at that meeting. The committee of the PCG (also the Structural Condensed Matter Group of the IoP) decide on the awardee and Philips sponsor the prize, which consists of a cash award plus expenses for attending the Spring Meeting to deliver the award lecture. The Award will be presented by a representative of Philips Analytical.

Nominations should include a brief CV of the nominee; copies of the papers on which the nomination is based (on which the main judgement is made); and a supporting statement from the nominator, including comments on the part the nominee has played in any research work published jointly with others. Optionally, a nomination form is available from the PCG/SCMPG Secretary ([C.C.Wilson@rl.ac.uk](mailto:C.C.Wilson@rl.ac.uk)) or from the Web at <http://bca.cryst.bbk.ac.uk/bca/PCG/PhForm.html>.

Nominations of candidates from the same Department as the nominator are not normally allowed.

Nominations for this Award should be sent, by **31 January 2002**, to the Chairman of the Group -

**Professor J L Finney**,  
Department of Physics and  
Astronomy, University College  
London, Gower Street, London  
WC1E 6BT  
(email: [j.finney@ucl.ac.uk](mailto:j.finney@ucl.ac.uk)).

### PCG Workshop: Introduction to the Principles and Practice of Rietveld Refinement.

#### Satellite meeting to BCA 2002 Spring Meeting

The workshop will take place immediately prior to the Nottingham BCA meeting, on Sunday 24 and Monday 25 March 2002 (see page 21 for details).

Contact the organiser Chick Wilson ([C.C.Wilson@rl.ac.uk](mailto:C.C.Wilson@rl.ac.uk)) for more details.

### PCG/SCMPG Bursaries

The PCG welcomes bursary applications from BCA or IoP members who are affiliated to the PCG or to the Structural Condensed Matter Physics Group of the IoP. These are intended mainly to help young scientists (students and post-docs) to attend meetings and conferences relevant to PCG/SCMPG areas of interest. Bursaries can be applied for at any time, through the PCG/SCMPG Secretary ([C.C.Wilson@rl.ac.uk](mailto:C.C.Wilson@rl.ac.uk)) and will be considered by the Group Committee. However, each year we expect to target selected meetings as highly relevant for the award of bursaries. The IUCR XIX Congress in Geneva will be a targeted meeting in 2002.

Applications for bursaries are expected to be received by the PCG Secretary at least two weeks prior to any early registration deadline - more details of deadlines will be publicised on the PCG Website. Recipients of bursaries are expected to write a brief report on the relevant meeting, and may be asked to report on a particular session. Session reports will normally appear on the PCG Website (<http://bca.cryst.bbk.ac.uk/bca/PCG/pcg.html>), but may also appear in Crystallography News.



## PCG/SCMPG AGM

The AGM of the BCA Physical Crystallography Group (also the Structural Condensed Matter Physics Group of the IoP) will be held at the 2002 BCA Spring Meeting at the University of Nottingham. The AGM will be held in Lecture Room C16 of the Chemistry Department, at 12:30 on Wednesday 27th March 2002.

There will be elections for Chair, vice-Chair, Secretary/Treasurer and also vacancies for Ordinary Members. Nominations (with name of seconder and note of acceptance from the nominee) for any of these positions should be sent to the Hon Sec by March 1st, 2002.

**Dr Chick C Wilson**  
([C.C.Wilson@rl.ac.uk](mailto:C.C.Wilson@rl.ac.uk))  
Hon Sec/Treasurer

## Biological Structures Group News

### BSG - Logo Competition



A logo for the Biological Structures Group would be helpful, for example in attracting the attention of readers browsing through the pages of Crystallography News or the BCA

website. We are therefore holding a logo design competition. A cash prize will be awarded for the design chosen at the Biological Structure Group Winter meeting. The logo should identify our group clearly, and designers should bear in mind that it will be used both in printed media (including Crystallography News, two tone only) and on the BCA and BSG websites. The ideal logo would therefore be recognisable in black and white, as well as in colour. Entrants should note the following information and conditions:

1. Logo designs should be submitted as graphics files. The preferred format is JPEG, but other common file types will also be acceptable.
2. The author of the winning entry must assign the copyright of their design to the Biological Structures Group of the British Crystallographic Association. The BSG reserves the right to modify the winning entry for use in different media.
3. The design should express the identity of the Biological Structures Group but there are no limitations to how this may be achieved. The design must be clear and attractive when reduced to a typical size used in BCA material - around 25 mm x 25 mm.
4. Entries should be submitted electronically to the group secretary ([a.t.hadfield@bris.ac.uk](mailto:a.t.hadfield@bris.ac.uk)) by December 10th 2001

## Biological Structures Group Winter Meeting 2001

The Winter Meeting of the British Crystallographic Association, Biological Structures Group: "Membrane proteins: Challenges to Structural Biology", will be held on Monday 17 December 2001 from 10:30 am - 6:00 p.m., in the Read Lecture Theatre, Sheffield Building, Imperial College, London.

The meeting will focus on the recent results in membrane protein research, including expression, crystallisation and structural studies. A wide range of methodologies will also be covered in the meeting, including kinetic crystallography, electron microscopy and single-molecule observation.

The registration deadline was 1st November 2001. Further information can be found at <http://www.ic-csb.ic.ac.uk/>

## Biological Structures Group Sessions at BCA Spring Meeting

**Nottingham**  
**25th - 28th March 2002**

BSG sessions organiser, to whom scientific enquiries/comments should be addressed:

Dr. Peter Moody  
E-mail: [pce1@leicester.ac.uk](mailto:pce1@leicester.ac.uk)

All potential registrants are reminded that a prize of £100 plus a Blue John trophy is awarded to the best BSG poster presented at the spring meeting.

Registration is free for graduate students and a limited number of bursaries will be available on a competitive basis to cover accommodation. See meeting main entry for further details of this and the sessions outlined below.

#### **Plenary Session: New Methods in Structure Solution and Phasing**

The meeting starts with an afternoon of plenary lectures, one from each special interest group within the BCA. These are designed to be of broad appeal across the crystallographic community. Kevin Cowtan will be giving the plenary lecture on the behalf of the Biological Structure Group including an overview of developments worldwide in structure solution and phasing.

#### **DNA Recombination and Repair**

A selection of talks looking at different structural aspects of DNA combination and repair.

#### **Crystallography of Drugs and Disease**

Speakers from both academic and commercial backgrounds will present their data on protein structures of biomedical interest and strategies for drug design.

#### **Detectors**

This session will bring us up to date with the latest developments in detectors.

#### **Crystallisation Workshop**

Tips on crystallising your (least?) favourite protein, and a chance to handle some of the wide variety of hardware now available for crystallisation.

#### **CCP4 Workshop**

Software demonstration including recent developments and overview of CCP4 software.

### **Biological Structures Group Winter Meeting 2002**

The BSG winter meeting will be held in Warwick in 2002. Suggestions for topics for this popular one-day meeting are welcomed by all the members of the committee.

### **International Course in Crystallography - Meeting Report**

**Erice, Scicily, May 23-June 3, 2001**

The 32nd Erice course in Crystal Engineering this year was entitled "Strength from Weakness: Structural Consequences of Weak Interactions in Molecules, Supramolecules and Crystals." As always the Erice course was an excellent meeting set in the beautiful surroundings of an ancient village high on a Sicilian hilltop. In this course, the bringing together of participants from many different disciplines lead to some interesting discussions both in and outside the lectures and new collaborations. Student participation, in the forms of posters, short presentations, and questions was strongly encouraged, and the length of the course - 10 days - gave everyone a chance to relax make friends and to find a chance to chat to lecturers without needing to make a formal question or point during or immediately after a lecture.

There was a strong emphasis on the study of interactions not just by crystallography, but also by techniques ranging from gas phase electron diffraction, IR and NMR to theoretical techniques. Excellent lectures gave an introduction and broad overview for participants unfamiliar with the techniques then, as the course progressed, the emphasis changed more to the uses of these techniques and results obtained.

Important points were raised about the meaningfulness of comparing measurements of parameters obtained by different techniques, given the fact that different techniques measure different things. Sometimes there is an obvious difference such as a difference in phase or experiments at different temperatures but often the differences are more subtle, such as the difference between a time averaged structure and a single 'freeze frame' snap shot of a molecule in motion or the differences between theoretical calculations calculated for an idealised case absolute zero and experimental results obtained at ambient temperatures for a molecule in a real system.

For me, however, the highlight of the meeting was the lively, (sometime heated!) debates on the nature of hydrogen bonds, especially the existence of 'blue shifted hydrogen bonds' (Hobza) and the classification of strong hydrogen bonds (Gilli), and on the virtues or otherwise of theoretical versus experimental techniques.

**Bursary Report**  
**Charlotte Broder**  
**University of Durham**

## European Crystallographic Meeting ECM20 Kraków, Poland - Meeting Report

25th-31st August 2001

### CCDC Poster Prize winners at ECM20

The CCDC poster prizewinners at ECM20 were:

L. Dobrzycki (Warsaw University, Poland).

*Structure of YAG crystals substituted with Erbium and Ytterbium.*

G. Paliwoda (Jagiellonian University, Krakow).

*Mutual recognition between diastereoisomers, quinine and quinidine, in the solid state.*

M.U. Schmidt (Clariant GmbH)  
*Ternary mixed crystal*

$C_{22}H_{12}C_{12}N_6O_4/C_{23}H_{14}C_{12}N_6O_4/C_{24}H_{16}C_{12}N_6O_4$   
*Structure solved by crystal structure predictions and X-ray powder diffraction*

The Prizes - an amethyst geode and \$250 to each winner - were presented by CCDC Scientific Director, Dr Frank Allen, at the Closing Ceremony on 31 August 2001.



CCDC Prize presentation to L. Dobrzycki (Warsaw University, Poland)

The CCDC Prize Committee comprised:

**Gautam R. Desiraju**  
(Hyderabad, India)

**Robert O. Gould**  
(Edinburgh, Scotland)

**Mariusz Jaskolski**  
(Poznan, Poland and ECA Executive Committee)

**Paul T. Beurskens**  
(Nijmegen, The Netherlands and ECA Executive Committee).

### Computing and Teaching Microsymposia at ECM

The ancient Jagiellonian University (founded in 1364) of the splendid architectural city of Kraków, was the host of one of the contrasting final morning Microsymposia on the contemporary topic of Computing and Teaching. Six speakers delighted the audience with a wide range of topics on using the Internet for distance learning, virtual courses in crystallography and a number of different models for delivery of the curriculum. Some key issues regarding the pace of introducing the new technologies, the role of government in delivering mass education and the pressures on institutions in responding to the novel methods of education were raised during the talks.

Y. Epelboin (CNRS, Paris) [1] in the opening address asked, "What can we learn from actual experience?" and compared the US experience with the European paradigm. He projected that the world education market [2] by 2005 would be worth an

estimated 90 billion US dollars. Distance learning would open up the accessibility to virtual documents and libraries facilitating politicians to contain the budget for education. However, the case was argued that the rich diverse tapestry of language and traditions that is European culture could not so easily be swayed by an economic model. Co-operation via Brussels would ensure that the "Revolution would go marching on..." was the idiosyncratic Gallic rally.

At the heart of G. Chapuis' talk (Lausanne, Switzerland) was the "nuts and bolts" of implementing interactive web applications of Java applets to provide simulation of some key crystallographic concepts. He listed the ingredients for a virtual course in crystallography concentrating on the tools for simulation and provided a number of real time demonstrations of the Ewald sphere, Laue pattern diagrams and Fourier transforms. The didactic road is long to a complete course on the Internet although within a Java environment using a web browser simulations can be performed, directly independent of the computer platform being used. This time the baton was passed on to the IUCr to promote and establish structured learning modules for potential crystallography students. C. Sansom (Birkbeck, London) described at length the Masters level distance learning courses in Structural Biology offered by Birkbeck College since 1996. She gave an overview profile of the

average student taking the course as mature with demanding professional careers quipping "that there were no typical students". The communication links between students and teachers were maintained using a purpose built Internet chat room or MUD for short (multi-user Dimension). Much of the material is written in simple HTML which can be run on a low specification computer, course material being made available at regular intervals throughout the year. It was stressed that fees were kept low to encourage wide student participation in the Advanced certificate on the Principles of Protein Structure (PPS) [4].

The first of two talks on powder diffraction commenced with A. Le Bail (Université du Maine, France) who challenged the audience to think "Where is all the knowledge." and reminded us that distance learning was in its centenary. The dangers of online education are well-established [5] with the automation of Higher Education likened to creating "Digital diploma mills" as the pervasive new information technologies advance. The provision of a powder diffraction course was inspired by the Birkbeck model and the speaker emphasised the deliberation in choosing between a synchronous and asynchronous mode of learning. The course material with pedagogic exercises is available on Structure Determination by Powder Diffractometry (SDPD) [6] and can be viewed on the web. Caution was advised that expert systems could kill the interest of deep

learning and that an explosion of software diversity could pose a nightmare for student and teacher alike. An anachronistic talk on Crystallographic Autostereograms was given by A. Katrusiak (Poznan, Poland) using handouts for the audience to practice on. The speaker presented a clear reminder of the optics of the eye and its ability to perceive perspective by binocular vision. An interesting talk that prompted a member of the audience, R. Shirley (Surrey, England), to remark that confusion over the term stereogram could be avoided if it referred only to that normally used in stereographic projection.

Returning to the topic of powder diffraction on the Internet J. Cockcroft (Birkbeck, London) stressed again the need for life-long learning and the proud tradition that Birkbeck has maintained in teaching during its 178-year history. The compatibility of the Powder Diffraction on the Web course [7] with both Netscape and Internet Explorer 3 was mentioned as well as being Java/Java script free. As it is easy "to get lost in hyperspace" the material makes extensive use of course navigation buttons on the web pages. With such an undertaking a priori knowledge cannot be assumed, but full use of colour is made in pictures and photographs contained in the HTML documents. Awareness of copyright is also an issue. The material itself is organised into three areas; experimental methods covering basic crystallography, diffraction and symmetry, data analysis covering

both quantitative & qualitative aspects and a project on Rietveld refinement. On the topic of programming options it was revealed that the space group diagrams used in the course were written in Fortran code, a spin off being a commercially available CD-ROM. The debate over interactive versus downloadable software was touched upon again. Finally the matter of assignments was mooted and their role in good housekeeping recorded. They act as an aid to learning, are complementary to the course material and provide model answers and feedback to the students in their distance learning environment away from the more traditional face to face approach that is being challenged more and more in the 21st Century.

#### References

- [1] <http://www.lmcp.jussieu.fr/~epelboin>
- [2] <http://www.wemex.com>
- [3] Chapius G. & Hardaker W., J. Appl. Cryst. (1999) 32, 1164-1168
- [4] <http://www.cryst.bbk.ac.uk/pps/index.html>
- [5] Noble D. - <http://communication.ucsd.edu/dl>
- [6] <http://sdpd.univ-lemans.fr/course/index.html>
- [7] <http://pd.cryst.bbk.ac.uk/pd/welcome.htm>

#### Bursary Report

**Jim Kelly**  
**Industrial Materials Group**  
**School of Crystallography**  
**Birkbeck College**



## Sensors

MDPI have launched another new journal in Basel, Switzerland. The new journal **SENSORS**.

<http://www.mdpi.net/sensors>

Volume 1, Issue 1 (June 2001) pages 1-52, Issue 2 (July 2001) pages 53-74 and Issue 3 (August 2001) pages 75-101 have been released. See published papers. It is FREE.

You can read the papers at the <http://www.mdpi.net/sensors/list01.htm#new> website.

Because it is a free online journal of high quality, papers published in SENSORS have very high publicity.

Contributions of manuscripts are greatly welcomed. You are invited to send your manuscripts to the Editor-in-Chief -

**Dr. Milan Antonijevic**  
by e-mail: [adanilo@ptt.yu](mailto:adanilo@ptt.yu)

If you have any suggestions, please kindly let us know.

## Sensors

## Organic Crystal Chemistry - Meeting Report

**20-24th August 2001**  
**Rydzyzna, Poland**

About every three years during the past two decades, the Adam Mickiewicz University, Poznan, has arranged an International Symposium on Organic Crystal Chemistry (SOCC) at Rydzyzna village in western Poland. The baroque chateau, situated between (but usefully distant from) Poznan and Wroctaw, painstakingly rebuilt and decorated after near destruction in 1945, now provides a congenial residential setting for small, closely interacting conferences. Support from the IUCr helped ensure the presence at the 11th SOCC of younger scientists from Russia, Moldova and Poland, while three or more of the orally presented papers came from each of Japan, Poland, Russia and the USA.

The predominant themes of the meeting were intermolecular interactions, including hydrogen bonding, supramolecular arrays, polymorphism and structure prediction. Each (fairly long) day there were about five 50-minute talks with several shorter ones, given in the exquisitely restored ballroom, while the evening poster session was stimulated by beer on tap. Pertinent comments, especially by the Programme Chair (and Photographer), Bill Duax, the local Organisation Chair, Teresa Borowiak, and Dario Braga, helped promote lively discussion.

Opening the Symposium, the Honorary Chairman, Nobel Laureate Jerome Karle (Washington DC), reviewed 20th century attempts to account for the attraction of molecules to form crystals through classical, empirical, and quantum-mechanical approaches, initially to fluids. Computer programs based on many-body symmetry-adapted perturbation theory (SAPT) have facilitated the computation of intermolecular interaction energies and may lead, with advancing computer speed and capacity, to packing energies in crystals. F. A. Allen (Cambridge) then embraced several Symposium topics in describing and illustrating the use of the Cambridge Structural Database (CSD) in the study of non-covalent so-called weak interactions; many of the, so far, less commonly observed unconventional intermolecular interactions are actually quite strong. Hydrogen bonding at C=S acceptors was instanced while non-H-mediated intermolecular interactions between carbonyls can approach hydrogen bonding energies. Allen emphasised that, in addition to maintaining the database (and capturing the more elusive data) CCDC's remit includes actual research, e.g. on genuinely weak interactions such as between N, OH and alkyl C-Cl. His final message on the role of informatics in helping better to predict molecular packing in crystals was to let the data speak. Problems in supramolecular chemistry would best be solved by mining the knowledge rather than merely the data. Among systematic users of the CSD, V. K. Belsky (Moscow) noted the



difficulty of predicting to which of four main structural types a complex formed by metal halides and crown ethers belonged, while L.N.Kuleshova (Moscow) noted the widespread occurrence of so-called polysystems, in which molecules occupy more than one set of independent positions, among crystals of hydroxy compounds that exhibit intermolecular hydrogen bonding. D.W.M. Hofmann (Bonn) had been attempting more general structure prediction and determination for molecules of <100 atoms by data (or knowledge) mining. He emphasised the importance of first trying to screen out any few remaining data of doubtful quality. Candidate structures were generated with FlexCryst, a program described at the preceding SOCC, and energy descriptors were 'trained' to discriminate between the observed structures and 'decoys' which deviate slightly. For crystal structures in space group  $p1$ , there was considerable success in both prediction and (utilising powder diffraction data) determination. A. Katrusiak (Poznan) recommended his single-image autostereograms: not motor-car sound systems but perspective drawings facilitating stereoscopic visualisation of structures.

In the first of several excellent presentations on the design and preparation of supramolecular networks, M.Wais Hosseini (Strasbourg) introduced molecular tectonics or molecular network engineering, where supramolecular chemistry meets materials chemistry.

Supramolecular structures with translational symmetry may be regarded as hypermolecules in which tectons (molecular components) are linked by non-covalent and/or reversible interactions (connections which Hosseini illustrated with cylindrical wine glasses). Hosseini looked forward to the utilisation of a wide range of physical data in the design of new materials based on functional molecular networks. From his work on materials with ion-exchange capability, W.Jones (Cambridge) described the use of a layered host as a design template to control the insertion of guest molecules. Co-crystals of, e.g., quinoxaline and succinic acid, formed by grinding powders, could be studied by powder diffraction, aided by molecular dynamics simulations of guest orientations and anionic motion. Anionic exchange clays were valuable because the layer charge could be controlled. Maria Gdaniec (Poznan) described how flexible organic molecules that are accommodated in a chiral host matrix may adopt a chiral conformation so that circular dichroism is detectable in the solid state. Cholic acid and deoxycholic acid are such versatile chiral hosts of known absolute configuration. With guest N-nitrosoamines in which the chirality is due solely to hindered rotation past a moderately high energy barrier, one may be able to separate a single enantiomer of the guest from the optically active host diols. Emphasising his organic chemistry credentials, D. Braga (Bologna) has exploited the strong intermolecular hydrogen

bonds that can form from -COOH groups in organic and organometallic polycarboxylic acids to form 1-, 2-, or 3-dimensional aggregates. With ions, charge-assisted O-H...O hydrogen-bonded networks can be strong and there is the possibility of exploiting metals with different charges, oxidation and spin states, and coordination topology. When the supramolecular bonding capacity of organic molecules is utilised as metal-bound ligands, electrostatic compression appears to permit close O(COOH)...O(H<sub>2</sub>O) approaches of 2.57Å.

Among several contributors on polymorphism and transformations, K. Ogawa (Tokyo), who also shone as an operatic tenor around the farewell bonfire, described solid-state thermochromism in salicylideneaniline and its analogues arising from proton-transfer tautomerism controlled by aggregation. In H. Birkedal's (Lausanne) study of polymorphism, stacking disorder and weak interactions in tris(bicyclo[2.1.1]hexeno)benzene, X-ray diffuse scattering is interpreted as heavily faulted layer scattering. The polished account of crystallographic and calorimetric studies of solid-state dynamics in hexafluorophosphate organometallic salts by Fabrizia Grepioni (Sassari) warned about true and pseudopolymorphism (possibly involving solvent) and of the dangers of mechanochemistry through grinding. S.Y. Chazhengina (St Petersburg) reported further progress in extensive studies of normal alkane C<sub>n</sub>H<sub>2n+2</sub> (n up to 37)

rotator crystals, both pure and as mixtures, which may undergo thermal transitions by torsional motion about the chain axis.

Linking polymorphism with biological activity, Elena Boldyreva (Novosibirsk) summarised her high-pressure X-ray and infrared results on the much-studied drug paracetamol, while Judith Flippen-Anderson (Washington DC) hinted how design of compounds to treat drug abuse and relieve pain can hinge on structure determinations of non-peptide ligands. In an enthusiastic account of ion transport in channels of gramicidin alkali-halide complexes, W.L. Duax (Buffalo) remarked on the uniqueness of gramicidin, the largest natural alternating d/l peptide, made by only one kind of bacteria. Paying tribute to her late collaborator Darshan Ranganatha (Bangalore), Isabella Karle (Washington DC) commented that their research was about the 'empty spaces' in pores, channels and tubules formed by self-assembly of cyclic hybrid peptides. Among successful tubule formers were polymethylene-bridged cystine-based cyclo bis ureas and cyclo bis amides, in which intermolecular hydrogen bonding (for which N-H and C=O groups must be in register) stabilises the walls.

Three speakers discussed charge-density measurements: after outlining topological analysis and the combination of X-ray and polarised neutron measurements, C. Lecomte (Nancy) compared N-bonds in  $-\text{NO}_2$ ,  $\text{NO}_2^-$ , and  $\cdot\text{NO}$  radicals; F.K Larsen (Aarhus) laid

stress on very-low-temperature X-ray and neutron data for characterising very short intramolecular hydrogen bonds; and M. Kubicki (Poznan) described how  $\rho(r)$  topological analysis revealed weak intermolecular hydrogen bonds in 1-phenyl-4-nitroimidazole. J. Meinel (Rennes) made use of both diffraction and inelastic scattering of neutrons in probing the nature of rotation and tunnelling of methyl groups in halogeno-methylbenzenes (and drew literally, analogies with tunnelling through the Alps. Very detailed optical-rotation tensor measurements figured largely in the survey by B.Kahr (Washington) of low-symmetry dye-inclusion crystals as a test of optical rotation theories; he looked forward to future chiro-optical imaging in biology. The seventy participants from a dozen countries are grateful to Chair Teresa Borowiak and Co-chair Maciej Kubicki for maintaining the best Rydzyna Symposium traditions of stimulating host-guest and guest-guest interactions in an unhurried ambience (without parallel sessions). For the wider organic crystal chemistry community, it is planned, as with recent SOCC, to publish selected papers in a special issue of *J. Molecular Structure*.

**Derry W. Jones**  
University of Bradford

## International Meeting on Ferroelectrics

**IMF-10, 3 -7 September 2001, Madrid**

After the opening on a warm Monday morning, Professor Blinc discussed the general topic of ferroelectrics between 1966 and 2001. At the last European ferroelectric meeting, just two years ago, the emphasis was on phase transitions and particularly the soft mode. At the present meeting the topics were already much more diverse, with interest in thin films and other areas becoming more significant. Ferroelectric smart cards are already a 2500 million dollar industry and non-volatile ferroelectric memories are already on the market.

Professor Ginzburg gave an interesting and amusing look at phase transitions in ferroelectrics in an historical context and emphasised toroidal moment as an important quantity. Professor Muller, the 1987 Nobel Prize winner, spoke about tricritical points and incommensurate phases, in a slight change to the advertised topic.

The first of the poster sessions followed these talks. I presented my work on computer simulations of the ferroelectric perovskite sodium bismuth titanate, and other titanates. This led to a number of interesting conversations.

Some presentations of particular interest to me were:

- A. Garcia, who described a 2-dimensional Ising-like model for

ferroelectric behaviour in the "Advances in Theory 1" session

- T.Egami's description of the atomistic mechanism in relaxor ferroelectrics in the "Phase Transitions and Critical Phenomena 1" session
- K. Parlinski's discussion of his "phonon" program and the results that can be gained from it in the "Computer Simulations" session
- P. Baranek's description of the use of Raman spectroscopy to measure complete dispersion curves in the "Spectroscopies" session
- S.Kamba's discussion concerning the importance of coupling between the modes for the soft mode phase transition, also in the "Spectroscopies" session.
- S. Said's description of work on the  $(\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3) - \text{PbTiO}_3$  solid solution in the "Mixed Systems" session

Wednesday morning consisted of a number of very interesting and enlightening talks about "Great 20th Century Solid State Physicists". All of these talks were of a high standard and gave a fascinating background to a number of names that are very familiar. Of particular note were A.M. Glazer's talk about the Braggs, E.Courten's discussion of Peter Debye and V.Ginzburg's description of Landau. The conference was busy and the packed schedule was very interesting. I would like to thank the BCA for allowing me to attend.

**Bursary Report**  
**Vincent Jenning**  
**University of Warwick**

## 8th CCP4 Glasgow Protein Structure Workshop

**Galashiels, September 5-7, 2001 -Meeting Report**

The first session of this year's Galashiels meeting was opened by Wulf Blankenfeldt (St. Andrews), with the structure of RmlD, the next instalment in the structures of the L-rhamnose pathway enzymes, a regular feature of the Galashiels meeting in the last few years. Stephen Muench (Sheffield) also continued a theme of previous meetings by describing his structural studies with acyl carrier protein enoyl reductase, this time from *Plasmodium falciparum*. Steve Prince (UMIST), describing structural studies and TLS refinement on the Opc adhesion protein from *Neisseria meningitidis*, challenged Wulf with "if you think your L tensors are large, you want to see mine!". Nick Hopcroft (York) described a variety of TRAP-RNA complexes and the session ended with a talk on matrix metalloproteinase-9 from Siân Rowsell (AstraZeneca).

After coffee, Iain Mitchell (Glasgow) described his experiences of characterising polypeptides from bacterial light harvesting complexes using MALDI-TOF mass spectrometry. The remainder of the session was compared to an AA meeting in which Jim Brannigan (York) and Stuart Annan (St Andrews) confessed that they were not crystallographers but actually molecular biologists and Bob Ford (UMIST) admitted he was 'sort of a crystallographer - an electron

crystallographer'. Tales of woe and cries for help from Colin James Bent and Claire Martin (both Glasgow) were also heard.

After dinner, those who managed to resist the temptations of TV rooms simultaneously showing the England and Scotland World Cup qualifier football matches were not disappointed. First we were treated to a double act from Konstantinos Beis and Simon Allard (St. Andrews) who again gave us an update on progress since last year's meeting with the various complex structures of RmlB which have allowed them to elucidate the enzymatic mechanism. John Rafferty (Sheffield) then described his work with the leucine responsive regulatory protein from the aptly named *Pyrococcus furiosus*, a denizen of deep sea black smokers. The evening was concluded by Iain Kerr (St. Andrews) who described his phasing experiences and difficulties with twinned crystals while working on the (still unsolved) structure of SSB from *Solfolobus solfataricus*.

Thursday morning was devoted to this year's specialist topic of data collection with talks in the first session from our two guest speakers, Jim Pflugrath (Rigaku/MSC) and Elspeth Garman (Oxford). Jim began by affirming that he was not a molecular biologist but a card carrying crystallographer. He went on to describe 'the diffraction experiment', taking us from Bragg's law through the Ewald sphere and ending with suggestions for data collection strategy, using a pepperoni pizza

to illustrate the differences between coarse and fine phi slicing. Elspeth was then billed by Richard Pauptit (AstraZeneca) as 'going to fill in the cheese in Jim's pizza'. In her talk entitled 'high quality cool data - optimising the chances' Elspeth gave us a comprehensive guide to cryocrystallography, advocating the use of acupuncture needles, 'the answer to a crystallographer's prayer', and offered a beer to anyone who could spot the 'deliberate mistake' in her slide on safe handling of liquid nitrogen.

After coffee, Bram Schierbeek (Bruker-Nonius) talked on the use of CCD detectors in the home laboratory and speculated on fully automated data collection, structure solution, publication and even deposition with the software prompting the user 'deposition complete, please check mobile phone for report'. Graham Fraser (Bede Scientific) described the Bede microsource, and Jim Pflugrath reassured 'flux junkie' Jim Naismith (St. Andrews) that there was only a 2-fold difference in flux between a rotating anode and a microsource. Liz Duke (Daresbury) then updated us on the plans for protein crystallography at Diamond, and the session was ended by Iain McNae (Edinburgh), who described a puzzling anisotropic mosaicity effect observed from his type I dehydroquinase crystals. There followed an afternoon advertised as free for 'shinning, shopping, shirking, shnoozing (or just sight-seeing)' on which Richard had the onerous task of testing all the hostelries in Jedburgh to find one

suitable for the walkers to relax in after their expedition with Lindsay, while others spent their afternoon playing golf, visiting a brewery or 'Bouldering'.

That evening, following the conference dinner, we were entertained by Andy Freer in full Scottish dress (which included a transgenic mouse hidden in his sporran) who addressed the Swiss roll (!) (aka myelin) in admirable Burns night fashion, and demonstrated the principles of selective protein extraction with the aid of the dismembered cake, a bottle of mineral water, Fairy liquid and a large quantity of salt. He alienated (presumably intentionally) all Manchester United fans with a half-time slide of Man United jokes, 'to regain our attention', which of course had never faltered anyway.

The final day of the workshop began with Mike Cianci (Manchester) who explained the differences in appearance between cooked and uncooked lobster while describing the structure solution of apocrustacyanin using xenon, sulphur and softer X-rays. Dominic Hunter (Edinburgh) then talked at length about bacterial ferric iron-binding proteins. Christine Thomas (Dundee) described the serendipitous binding of citrate to the PH domain of TAPP1. Christos Tzitzilonis (UMIST) talked about his structural studies of *N. meningitidis* outer membrane antigen analogues binding to antibodies. Sheelan Jamal (York) closed the session by showing how the structure of complex between a carbohydrate binding

module and its substrate explains specificity for xylosugars.

The final session was kicked off by Andrew Pannifer (AstraZeneca), who warned of the dangers of working with a mutant rather than the genuine wild-type structure. Jim Pflugrath then gave a second talk describing how it is possible to collect sulphur anomalous data using a rotating anode source, avoiding the need to collect data at the synchrotron, allowing you to "stay home, relax, drink beer...". Jim Naismith stepped in at short notice to continue the rhamnase pathway saga, and described complex structures of RmlC from four different bacterial species. Julie Tucker (AstraZeneca) then described the structure of phosphorylated CDK2-cyclin A depressing the audience with the news that they were probably unable to repair the brain cells damaged in the informal discussion sessions held the night before. The final talk of the meeting was given by Alastair Gardiner (Glasgow), another self-confessed non-crystallographer, who described the perils of using a *Rhodobacter sphaeroides* zinc-binding mutant reaction centre for the study of unpaired electrons in this system.

The organisers gratefully acknowledge the BCA, CCP4, AstraZeneca, Bruker AXS, Bede Scientific and Molecular Dimensions for financial support. The next workshop will be held at Galashiels, September 4-6, 2002.

**Siân Rowsell & Julie Tucker,**  
AstraZeneca, October 11, 2001

### Post-doctoral positions in Protein Crystallography

Applications are invited for post-doctoral positions in protein crystallography at St. Vincent's Institute of Medical Research in Melbourne, Australia. Major areas of interest include studies of receptors and ion channels with the aim of developing therapies towards a variety of diseases such as Alzheimer's disease and epilepsy. Exciting projects at all stages are available. For more information on the Laboratory and recent projects, see <http://www.svimr.unimelb.edu.au/parker.htm>

For more information on Melbourne, see <http://www.australia.com/>

Excellent facilities are available including two imaging plate detectors with focusing mirror optics, cryo-cooling systems and a computer network of 9 SGLs. We have ready access to synchrotron radiation when required. The crystallography effort is supported by well-equipped Biochemistry, Molecular Biology and Structure-based Drug Design Laboratories.

Applicants must have experience in determining protein structures by X-crystallography. Applications will be accepted until the positions are filled. Applicants should send their curriculum vitae with full details of qualifications and research experience together with names and addresses (include phone,

fax and e-mail) of three referees to: Prof Michael Parker, St. Vincent's Institute of Medical Research, 9 Princes St, Fitzroy, Victoria 3065, Australia  
Tel.: +61 3 9288 2480  
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### Physics Jobs

The Institute of Physics' online job service is being relaunched with lots of new services including a searchable database of CV and e-mail alerting of vacancies. Other services including an online career manager will be added in the coming months.

#### Website

<http://recruitment.iop.org/cvs/>

### Errata

Crystallography News, Issue No. 78, page 5, 2nd column. Title should read 'Dame Julia Higgins' not 'OBE for Professor Julia Higgins'.

### Meetings of Interest

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](mailto:cockcroft@img.cryst.bbk.ac.uk) or to the Editor, [bob@gould.ca](mailto:bob@gould.ca)

#### December 17, 2001

British Crystallographic Association/ Biological Structures Group: "Membrane proteins: Challenges to Structural Biology", Read Lecture Theatre, Sheffield Building, Imperial College, London. [<http://www.ic-csb.ic.ac.uk/>]

#### March 4-7, 2002

10th Annual Meeting of the German Society for Crystallography (Deutsche Gesellschaft fuer Kristallographie / DGK) Kiel, Germany [<http://www.ifg.uni-kiel.de/dgk2002>]

#### March 23-28, 2002

9th International Conference on the Crystallization of Biological Macromolecules, Jena, Germany, [<http://www.conventus.de/iccbm9/>]

#### March 25 - 28, 2002

BCA Annual Meeting, Nottingham University (Full details in this issue)

#### April 2 - 4, 2002

Spring Meeting of the Materials Research Society, San Francisco, CA, USA [<http://www.mrs.org/meetings/spring2002/>]

#### May 23 - June 2, 2002

From Genes to Drugs via Crystallography, Erice, Italy [<http://www.geomin.unibo.it/orgv/eric/drugdesi.htm>]

#### May 23 - 26, 2002

EPDIC-8 - 8th European Powder Diffraction Conference, Uppsala, Sweden [<http://www.mkem.uu.se/epdic8>]



## May 25 - 30, 2002

ACA American Crystallographic Association Meeting, San Antonio, Texas, USA  
[\[http://www.nexus.hwi.buffalo.edu/ACA/ACA-Annual/futuremeetings.html\]](http://www.nexus.hwi.buffalo.edu/ACA/ACA-Annual/futuremeetings.html)

## June 24 - 26, 2002

Time-Resolved Chemistry: From Structure to Function, Manchester, UK  
[\[http://www.rsc.org/pdf/conf/faradisc/fara122/pdf\]](http://www.rsc.org/pdf/conf/faradisc/fara122/pdf)

## July 14 - 19, 2002

International Conference on the Physics and Chemistry of Ice, Newfoundland, Canada  
[\[http://www.housing.mun.ca/conf/pci/\]](http://www.housing.mun.ca/conf/pci/)

## July 29 - August 2, 2002.

Denver X-ray Conference, Denver, USA  
[\[http://www.dxicdd.com/02/\]](http://www.dxicdd.com/02/)

## August 6 - 15, 2002

IUCr XIX - XIX Congress and General Assembly of the International of Crystallography, Geneva, Switzerland  
[\[http://www.kenes.com/iucr/\]](http://www.kenes.com/iucr/) also at <http://www.unige.ch/crystal/ahdf/geneva02.html>]

## August 25 - 29, 2002

SAS 2002, XII International Conference on Small Angle Scattering, VENICE, Italy with some satellite meetings at ELETTRA in Trieste. [Contact: A.Benedetti, Dipartimento di Chimica Fisica, Calle Larga S.Marta D.D. 2137, 30123 Venezia - ITALY [fax +39 041 257 8594, E-mail: [sas2002@unive.it](mailto:sas2002@unive.it) <http://www.isf.unian.it/isf/SAS/Home-SAS.htm>]

## April 14 - 17, 2003

BCA Annual Meeting, York University last day is Maundy Thursday

## August 2005

XX Congress of the International Union of Crystallography, FLORENCE, Italy [Carlo Mealli, email: [mealli@fi.cnr.it](mailto:mealli@fi.cnr.it)]

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**Final Accounts**

**INCOME**

Sponsorship	£5,328.28
Registration	£41,782.35
Exhibition	£9,242.00
<b>TOTAL INCOME</b>	<b>£56,352.63</b>

**EXPENDITURE**

Accommodation & Meals	£20,066.10
Facilities	£8,929.62
Catering	£7,257.30
Social Event	£1,975.50
BCA Speakers Expenses	£2,605.78
Abstract Book	£2,512.74
Postage & Advertising	£2,201.94
NN Fee & Expenses	£7150.21
BCA Administration	£944.97
Stationery & Copying	£700.02
Bursaries	£2,000.00
<b>TOTAL EXPENDITURE</b>	<b>£56,344.18</b>
<b>MEETING SURPLUS (-DEFICIT)</b>	<b>£8.45</b>

**Dr Christine Cardin (University of Reading)  
& Mr David Taylor (BCA Treasurer) 30/10/2001**

*Note: The BCA deposit of £3098.20 paid in 1999 has been refunded.*

*To expedite closing the account some transactions have been made through the BCA accounts.*

*The net contributions to speakers expenses which will appear in restricted funds of the BCA accounts have been included.*

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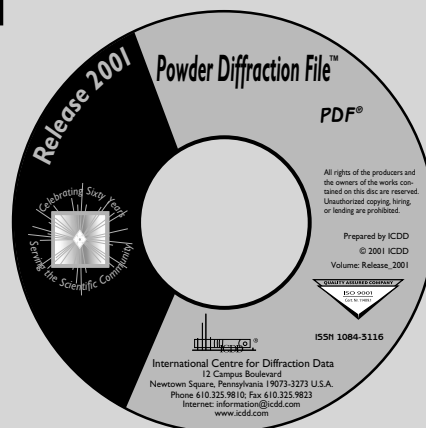
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