

# CRYSTALLOGRAPHY NEWS

## British Crystallographic Association

No.82

September 2002

Join the BCA!  
Education News  
Durham School 2003



Quarterly

Authorship at the BCA  
Agony Column  
Book Reviews





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

**NEXT ISSUE OF  
CRYSTALLOGRAPHY NEWS**

**CRYSTALLOGRAPHY NEWS** is published quarterly (March, June, September and December) by the British Crystallographic Association. Text should preferably be sent as MSword documents (any version - .doc files) or else as .rtf on a PC disk or electronically. Diagrams and figures are most welcome, but, if possible, please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (e.g. awards, honours, retirements etc.), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews. Please ensure that items for inclusion in the **December 2002** issue are sent to the Editor to arrive before **18th October 2002**.

**BOB GOULD**  
EDITOR, CRYSTALLOGRAPHY NEWS  
33 Charterhall Road  
EDINBURGH EH9 3HS  
Tel: 0131 667 7230  
E-mail: bob@gould.ca

*The British Crystallographic Association  
is a Registered Charity (#284718)*

As required by the DATA PROTECTION ACT, the BCA is notifying members that we store your contact information on a computer database to simplify our administration. These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting or any time on application to them at the BCA Administrative Office, when we will be happy to make corrections.

# Contents

From the President .....2

Council Members .....3

From the Editor .....4

ACA San Antonio .....5

Towards an ERC? .....8

Education News .....8

Anchorage .....10

Agony Column .....11

Obituary - Ron Jenkins .....12

BCA/CCG School .....13

BCA/CCG Course Application Form .....14

Group Meetings .....15

Join the BCA! .....16

BCA Membership Form 2003 .....17

Book Reviews .....18

L'Oréal Winner .....26

New Journal .....27

Puzzle Corner .....28

News from bede .....29

Meetings of Interest .....30

Corporate Members .....33

*President's Remarks*

*I am just off to Wyoming for a few weeks of climbing in the Wind River Mountains and then on to Geneva for the IUCr Congress. Last time I checked, there were about 1700 delegates registered so it is shaping up to be a major event in the world of science this year. It brings back memories of this time three years ago before the Glasgow IUCr Congress. You may be surprised to learn that 99% of my memories of this are really pleasant ones: the way the UK community worked together, Northern Networking, the staff at the conference centre, the sponsors and, not least, the science - it really was a privilege to work in such an environment.*

*Three years on and a lot has changed in the BCA. We have professionals organising the day-to-day running of the BCA, a new newsletter format, and a deal with Crystallography Reviews to publish the plenary lectures and associated sessions in a special issue of the journal rather like the Transactions that the ACA produce each year. All this reflects well on the BCA in particular and UK crystallography in general.*

*Where do we go from here? In my own view (the Treasurer will probably disagree!), our annual subscription is low in relation to the services we provide. (How many scientific societies operate on this sort of a budget?) With a larger guaranteed income we could be on a surer financial footing for our annual meeting and for a continued, strong student bursary plan. Should we have different grades of professional membership rather like the RSC? We are*

*crystallography professionals, and perhaps the BCA membership should reflect this. I would be interested to know what you all think about these issues. The AGM is a rather limited forum for these sorts of discussions.*

*The annual meeting has also been discussed on many recent occasions, not because of its science or quality, but because the BCA would like to do more to interact with the protein crystallographic community. There are a lot of meetings each year, and the choice is extensive; for macromolecular crystallographers the choice is simply enormous when you include all the biologically relevant meetings. And funding is finite. Next year at the BCA Meeting in York we will be experimenting with one-day registrations to attract such people - they are cheap and only involve a one night stay, and the scientific programme has been designed accordingly. We have also shortened the meeting by one day to make it a two-night commitment overall. Financially this is a gamble, and if it is a successful format, long term funding may have to be an issue. One thing is for certain - standing still is not an option.*

*The mountains are waiting. I hear that grizzly bears are making a comeback in Wyoming....*

**Chris Gilmore**  
September, 2002

## Cover pictures left to right:

Trevelyan College in the Spring – home of the BCA/CCG School

A Holliday Junction!

Anchorage – how far can you go with a BCA Bursary?

A Mineralogical Dragon!

The River Center in San Antonio

## BCA Council Members 2002 - 2003

### *President (2003)*

Prof. Chris J. Gilmore  
Department of Chemistry  
University of Glasgow  
GLASGOW G12 8QQ  
tel: 0141 330 3716  
[chris@chem.gla.ac.uk](mailto:chris@chem.gla.ac.uk)

### *Vice President (2004)*

Prof. Paul Fewster  
Philips Analytical Research Centre  
Cross Oak Lane  
Redhill RH1 5HA  
tel: 01293 815714  
[paul.fewster@philips.com](mailto:paul.fewster@philips.com)

### *Secretary (2004)*

Dr. Christine Cardin  
University of Reading  
Dept of Chemistry  
Whiteknights  
Reading RG6 6AD  
tel: 0118 9318215  
[c.j.cardin@reading.ac.uk](mailto:c.j.cardin@reading.ac.uk)

### *Treasurer (2003)*

Mr. David J. Taylor  
35 Birchley Road,  
Billinge  
WIGAN  
Lancs WN5 7QJ  
tel: 01744 893108  
[djtaylor@lineone.net](mailto:djtaylor@lineone.net)

### *Ordinary members*

Dr Margaret J. Adams (2003)  
Lab. of Molecular Biophysics  
Rex Richards Building  
South Parks Road  
OXFORD OX1 3QU  
tel: 01865 275391  
[margaret@biop.ox.ac.uk](mailto:margaret@biop.ox.ac.uk)

Dr Jeremy K. Cockcroft (2003) (Web  
Master)  
School of Crystallography  
Birkbeck College  
Malet Street  
LONDON WC1E 7HX,  
tel: 020 7631 6849  
[cockcroft@img.cryst.bbk.ac.uk](mailto:cockcroft@img.cryst.bbk.ac.uk)

Prof. Paul R. Raithby (2003)  
Department of Chemistry,  
University of Bath,  
Claverton Down  
BATH BA2 7AY  
tel: (01225) 323183,  
[p.r.raithby@bath.ac.uk](mailto:p.r.raithby@bath.ac.uk)

### GROUP REPRESENTATIVES

#### *Biological Structures*

Dr. A. Hadfield (2002),  
Department of Biochemistry,  
University of Bristol  
BRISTOL BS8 1TD,  
tel: 0117 928 7436,  
[A.T.Hadfield@brist.ac.uk](mailto:A.T.Hadfield@brist.ac.uk)

#### *Chemical Crystallography*

Dr Harry Powell (2002)  
MRC Lab. of Molecular Biology  
MRC Centre  
Hills Road  
CAMBRIDGE CB2 2QH  
tel: 01223 402423  
[hrp1000@cus.cam.ac.uk](mailto:hrp1000@cus.cam.ac.uk)

#### *Industrial*

Prof. Christopher S. Frampton  
Department of Chemistry  
University of Southampton  
Highfield  
Southampton SO17 1BJ  
tel: 02380 594167  
[chrisf@soton.ac.uk](mailto:chrisf@soton.ac.uk)

#### *Physical Crystallography*

Dr P.A. Thomas  
Department of Physics  
University of Warwick  
COVENTRY  
[phrve@csv.warwick.ac.uk](mailto:phrve@csv.warwick.ac.uk)

#### *Co-opted Members*

Prof. P. Barnes,  
Department of Crystallography,  
Birkbeck College,  
Malet Street,  
LONDON, WC1E 7HX  
tel: 020 7631 6817  
[barnes@img.cryst.bbk.ac.uk](mailto:barnes@img.cryst.bbk.ac.uk)

Prof. Chick Wilson,  
Rutherford Appleton Laboratory,  
ISIS Facility,  
CHILTON,  
Oxon OX11 0QX  
tel: 01235 82 1900 ext 5137 or 01235  
44 5137,  
[C.C.Wilson@rl.ac.uk](mailto:C.C.Wilson@rl.ac.uk)

### *Ex-officio Members*

#### *Editor "Crystallography News"*

Dr Robert Gould  
33 Charterhall Road  
Edinburgh EH9 3HS  
Tel: 0131 667 7230  
[bob@gould.ca](mailto:bob@gould.ca)

#### *Education Officer*

Mrs K.M.Crennell  
'Fortran Friends'  
P.O.Box 64  
Didcot  
Oxon OX11 0TH,  
tel: 01235 834 357  
[bca@isise.rl.ac.uk](mailto:bca@isise.rl.ac.uk)

### GROUP CHAIRMEN

#### *Biological Structures Group*

Dr. Richard Pauptit  
Protein Structure Lab  
AstraZeneca,  
Mereside,  
Alderley Park,  
Macclesfield  
SK10 4TG,  
tel: 01625-516135  
[richard.pauptit@astrazeneca.com](mailto:richard.pauptit@astrazeneca.com)

#### *Chemical Crystallography Group*

Prof. Paul R. Raithby  
Department of Chemistry  
University of Bath  
Claverton Down  
BATH BA2 7AY  
tel: (01225) 323183  
[p.r.raithby@bath.ac.uk](mailto:p.r.raithby@bath.ac.uk)

#### *Industrial Group*

Prof. Christopher S. Frampton  
Department of Chemistry  
University of Southampton  
Highfield  
Southampton SO17 1BJ  
tel: 02380 594167  
[chrisf@soton.ac.uk](mailto:chrisf@soton.ac.uk)

#### *Physical Crystallography Group*

Dr Pamela A. Thomas  
Department of Physics  
University of Warwick  
Coventry CV4 7AL  
tel: 0113 233 2538  
[p.a.thomas@warwick.ac.uk](mailto:p.a.thomas@warwick.ac.uk)

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



Welcome to September! We hope to get this issue to more than our usual readers, and I hope you like it! There is little to report of our own meetings here, so I have tried to take in some things for which we didn't have space last issue. The next issue will have reports from the International Union of Crystallography in Geneva, and the outline of our annual meeting next March.

Many thanks to all our contributors. One of the main

items in this issue is Book Reviews, particularly of two new introductory books on biological crystallography, which look very promising. There is a lot of news, including a student report from Alaska.

We are sad to report the death of Ron Jenkins in this issue, and our Treasurer Dave Taylor has written about him. We have a much happier event to report, a child born to Andrea Hadfield in April, to whom we give our congratulations.

Another happy piece of news from the Treasurer is that we will receive £708.37 from the Inland Revenue as the Gift Aid recovered on behalf of 210 members. These proceeds are destined for the Arnold Beevers Bursary Fund.

I continue to look for new ideas for features in CN that would appeal more widely. Small, but non-zero, replies come in for the Puzzle Corner. This month's is

very easy. Why not have a go? A new feature is "Dear Expert", the next best thing to an agony column. The contents of this one I picked up from an Internet newsgroup, and many of them do turn up answers worthy of a much wider audience. Is the list of meetings helpful? Should more information be included? Of course, most factual information is available on the Internet, so it is important that we put in enough to turn serious enquirers in that direction. I would, as always, greatly value suggestions from you, our readers.

Finally, this is your magazine; things you contribute have a very high chance of acceptance, so do let us hear from you.

**Bob Gould**  
September, 2002



## *Acknowledgements*

### *BCA Sponsors*

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

### ACA San Antonio, May 2002 - Session on Authorship Issues

The American Crystallographic Association held its meeting early this year (May 25-30) in Texas. The participation of British Crystallographers continues to grow, and almost dominated some sessions! San Antonio is a beautiful and varied place; the pictures shown were within walking distance of the conference!

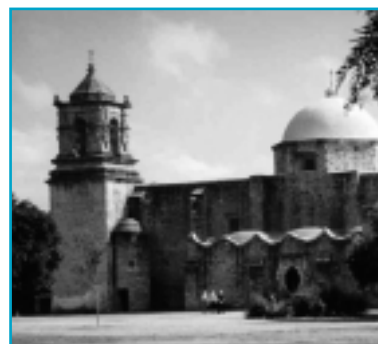
Particularly interesting was this lively evening session, rounding off a full day and ending after 10 p.m., not counting the sessions in a bar afterwards. It was organised by Larry Falvello and ably chaired by Carol Brock, from the University of Kentucky, Lexington and was both lively and worthwhile. Nearly all of the session was concerned with papers emanating from academic institutions, since government and industrial institutions have very different priorities.

The first speaker was Stephen Ritter, Senior Editor of Chemical and Engineering News. He emphasised a theme, taken up many times, that *Science* is a great career, and that scientists are generally benevolent, but the need to write to get and keep jobs does occasionally blunt this benevolence! Gross misconduct is rare, and smaller complaints on ethical matters are generally solved. The main subject of discord is over who gets to be on what paper and in what order. The ACS is the largest publisher of scientific work in the world, but it is medical journals,

followed by *Science* and *Nature* that have led the way in developing conflict policies, although they are actually rarely needed. Since 1985, the ACS has had guidelines, and these state that all persons whose contribution to the work is significant should be included and consulted on the total contents of the manuscript, and that no others should be included. There is a suggestion that the nature of each author's contribution should be specified, in the abstract or otherwise. Some of the problems which do arise are the holding back of junior authors' work to protect patent possibilities and students beginning to assert rights by withholding work. Training in Ethics is good, but does often miss concern with common problems like the assigning of credit. The most important thing is training in mutual respect when working together!

Larry Falvello (Zaragoza) entitled his contribution, "More to the bye-line than meets the eye". He illustrated this with the first pages of a number of important papers covering more than a century by Bravais, Hermann, Mauguin (who published separately!), Bragg and Pauling, all of which had a single author. The "first" paper on X-ray diffraction was divided into a "theoretical" part by von Laue, and a "practical" part by Friedrich and Knipping. After 1950, however, things changed, and there were more authors; at present, Acta A has mainly two-author papers, while Acta B and Acta C show broad peaks at three authors. Senior people

tend to insist on always being authors of papers from their research groups. A notable exception is the famous paper in *Nature* on DNA by Watson and Crick, a post-doc and a graduate student with no one more senior! Generally, students are regarded as paid servants, and should a supervisor allow them to publish on their own, colleagues are upset! As far as crystallographers are concerned, they are often regarded partly as technicians, and partly as a sort of Cerebus, guarding the gates



Eighteenth Century Mission in San Antonio

of the Hades of publication, and thus recipients of some jealousy.

Ton Spek, the director of the Netherlands Centre for Crystal Structures in Utrecht, emphasised the different approaches possible to publication. Most of the structures in which he is involved are coordination or organometallic compounds. These frequently have structures significantly different from what the synthetic chemists have predicted, making it undeniable that crystallography has greatly added to the value of the work. Like most of us, he likes to be included in good papers and left

off bad ones. Frequently, he publishes structural details separately, and in any case will not supply a .cif or .fcf file before a publication has been submitted. Before this, a "client" will only be given printed output and a SHELX .res file. The price of not taking the crystallographer seriously was recently shown by the 2001 report in *Angewandte Chemie* of a novel (cp\*)<sup>+</sup> cation. From the drawing and the bond lengths, it was obvious that this ion actually was 1,2-dihydro-pentamethylcyclopentadienyl, but no one had noticed this. What had the referees been doing? It seems that no crystallographer had reviewed it and the one who had done the work was only "acknowledged" in the paper. When Ton is asked to referee a paper with a crystal structure but with no crystallographers in the author list, he makes a point of asking questions which only a crystallographer can answer! In this way, the "added value" can be made more explicit!

Philip Fanwick from Purdue directly addressed the role of the "service" crystallographer, distinguishing two types: those who maintain a lab for users to collect data and solve structures, and those who do all the work. In paper preparation, the role of crystallographers may be limited to producing "canned" tables and figures. On the other hand, they may provide customised figures and even initiate part of the discussion. Journals have very different assumptions: in *Inorganic Chemistry*, where there are often 6 structures per paper, it is normal for a crystallographer

to be an author, while the *Journal of Organic Chemistry* is happy with the somewhat tautologous statement that "the structure has been supported by an X-ray structure determination". To some extent this correlates with the likely position of a structure in the two journals on the scale: 1:chemist has it right; 2:chemist has it almost right; 3:chemist has no idea; and 4: chemist has the



River Center in San Antonio

wrong idea! In this system, an issue of IC may average in excess of 2.5, while JOC will hardly exceed an average of 1.5. A further complication arises in complex structures involving  $Z' > 1$ , twins, or generally poor data. In these cases a lot of work may be involved which is of no interest at all to the chemist. In general, he felt that many crystallographers had to take the attitude, variously ascribed, that "there is no limit to what a man can do, providing he doesn't give a damn who gets credit for it!" Whoever gets the credit, concern must also be felt for accuracy. The fact that *J. Org. Chem.* rarely uses a crystallographer as a referee, while the RSC has a crystallographer on the staff to check structures shows the wide

variety of practice. He finished by wondering what should be done about structures determined from powder data, which are becoming more common, and for which most of the usual tests for accuracy are inapplicable.

The following talk, by Andrew Bond (Cambridge) was well the most outspoken of the evening. He pointed out that while the work done in crystal structure determination had changed out of all recognition in the last 50 years, publication policies had changed very little, and we should not find it odd that they should begin to do so. Going step by step through the process of generating a structure for publication, he pointed out that in most cases there was little done that could give any more right to authorship than what was done by the mass spectroscopy technician. He asked if he is selling himself short by not asking to be an author, even when his advice on some matters has to be sought. He said no, and was quite happy to separate "technical" crystallography, which got no authorship and for which data were simply sent to the CCDC from "scientific" crystallography, when separate publication is appropriate.

Fred Hollander (Berkeley) emphasised that academic scientists must justify a position that authorship rights are actually important. In practice, professional courtesy and ethics can be summarised by the phrase, "Play nice and share the toys." In general there is no problem when a contributor may

be seen to have contributed about 30% of the work and a comparable part of the write-up. Below that it becomes controversial. Obviously there may be problems over measuring "content". He favours the somewhat whimsical LPU (least publishable unit) and in this, 1 structure = 1 LPU. Synthesis, kinetics, spectroscopy, etc. can contribute other LPUs. Other matters, such as leadership are not quantifiable and are thus ignored, and in any case a suitable weighting scheme has to be applied, so that in the end,  $Cont = \sum(w_{ic} LPU_{ic}) / \sum(w_{it} LPU_{it})$  where the subscripts c and t refer to crystallographic and total.

There is then the sensitive question of who gets to award the weights, generally these being in the order: 1: head of research laboratory, 2: journal; 3: general policy and 4: the crystallographer.

Richard Eisenberg, the Editor of *Inorganic Chemistry*, could claim (like few in the audience) to have solved crystal structures based on intensities he had visually estimated himself! At present, 70% of papers in *Inorganic Chemistry* contain at least one crystal structure.

Crystallography generates more data than do other methods, and the quantity of data is increasing. Automation means that more students are doing some crystallography than ever before, and it is important that they learn something. Editors exist to assess and to archive, and must seek to publish the best science. Eisenberg supports peer review,

which often gives added value to a publication. There has been much change in submission technique:

#### pre 2001

no electronic submission  
 .cifs on disc and hard copy  
 .cif *after* paper and review by IC  
 .cif forwarded to server

#### now

electronic submission possible  
 .cifs electronically  
 .cif with submission  
 hard copy only accepted if .cif cannot be generated.

Some reviewers complain that they can't read .cifs easily, and some don't look at them. A questionnaire for referees is being sent to see whether they are coping, and how much they bother to do! The main problem is that there are too many structures and too few referees. In fact, most structures are fairly routine, and probably good. Eisenberg would like input from the crystallographic community over whether an automatic .cif check and viewer are required.

The final speaker was Frank Allen of the CCDC, who emphasised that the CSD records authorship exactly as it is on the paper. At one time a trial was made of recording crystallographers mentioned in the paper who were not authors, but this was given up as too inaccurate. Some non-author crystallographers do need to be contacted, and they are usually very helpful. The CCDC also writes for data on structures mentioned in a paper

without supporting data. About 25% of these are not answered. The idea of the CSD is to get as many structures as possible, but many are not published for lack of time, etc. Authorship of paper and responsibility for data can be separated, and three suggestions are:

Publication with no crystallographer – introduce a new cif data name to indicate responsibility.

Separate formal publication by crystallographer, e.g. in *Acta E*.

Personal communication to CSD. Authors are recognized, but this may not be a sufficient recognition.

These distinctions are becoming fuzzy, and the CCDC is more and more coming to support publication rather than deposition. The IUCr database committee must be kept in communication to get eventual improvement. Whatever authorship issues are involved, Frank's own strongly held feeling is that *all* crystal structures have some value, usually greater than the authors assume!

The general feeling of the meeting was definitely positive, and everyone realised that genuinely difficult problems are rare.

Bob Gould



## Towards a European Research Council?

*The following letter has been circulated by the Office of the Secretary General of the European Science Foundation to seek views about the possible formation of a European Research Council.*

Dear Colleagues,

The debate on the case for and against a European Research Council is now well underway. The European Science Foundation (ESF) has taken on itself to lead the debate on this important topic. We have established a high level group to provide advice and we are also partners with the Danish Presidency in arranging a major meeting which will take place in October. The issue will also be the focus of the debate at the ESF's own Annual Assembly of its Member Organisations in November and we aim to publish a major position paper on the outcome of these debates early next year.

We are particularly keen to have the views of the wider scientific community in Europe (especially young scientists and scholars) as such a major structural change in European research funding will be bound to have major repercussions. Therefore, we particularly want to have the views of people and organisations connected with ESF, especially through the EURESCO activities.

The issues on which we would welcome views are:

- Is there a need for European Research Council funding fundamental research at a European level or is the present system of national funding agencies and the EU Framework Programme appropriate for Europe?
- Would a new European Research Council structure contribute to the promotion of excellence and make European science more competitive on the World stage?
- Should such a Council cover all areas of the research spectrum or should there be a series of disciplinary focused research councils?
- How could a European Research Council be funded?
  - i. by the European Union from common funds?
  - ii. from a transfer of national funds to the new body?
  - iii. from a mixture of national transfers and EU funds?

I very much hope that you will be able to respond.

Please send your views to:  
[erc@esf.org](mailto:erc@esf.org)

Many thanks,  
Sincerely,

A E S (Tony) Mayer  
Head, Secretary General's Office  
European Science Foundation  
1 quai Lezay-Marnesia  
67080 Strasbourg, Cedex  
France  
Tel: +33 (0)3 88 76 71 02/46  
Fax: +33 (0)3 88 36 69 45  
email: [amayer@esf.org](mailto:amayer@esf.org)  
ESF Web Site: [www.esf.org](http://www.esf.org)

## Education News

### 1. BCA Survey of UK Undergraduate Crystallography courses

The June issue of 'Crystallography News' had a survey form on page 16 and an A4 loose sheet of paper with the same survey was enclosed with the newsletter. We are trying to find out how much crystallography is taught in Undergraduate courses of all kinds. Readers were asked to complete the form, and return it by post to the Education Officer or to save the electronic form on the BCA website at

<http://bca.cryst.bbk.ac.uk/BCA/ed/survey/Survey.html>

and return it by email to  
[BCA@isise.rl.ac.uk](mailto:BCA@isise.rl.ac.uk)

Today is the 17th July 2002; I have received 16 replies by post and 5 by email and none during this last week. This is a very disappointing response. Perhaps the state of crystallographic teaching is worse than we thought, and we should resign ourselves to there being no crystallographers in future. Assuming that surveys get on average a 20% response and there are 600 UK members of the BCA I expected up to 120 forms to be returned.

Here are some replies to the question:

'What might the BCA do to help teach crystallography better?'

1. Act as a clearing house for interchange of teaching materials

2. Provide on-line (web based) self-teaching materials
3. Increase general public awareness of crystallography, particularly in schools
4. Provide a library of teaching aids, videos etc
5. Provide exercise sheets giving students practice with symmetry operations and applications to point groups
6. Produce a teaching aid pack of standard definitions and nomenclature with perhaps some good graphics support to enhance the lectures
7. Provide interesting examples, case studies, demonstrating the application of basic principles of crystallography in materials studies
8. Currently the BCA does not seem to have much focus on or interest in undergraduate teaching as opposed to research. The question is can the BCA really sustain enough interest in teaching development amongst its members to add anything to the role of the professional bodies in this area?

One respondent helpfully enclosed some sheets from their laboratory practicals, which I may be able to convert to web pages to store on the BCA web site to help others.

A further form is enclosed with this newsletter. If you have not already done so, PLEASE COMPLETE AND RETURN YOUR FORM NOW.

## 2. BCA Bursary reports

The BCA provides bursaries to enable students to attend meetings and conferences. The

recipient is expected to write a concise summary report in grammatical English, correctly spelt, and send it preferably in electronic form to the BCA Admin office within a short time of their return from the meeting. The student is expected to describe the scientific highlights as they saw them. The editor of 'Crystallography News' may merge several reports from the same meeting into one article for publication if space permits, or if the report is unsatisfactory comment on how it can be improved. Writing good reports to a short deadline is not easy, and the BCA hopes students will profit from this training.



**3. The Mineralogical Society** have just set up an educational page for young mineralogists on their website at

<http://www.minersoc.org>.

It has links for schools, to museums with mineral collections, to mineral dealers and 'The Dragon's Cave' where you visit the cave to see its scary eyes looking at you and search for stars using the computer mouse to find minerals in the stars.

**4. 'The American Scientist'** Vol 90 no.4, July - August 2002 has an interesting article on the history of the determination of protein structures, "Protein Structures: From Famine to Feast" by Helen Berman, David Goodsell and Philip Bourne." Copiously illustrated, the article relates the pioneering work of Hodgkin, Bernal, Perutz and Kendrew, the founding of the Protein Data

Bank in the 1970s, and its phenomenal growth since then. The number of structures is expected to reach 20,000 by the end of 2002.

Links to Internet Resources for further exploration of protein structures are available on the American Scientist website at <http://www.americanscientist.org/articles/02articles/berman.html>

**5. The Institut Laue-Langevin Annual Report 2001** is now available in 3 formats:

- a. an A4 sized paperback booklet with colour printing
- b. a CD-ROM which holds the Annual Report and the Interactive Yellow Book, (describing the ILL instrument suite) supplied in a folder at the back of the A4 booklet
- c. on the ILL website, look for 'publications' on <http://www.ill.fr>

Giovanni Cicognani is asking for advice from ILL users as to which format they prefer, and comments on the content and presentation of the Annual Report.

He asks you to rank the options, 1 is the best, 3 the worst.

- paper version sent by post  
 Web version with email notification when it is ready  
 CD-ROM sent by post

You can return your comments by email to [cico@ill.fr](mailto:cico@ill.fr) or by post to

Giovanni Cicognani,  
 Institut Laue-Langevin,  
 6, rue Jules Horowitz,  
 BP 156 - 38042 Grenoble Cedex 9-  
 France

## Third International Symposium on Pneumococci and Pneumococcal diseases

Anchorage, Alaska, 5-8 May, 2002



*This report is from a student doing protein crystallography at the University of Glasgow, who received a BCA grant to help him attend the meeting. In his letter, he says, "Although the conference was in no way, shape or form crystallographic, it did provide me with an excellent knowledge of current research into pneumococcal disease, which should stand me in good stead when it comes to taking my viva in the coming months."*

On Friday 3rd May we flew out from Glasgow Airport to Anchorage, Alaska (a mere 26 hour trip!!!). Saturday was a well-earned rest day. The conference was kicked off on Sunday 5th May by two leading lights in the pneumococcal field, Prof. Robert Austrian and Prof. Helena Makela, who gave very general presentations about the history of the pneumococcus and pneumococcal vaccines. The main symposium began in earnest on the Monday and lasted until Wednesday with a total of 8 groups presenting.

### *Group 1: Global Epidemiology.*

Within this group there were some startling statistics about the prevalence of pneumococcal disease, mainly in the developing world. In Bangladesh and China, 33% of deaths in children <5 years old are due to pneumococcal infections. The fact that the prevalence of different serotypes changes constantly causes even more problems, in that current polysaccharide vaccines have become even less effective than usual. These facts, combined with the high rate of antibiotic resistant strains being discovered, leads to a serious problem, which is mirrored in large areas of Asia and Africa. Africa has been hit especially hard because of the high levels of HIV infection in small children.

### *Group 2: Determinants of Virulence and pathogenesis.*

The overall take-home message from this group is that they are not sure how genetics and biochemistry are linked to virulence and pathogenesis.

### *Group 3: Carriage and transmission*

Native Alaskans have been shown to have high infection rates. This tends to be due to household crowding and large families. When living with children under 5 years old the risk of adult pneumococcal disease increases with the number of children under 5. Thus, in Alaska, there is 18%

chance of adult infection if there is 1 child, 26% for 2 children and 34% for 3 children. The underused method of real-time PCA gives a good indication of carriage and is a good marker for infections and is much faster and more accurate than traditional haemolytic tests.

### *Group 4: Molecular and Genetic studies*

The complete R4 and A6 strain genomes were presented, which, to be fair, was a bit dull and uninteresting.

### *Group 5: Immune response to pneumococci and vaccines*

Conjugate vaccines for pneumococcal disease differ from those of *H. influenzae* in that they don't elicit higher immune responses in adults than the current polysaccharide vaccine. These conjugates are also less effective for otitis media in infants, suggesting that conjugate vaccines for pneumococcal disease have not been optimised well enough.

### *Group 6: Antimicrobial resistance*

South Korea has had a massive surge in fluoroquinolone and penicillin (60-80%) resistance. In fact, Asian countries have the highest rate of resistance in the world, and as yet no vaccines are being made available to them at a reasonable price. In areas of the USA in the 1990s, resistance to penicillin increased 3-fold to 27%, because doctors were

giving out penicillin for every cold/flu-like symptom a patient had. Over the last 5 years, strict guidelines have been implemented to halt this resistance problem, and these guidelines seem to be having the desired effect.

#### Group 7: Current Pneumococcal vaccines

Overall, new vaccines seem less than impressive against antibiotic resistant strains of pneumococci. Several serotypes which are not in the current 23-valent polysaccharide vaccine are making more of an impact in Africa and Asia. The situation is only going to get worse unless governments in both developing and developed worlds design a strategy that drug companies and shareholders will stick to. There are vaccines available that could save millions of lives each year, but they are not being made available to the people who need them most.

#### Group 8: Future Pneumococcal vaccines

Ppp1: Novel intranasal candidate for pneumococci. Good signs for anti-otitis media drug.  
PspA: Showed good antibody response and good booster response. DNA vaccines give good cellular immune response and good protection against pneumococci; these vaccines are, however, still in their infancy.

Colin James Bent

## Agony column

Dear Expert,

Well, what about an agony column? Some of the things that get sent to me on the web contain very good answers to simple questions, and deserve a wider audience than that particular list gets. Here is one on powder patterns. I'd welcome similar suggestions for future issues.

Editor

Hi everyone. I was wondering if anyone had a suggestion as to which program is best for indexing powder patterns.

Thanks  
Cara Nygren

Just relying on a single indexing program can be problematic given each program has its individual strengths and weaknesses. Available indexing programs and suites that interlink the various programs are visible via:

<http://www.ccp14.ac.uk/solution/indexing/>

At present, Robin Shirley's Crysfire 2000 links to the widest range of indexing programs:

Crysfire 2000 Tutorials:  
<http://www.ccp14.ac.uk/tutorial/crys/>

Crysfire 2000 Download:  
<http://www.ccp14.ac.uk/ccp/web-mirrors/crys-r-shirley/>

(the new Crysfire 2002 will be out any day now (which has some major usability and feature improvements over Crysfire 2000) - a few last minute bugs have

been found which Robin is stomping on)

Crysfire also interlinks into Chekcell by Jean Laugier and Bernard Bochu for graphically evaluating the results:

Tutorials:  
<http://www.ccp14.ac.uk/tutorial/mgp/index.html#chekcell>

Download:  
<http://www.ccp14.ac.uk/ccp/web-mirrors/mgp-laugier-bochu/chekcell.zip>

Lachlan

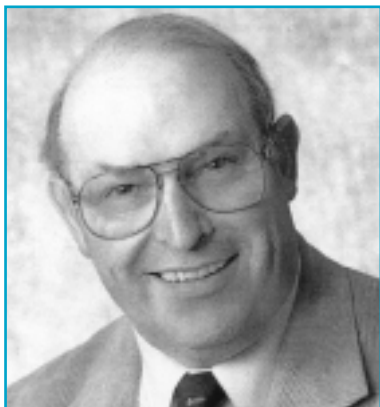
PS: After finding some good trial cells - always consider running Ton Spek's LePage program and search for sub-cells and super-cells. (A. L. Spek, J. Appl. Cryst., 21, (1988), 578-579) This is provided with Chekcell

A web example showing LePage in action is at:

Using Ton Spek's Lepage within Chekcell to find super-cells and better trial cell solutions:  
[http://www.ccp14.ac.uk/tutorial/mgp/chekcell\\_lepage.html](http://www.ccp14.ac.uk/tutorial/mgp/chekcell_lepage.html)

Lachlan M. D. Cranswick  
<http://www.ccp14.ac.uk/>

## Ron Jenkins 1932 -2002



Dr Ron Jenkins, born 10th April 1932 died peacefully at his home in Downingtown Pennsylvania on 19th June 2002. He was one of the great pioneers, teachers and leaders in the field of X-ray analysis, well known and highly respected in materials science circles around the world. A devout Christian and devoted family man, he is survived by his wife of 47 years, Phyllis, five children and five grandchildren.

Ron was born in Oxford and awarded a scholarship to the City of Oxford High School. He studied Physics and Metallurgy at the University of London, Chemistry at the Oxford Polytechnic Institute (ONC, HNC, LRSC) and was awarded his Ph.D. (Chem. Phys.) at the Polytechnic Institute of New York.

Ron started his career as an Analytical Chemist at Esso Research in Abingdon in 1953. At this time he served two years national service as a meteorologist in the RAF. In 1962 he became manager of the X-ray applications Laboratory for Philips Research and Control Instruments

in London. In 1967 he moved to Philips in Eindhoven to head the X-ray Applications Laboratory and in 1971 to Philips Electronic Instruments in Mahwah New Jersey as Principal Scientist. He took up the post of Principal Scientist with ICDD in 1986 becoming Executive Director in 1996 and serving as Corporate Secretary and member of the Board of Directors. His ceaseless efforts saw the introduction of CD-Rom Technology, the growth of membership and massive expansion of the PDF file.

The X-ray community has lost one of its leaders, but Ron's legacy of teaching X-ray science will live on. It is estimated that 5000 students attended his workshops around the world. Many will fondly remember his BCA workshops in Leeds, Cardiff, UMIST and Daresbury, especially those fortunate to receive one of his textbooks and have it personally signed. He wrote 10 textbooks and contributed 11 book chapters on x-ray methods, presented over 200 scientific papers on the subject and prepared two audiovisual courses for the American Chemical Society.

His technical achievements were recognised by the scientific community, and he received many awards and honours including: Gold Medallist, Society for Applied Spectroscopy 1982; Birks Award in X-ray Spectrometry 1986; Barrett Award in X-ray Diffraction 1993; Jenkins Award for Lifetime achievements in X-ray Analysis 2002. He is the only person to receive both the Birks and Barrett awards. Ron's ability to tell a good story was

suitably rewarded by his easily winning a light hearted after-dinner competition at the 1998 Denver Conference. The Denver Conference owes much to Ron for his unstinting and dedicated work as chairman of its organising committee since 1981.

In addition to his technical achievements, Dr. Jenkins was a member of STURP (Shroud of Turin Research Project) and lectured over 50 times to about 6000 people regarding the artefact. His book "Closing the Gap between Science and Religion" outlines his dedication to the Christian faith. He was most recently a member of the Church of the Nazarene, where he served as Council member, Choir Director, Vocal Soloist and Sunday School teacher. He was also a trustee of the Eastern Nazarene College in Quincy, Massachusetts, for many years. His love of music was expressed as a vocal soloist and by playing the trombone in a local brass ensemble. Denver Conference attendees will doubtless remember his participation in post-banquet entertainment, as a member of the "Powdermen" Barbershop Quartet!

Ron was a compassionate man with a charismatic sense of humour who brought leadership and enthusiasm to all aspects of his life. A Celebration of Life Service was held at the West Chester Church of the Nazarene, Pennsylvania on the 22 June. He will be lovingly remembered by many people around the world who were touched by his life.

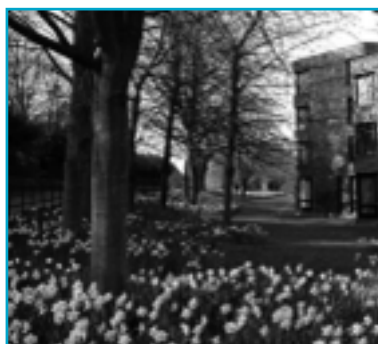
David Taylor

## British Crystallographic Association / Chemical Crystallography Group Ninth Intensive Course in X-ray Structural Analysis

University of Durham, England  
7th - 15th April 2003



The Course is intended primarily for younger scientists with some experience of structure analysis and other scientists who wish to improve their understanding of the underlying principles and practice. Although modern structure analysis systems enable many structures to be determined with very little formal crystallographic training, such training is essential to ensure that work is carried out correctly and to allow difficult problems to be identified and handled.



### Topics covered include:

- crystal preparation
- data collection
- data reduction
- structure solution by direct and Patterson methods
- refinement
- structure evaluation
- presentation of results
- Crystallographic Information Files (CIFs)

The Course has five principal lecturers and eight tutors, who each work with a group of 8-10 students throughout the course. The atmosphere is friendly, the accommodation and food in Trevelyan College are excellent and the work schedule is intensive. The lectures and all main activities take place in the College.

Participants **MUST** have a good understanding of spoken English since there is a lot of challenging material to be covered in a relatively short time. The cost of the course is £500, which includes registration, accommodation, all meals for the whole course and a full set of course notes. There will be some grants available for both UK and overseas participants.

The deadline for applications is the 6th January 2003 but the number of places on the course is strictly limited SO APPLY EARLY.

A registration form which may be photocopied is printed here. For more details contact:

Dr Claire Wilson  
School of Chemistry  
University of Nottingham  
Nottingham NG7 2RD  
UK

Fax: +44-(0)115-951-3563  
Phone: +44-(0)115-951-3511  
Email:

[Claire.Wilson@nottingham.ac.uk](mailto:Claire.Wilson@nottingham.ac.uk)



Students at the 2001 BCA/CCG school

**BCA/CCG Ninth Intensive Course in X-ray Structure Analysis  
7th - 15th April 2003, Trevelyan College, Durham, UK.**

**APPLICATION FORM**

The course is intended primarily for younger scientists with some experience of structure analysis who wish to improve their understanding of the underlying principles and practice. Subjects covered by the course include crystal preparation, data collection, data reduction, structure evaluation and presentation of results, including the use of Crystallographic Information Files (CIFs). The work schedule is intensive, with lectures starting at 4pm on Monday 7th April 2003. The atmosphere is friendly and the accommodation and food are excellent. **Participants must have a very good understanding of spoken English** since there is a lot of material to be covered in rather a short time.

The total cost of the course is £500, which includes registration, accommodation, all meals for the whole course and a full set of course notes. There will be some grants available towards the course costs for both UK and overseas participants. The deadline for application is the **6th January 2003** but the number of places on the course is strictly limited SO APPLY EARLY.

Name .....

Position .....

Background (Chemistry/physics/biology etc) .....

Address .....

.....

.....

Telephone .....

Fax .....

Email .....

**Grant Application**

Do you wish to apply for a grant towards LOCAL expenses for the course? **YES/NO**

If YES, please send with your completed application form (a) a brief explanation of why you should be considered for one of these grants and (b) a letter of support from your supervisor.

Are you a research student currently funded by EPSRC? **YES/NO**

Are you a research student currently funded by another of the UK research Councils? **YES/NO**  
If YES, please state which one.

-----

Please return your completed form, with the £50 registration fee (or a copy of the bank transfer), to:  
 Dr Claire Wilson                      Email: [Claire.Wilson@nottingham.ac.uk](mailto:Claire.Wilson@nottingham.ac.uk)  
 School of Chemistry                      Fax: +44 (0)115-951-3563  
 University of Nottingham              Tel: +44 (0)115-951-3511  
 Nottingham NG7 2RD, UK

**The £50 registration fee must accompany this form. The remaining £450 to be paid before 31st January 2003.**

<b>Bank Details</b>		
Cheques should be made payable to: <i>The BCA/CCG Intensive Course</i> . Bank transfers should be made to:		
Lloyds Bank	Sort Code	30-92-79
19 Market Place	Account Number	0794499
Durham DH1 3NL, UK	Account Name	BCA/CCG Intensive Course
For bank transfers from overseas, please transfer an additional £2 for the deposit and £7 for the remaining £400 to cover our bank charges as well as your own.		

## BSG: Winter Meeting 2002



### Structural Studies of Macromolecular Assemblies

The winter meeting of the Biological Structures Group will take place on Friday 13th December 2002 at the University of Warwick, Coventry. Invited speakers will include:

Dr. Ben Berks (University of Oxford)  
'The Tat protein translocation system'

Professor Neil Isaacs (University of Glasgow)  
'The structure of a photosynthetic bacterial core complex'

Professor So Iwata (Imperial College)  
'Evolution of the respiratory membrane proteins by shuffling of electron transfer modules'

Dr. Kiyoshi Nagai (MRC-LMB Cambridge)  
'Signal recognition particle'

Dr. Robert Robinson (Uppsala University)  
'Structures of gelsolin and arp2/3: Implication for cell movement'

Dr. Dale Wigley (Cancer Research UK)  
'Structure and mechanism of DNA helicases'

For further details and up to date information, see the website:

<http://globin.bio.warwick.ac.uk/~vilmos/bca/bca.html>

or E-mail me at:  
[vilmos@globin.bio.warwick.ac.uk](mailto:vilmos@globin.bio.warwick.ac.uk)

Vilmos Fülöp

## CCG Autumn Meeting 2002 Dealing with Difficult Data Sponsored by Bruker-Nonius



The CCG Autumn meeting 2002 will take place at King's College, Strand, London WC2R 2LS, on Wednesday November 13, 2002. The local organizer is Jon Steed. There is no car parking available on site.

The timetable for the day has not yet been finalized. For the moment, the list of speakers and titles of their talks is as follows;

- Simon Coles (Southampton) *Getting good data out of bad crystals*
- Simon Parsons (Edinburgh) *Difficult datasets - an overview*
- Simon Teat (Daresbury) *A bright way of handling difficult data*
- David Watkin (Oxford) *Weak data can still be good data*

Offers of short presentations (up to 20 minutes) should be sent to the programme organizer, Dr Sandy Blake, School of Chemistry, University of Nottingham, Nottingham NG7 2RD  
Tel: (0115) 951 3488  
Fax: (0115) 951 3563  
E-mail: [A.J.Blake@nott.ac.uk](mailto:A.J.Blake@nott.ac.uk)

Registration forms are available as PDFs and in MS-Word 97 (Mac Word 98) Format (as e-forms) on the CCG home page (<http://bca.cryst.bbk.ac.uk/BCA/CCG/>) and should be sent to Dr Harry Powell, MRC-LMB, Hills Road, Cambridge, CB2 2QH (e-mail [hrp1000@cam.ac.uk](mailto:hrp1000@cam.ac.uk)) with correct remittance. The timings shown below should be taken as a loose guide only!

1020-1035: Registration  
1035-1040: Welcome  
1040-1230: Speakers 1-3  
1230-1310: Lunch  
1310-1500: Speakers 4-6  
1500-1520: Tea  
1520-1600: Speakers 7-8  
1600: Closing Remarks  
1615-1730: CCG Committee Meeting

Harry Powell

## Industrial Group Autumn Meeting Sample Preparation

Thursday November 7th  
A one-day meeting at Hulme Hall,  
Oxford Place, Manchester.

The meeting is designed to be informal, to allow practitioners to seek advice and to share their own knowledge. It's aimed at all levels of experience from industry and from Universities. All types of samples will be discussed, powders, metallurgical, reactive etc.

There will be an open forum to discuss hints and tips as well as talks on specific aspects.

The objective is to share out our collective expertise. Do you have any recipes, which you are particularly proud of? Please come and throw your hat into the ring. Do you have colleagues or students who may be interested?

The registration fee is £30, which includes lunch.

Please contact - **Judith Shackleton**  
Manchester Materials Science Centre,  
Grosvenor Street,  
MANCHESTER, M1 7HS.  
Tel. 44 (0) 161 200 3584  
Fax. 44 (0) 161 200 3584  
Email. [judith.shackleton@man.ac.uk](mailto:judith.shackleton@man.ac.uk)



## On being a BCA member...

If you are reading this and it's not your copy, there are several possible reasons. The first and worst (but it happened in my lab last week) is that although you're a member of the BCA, the Administrative Office has for some reason not been sending your own copy to you. If that's so, please email them immediately and they'll take prompt action.

But perhaps you are aren't actually a member, and are browsing through a copy which some good kind person has thoughtfully left in your lab, library, coffee room or bedroom (I'm thinking of the state of my family home at this stage in the summer holidays). In that case, take action now and join! You should be reading this at the start of a new academic year, everyone fresh back from holidays and conferences and full

of enthusiasm for new techniques and crystals to measure. If you are a student, join now at our incredibly low rate of £7.50 for a whole year, and you will be eligible for a bursary to attend the Spring Meeting in York next April (15-17th – three days of concentrated crystallography and two nights of serious socialising). There will be lots about it in the December issue. What's more, we give bursaries for other meetings too – see Colin Bent's report in the issue on his trip to Alaska!

Even if you aren't a student, then BCA membership has got to be the best bargain going in society memberships. At £15 for four issues of this newsletter, you can become a member of the world's second biggest crystallographic association, whose founder members included Dorothy Hodgkin, David Blow and David Phillips (the first three original signatures in the beautiful old

Minute Book which lives in my office). There are now about a thousand members but by no means all crystallographers in this country are members, no doubt a simple oversight in many cases.

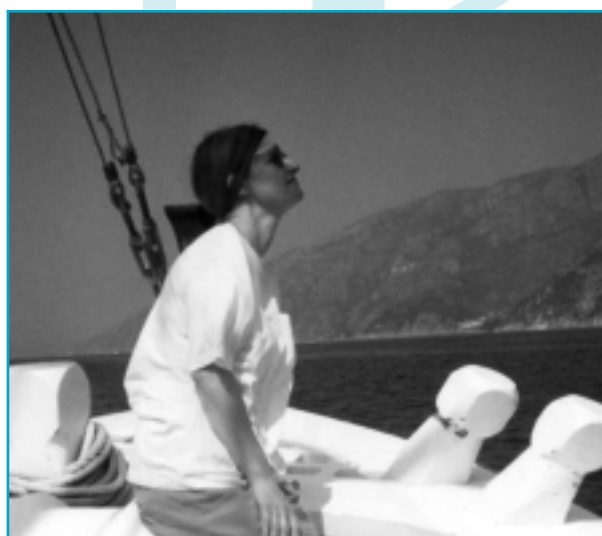
And there's more. Our editorial assistant, Ms Assyna Speys-Groop, has found an as yet unpublished photograph of the Editor at a meeting in France, wearing the internationally recognised BCA tie (available in three colours) and of me on a Crystallographic expedition in Greece.

So, please fill in one of the forms enclosed with this issue. We have a special prize for the person who introduces the most new members, so please write the name of the person who introduced you on the top of your application form.

**Christine Cardin**  
Secretary, BCA



The Editor flaunting a BCA tie in France



The Secretary doing Crystallography in Greece



# Membership Form 2003

Please photocopy

## British Crystallographic Association

Charity Registration Number 284718

WEB SITE: <http://bca.cryst.bbk.ac.uk/BCA/index.html>

Return this form to: **British Crystallographic Association, Administrative Office, 1 Tennant Avenue, College Milton South, East Kilbride, Glasgow G74 5NA UK.** Tel +44 (0)1355 244966, Fax +44 (0)1355 249959, E-mail: [BCA@glasconf.demon.co.uk](mailto:BCA@glasconf.demon.co.uk).

**Your details:** Please fill in in black ink using BLOCK CAPITALS

Title \_\_\_\_\_ Initials \_\_\_\_\_ Name \_\_\_\_\_

Institution \_\_\_\_\_ Department \_\_\_\_\_

Address \_\_\_\_\_

Postcode \_\_\_\_\_ Country \_\_\_\_\_

Phone: \_\_\_\_\_ Fax: \_\_\_\_\_ e-mail: \_\_\_\_\_

Please tick your membership status in a box below and to apply for reduced rates. The BCA has four groups to cater for specific interests of members. Please tick ONE Main Interest Group and any number of Special Interest Groups. The Groups which you select will inform you of their activities.

<b>MEMBERSHIP DETAILS:</b>	A current BCA Member	<input type="checkbox"/>	<b>Main</b>	<b>Group</b>	<b>Special</b>		
	A lapsed BCA Member	<input type="checkbox"/>					
	Not previously a BCA Member	<input type="checkbox"/>				Industrial	<input type="checkbox"/>
	Unemployed*	<input type="checkbox"/>				Chemical Crystallography	<input type="checkbox"/>
	Retired*	<input type="checkbox"/>				Physical Crystallography	<input type="checkbox"/>
	A full time student*	<input type="checkbox"/>				Biological Structures	<input type="checkbox"/>

**For Students only** - Signature of Supervisor: \_\_\_\_\_

Course completion date: \_\_\_\_\_

**FEES:** Full      \*Reduced      \*ONLY Students, Retired and Unemployed  
 £15      £7.50\*      in Pounds Sterling by cheque (UK Bank) or credit card (Mastercard, Visa, Delta ONLY)  
 £12      £6\*      by Banker's Order (drawn on a UK bank)  
 £12      £4.50\*      ONLY for members of the Structural Condensed Matter Physics Group of the Institute of Physics  
 £75 Term Payment for 5yrs (For **Overseas members only**) *Note: Payment by credit card is the best option for overseas members.*

£.....p **MEMBERSHIP FEE DUE**      I wish to add a donation to my fees as specified below:  
 £.....p to the **General fund** of the British Crystallographic Association.  
 £.....p to the **Arnold Beevers Bursary Fund** of the British Crystallographic Association.  
 £.....p to the **Dorothy Hodgkin Prize (DHP) fund**.  
 £.....p **TOTAL PAYABLE to British Crystallographic Association in pounds sterling.**

**A. PAYMENT FORM** I wish to pay by:  
 Cheque - please enclose your cheque drawn on UK bank made out to *British Crystallographic Association*  
 Banker's Order - please complete section (B) below.     Credit card - please complete the following: (eg Visa, Mastercard, Delta NOT Switch)  
 Name on card (IN CAPITALS)..... Card Type .....  
 Billing Address .....  
 Card No \_\_\_\_\_ Expiry Date .....  
 Signature ..... Date .....

**B. BANKER'S ORDER** Please return this form to the BCA, NOT to your bank  
 To the Manager ..... Bank  
 Branch address .....  
 Sort Code \_\_\_\_ -- \_\_\_\_ -- \_\_\_\_ Account no: \_\_\_\_\_

Account in the Name of .....  
 Please pay the British Crystallographic Association, HSBC, 56 Queen Street, Cardiff, CF1 4PX, Account no. 81157981, Sortcode 40-16-15, the sum of £ ..... (amount in figures) ..... (amount in words) on 1st January 2003 and thereafter on 1st January each year until further notice in writing or until ..... (date of last payment). This supersedes any other standing orders from my account (as above) in favour of the BRITISH CRYSTALLOGRAPHIC ASSOCIATION.

Signed ..... Date.....

Thank you for supporting the British Crystallographic Association

## Crystal Structure Determination

Werner Massa, *Marburg University, Germany (English translation by Robert Gould)*  
Springer Verlag, 2000.  
Price £24.00 (softcover)  
ISBN 3-540-65970-6, xi+206 pp

One trepidation about writing a review on the English edition of Werner Massa's "Crystal Structure Determination" is that it cannot do justice to the conciseness and clarity of this highly useful single-crystal crystallographic text. It not only provides a very clear exposition of crystallographic theory, but also the practice and "real world" tricks, hints and expectations of what is possible. Starting with the crystallographic theory (and various tricks and limitations of the method), it continues onto experimental methods (including the growing of crystals); mounting and indexing the cell; structure solution; structure refinement; additional topics such as absolute structure, extinction and the lambda/2 effect, etc; errors and pitfalls, disorder, false unit cells, twinning, false spacegroups, misplaced origins, etc; interpretation and presentation of results; crystal structure databases; and finally a worked structure solution using SHELX.

While some crystallographers might put the charge of "corrupting the youth" on the author by his emphasizing the use of F-square intensity data over F's for structure solution and refinement; there is almost

nothing significant on which to try and condemn this book. It is excellent. Though trying to find some criticisms; an extra emphasis on the use of CCD diffractometers and the various practical pitfalls and tricks of the trade in using CCD instruments would be useful. Another addition could be to point out the quite sophisticated automatic validation options in CIFCHECK as well as Platon, and how to interpret and make use of the validation output (different alert levels, A, B and C). Given the usefulness of the Worked Example of solving and refining a structure using SHELX, it could be nice to have worked examples of other programs showing their different approaches and advantages - but this is a personal and probably unimportant comment.

Another issue is that of the price. At £24.00 EUR 39.95, it is affordable by individuals (though half that cost would probably be nicer for the student budget). This price compares in a favourable manner to recent trends in published scientific texts that have the apparent primary aim of being a rip-off, rather than a useful scientific text deserving of being read. A possible equivalent of the Massa book in the powder diffraction field is priced at well over US\$ 100.00; with the added disadvantage of not having the conciseness, coherency and clarity that a single author like Massa should allow. The Massa book on Crystal Structure Determination is highly useful. Unlike other emerging scientific and crystallographic texts, it is

priced in an affordable range making it easily available to anyone involved in performing crystallography using single crystal methods.

As it is reported there is a 2nd German edition of this text in print, assuming it builds on the high quality of the first edition, it would be of major benefit to see this new edition translated into English (and other languages). This would not only benefit crystallographic teaching and education, but also people such as synthetic chemists and solid state chemists who use crystallography as a "part time" tool; and do not have access to formal crystallographic teaching courses.

Springer website:  
<http://www.springer.de>

Werner Massa's Website:  
<http://www.chemie.uni-marburg.de/~massa/>

Lachlan Cranswick

**"Symmetry 2000":**

Proceedings from a symposium held in Stockholm September 2000. (Volume 80 of the Wenner-Gren International Series)

**Editors: I. Hargittai and T.C.Laurent**

Portland Press Ltd, London 2002

**Price £110 (hardback bound in 2 parts)**

ISBN 1 85578 149 2 627pp total.

This symposium had three inter-related aims: (i) to demonstrate the use of the concept of symmetry in diverse fields, and to think of future applications (ii) to encourage inter-disciplinary dialogue between those using symmetry (iii) to identify the potential of the concept of symmetry in general education and in the public understanding of science. Most of the articles were presented at the symposium, but the editors have also included a few from other contributors which help to fulfil their aims. This is not a textbook where one chapter follows logically from the next, instead the 52 individual articles are grouped into like topics in six sections; in part 1, *Shapes and fractals, Properties and regularities, Symmetries and chiralities* and in part 2 *Molecules and assemblies, Social culture, Artistic symmetry*. Notes and references for each article are printed at the end of the article. The contents of both parts are printed in both volumes, the subject index only at the end of the second part.

There is plenty here to interest a crystallographer; articles written by acknowledged experts in their

fields include that by Alan Mackay "*The shape of two dimensional space*", and that by Jack Dunitz, "*Space filling in molecular crystals*". "*Crystal optics and the symmetry principle: an update*" has a summary by W. Kaminsky and B.Kahr of the history of optical rotation in crystals. There are several articles on symmetry concepts in NMR Spectroscopy including "*Seven-fold dynamical symmetry in solid-state NMR*" by M.Levitt who has been studying the detailed geometric structure of rhodospin before and after absorbing light. Perhaps the most fundamental concepts are those described by D.Rouvray in "*Symmetry in Action: the laws of Nature*" which includes a summary of the work of William Hamilton and Emmy Noether's theorem relating symmetries to conservation laws in chemistry.

Those interested in geometrical shapes will enjoy H.S.M.Coxeter's "*The rhombic triacontahedron*", or M. Longuet-Higgins' "*On the use of symmetry for constructing polyhedral models*" or the summary by I.Bergstrom and S. Frefert "*On the origins of the Platonic bodies and some of their relatives*" which discusses how the recent discovery of C<sub>60</sub>, which has the form of a truncated icosahedron, one of the Archimedean solids, has prompted a renewed interest in polyhedral forms. Marjorie Senechal contributes "*Reflections on the Kaleidoscope*", Benoit Mandelbrot "*Symmetry by dilation, reduction, fractals and roughness*" and Doris Schattschneider "*The many faces of symmetry in the work of M.C.Escher*".

The inter disciplinary nature of the books means that you may be able to persuade your University Library to buy it since there are articles of interest to historians, artists, students of foreign cultures and information technology as well as mathematicians and scientists. P.Gerdes writes on symmetry in African cultures, T Kobayashi on "*What was known about the polyhedra in Ancient China and Edo Japan*" where he describes early seventeenth century texts on the Platonic and Archimedean solids, but failed to look closely at the lion dogs which guard Chinese temples; some of these sculptures date from the Ming Dynasty (1368 - 1644). While visiting the IUCr Congress in Beijing in 1993, I. Hargittai photographed the ball held in the claw of one of the lion dogs and saw that it resembled a "bucky ball", (see "*The Crystallographic Tourist*". page 50 "*Crystallography News*" No 63 December 1997.) Those who attended the IUCr Congress in Glasgow will have seen the textile exhibition organised by Annegret Haake on crystallographic themes and be interested in her description of how it started, "*XX-TEX - textiles and crystallography*". I also liked J.Beyers' "*Symmetry concepts in quilt and fabric design*", but I am not sure whether to take seriously "*The songs of the double helix: symmetry and lyrical conceptualism*", where Paul Hartel quotes Kepler's "Harmonica Mundi" of 1618 describing the music of the spheres, the sun and planets which he associated with the geometrical forms of the 5

Platonic solids. Hartel thinks that music is embedded within the essential building blocks of DNA; some composers have assigned musical notes to DNA's constituent molecules and found that members of the audience likened the resulting melodies to little known works by Bach, Brahms or Chopin! Students having difficulty in understanding the concept of symmetry in introductory crystallography courses may find it helpful to read some of the papers in the "Social Culture" and "Artistic Symmetry" sections.

I found these volumes fascinating with their interesting mix of articles showing many aspects of symmetry in our culture. However, they are expensive, costing more than many hardback textbooks, so I doubt whether University Research Groups can afford them. Try to persuade your University Library to buy them and then take them out on permanent loan.

#### Kate Crennell

#### Notes:

These volumes can be purchased direct from the publisher via their web site at <http://www.portlandpress.co.uk/>

Click on their 'Book catalogue' entry and then search for these volumes to find the page with a complete listing of the contents of these volumes with the titles of all the articles.

### The Road to Stockholm. Nobel Prizes, Science, and Scientists.

**István Hargittai**, Budapest Technical University, Hungary. Oxford University Press, 2002  
**Price: £19.99 (hardback)**  
 ISBN 0-19-850912-X 360 pp 24pp halftone plates

The year 2001 was the centennial of the first award of the Nobel prizes. They remain the only science prizes widely recognized by the general public and the media; for a few days each Autumn there is international and local news, sports news and *science news* when the achievements of the year's Nobel Laureates are acclaimed. There are many other science prizes, how has this one captured the public attention? Have you ever wondered how the selection process works? Or whether the award of this prize changes the lives of those who receive it? István Hargittai has thought about this for some years; he has interviewed some 70 Nobel Laureates and other distinguished scientists in the fields of "chemistry", "physics", and "physiology and medicine" and distilled his findings into this book, where he explores the answers to these questions. This book is not concerned with the Prizes in economics and literature and although the title includes the word "science", this is incidental to the sociology; these people happened to be scientists; the author has sensibly refrained from trying to describe the science itself in detail, that would have made a much longer book. If you want to learn more of the

science there are copious references in the Notes section which is almost 50 pages long; I expect that most BCA members will already be familiar with the science.

The first chapter explains the history of the Nobel Prizes and the annual selection process and mentions other science prizes, including the "reverse Nobel prize" known as the "*Ig Nobel prize*" bestowed by the *Annals of Improbable Research* on individuals whose "achievements cannot or should not be reproduced".

The next chapter "**Nobel prizes and National Politics**" explores the distribution of prizes amongst scientists of various nationalities. One problem is that the scientists themselves are more often citizens of the world than of any one country, and may not themselves have the aspirations attributed to them by others. We read (p 29) that Boris Vashteyn, evaluating the life and work of Dorothy Hodgkin, noted that she "*has done much for the glory of her homeland*". As Hargittai remarks "*This reflected more Vashteyn's way of thinking than Hodgkin's aspirations*". Scientists naturally migrate to other countries even in peace time, and in the 1930s many who later became Nobel Laureates fled Nazi Germany. The small number of prizes for Japanese scientists may also be an indication of the timidity of Western Science towards Japan. We see this also in the IUCr where an excellent Japanese bid to host the 2005 Congress was rejected in favour of one from Florence.

"Who wins Nobel prizes?" is the question posed in the third chapter. The author tries to assess the common qualities which Nobel laureates possess, and speculates on whether it may be possible to train people to become Prize winners. A later chapter on "Mentors" describes how students naturally wish to work with inspiring eminent scientists who may later win Nobel prizes; some famous examples are Frederick Sanger (winner of the Chemistry prize in 1958 and again in 1980) and his research student César Milstein who won one in medicine in 1984.

Equally interesting is the last chapter, "Who did not win?", where possible reasons are discussed as to why those who surely deserved a Nobel prize did not receive one. J.D.Bernal is perhaps the most notable crystallographer; another example is Isabella Karle, who played a significant role in putting the direct method into practice but was not awarded the Nobel prize with Herbert Hauptmann and Jerome Karle in 1985. She was given the Swedish Aminoff prize for crystallography in 1992. There are also some important newly discovered topics such as "quasi-crystals" whose discoverers have not yet received a Nobel Prize. Dan Shechtman received the Aminoff Prize for his discovery of quasi-crystals in 2000. Hargittai speculates that the Aminoff Prize may be becoming a "consolation prize" for those not awarded a Nobel prize.

The book lists the Nobel Prizes awarded in scientific fields up to

2001; it has an index to the names of the scientists but *no subject index*. This would have made it a much better reference tool for those who wonder which important scientific discoveries have been awarded a Nobel prize. Nevertheless, the book is very good value for money, a well produced hardback for just under £20, but the publisher saved money by binding all the photographs together in one place; I would have preferred them distributed throughout the text. If you are interested in the history and sociology of science or just wondering how to groom your students to become future Nobel prizewinners buy this book.

Kate Crennell

#### Relevant Web Addresses

1. The Oxford University Press site is <http://www.oup.co.uk/> search their books catalogue for the ISBN or author to find the publishers press release. You can buy the book at full list price through this site, but you may find other Internet book sellers with discount prices.
2. A site devoted to this book is <http://www.roadtostockholm.com/> it has extra information, including reviews, photographs not featured in the book itself and information about the author. This site is not always obtainable, and alternate URL is: <http://www.princeton.edu/~eszter/rs/>
3. The *Electronic Nobel Museum* is at <http://www.nobel.se> which has full details of all the Nobel Laureates, with portraits and bibliographies. Philatelists can also access the catalogue of Swedish postage stamps now issued annually to commemorate the Nobel Prize winners.
4. The *Nobel Prize Internet Archive* at <http://www.nobelprizes.com> has more indexes, including the "Nobel Laureates Alma Mater", an alphabetic index of all the Nobel Laureates and a "Nobel Trivia Quiz" which could be useful for those arranging a scientific social "Quiz Night".
5. The Stanford University Library has a set of useful links at: <http://www.slac.stanford.edu/library/resources/more.html#Nobel>
6. The results of a "Prize Competition" in "Crystallography News" lists those Nobel Laureates who the editor thought could be described as "*crystallographers*" together with links to other pages giving details of their achievements <http://bca.cryst.bbk.ac.uk/BCA/CNews/1997/Sep97/nobels.htm>

Please send news of other relevant web sites to the BCA Education Officer preferably by email: [BCA@isise.rl.ac.uk](mailto:BCA@isise.rl.ac.uk)

## The Chemical Bond in Inorganic Chemistry: The Bond Valence Model

I. David Brown, Macmaster University, Hamilton, ON, Canada  
IUCr Monographs on Crystallography, Oxford University Press, 2001.  
Price: £75.00 (hardback)  
ISBN 0-19-8508700 x + 278 pages

Although the idea of the chemical bond is of some importance in chemistry, it has proved to be difficult to describe quantum mechanically. As Brown puts it on the first page of this excellent book, *it is unlikely that, left to themselves, theoretical chemists in the twentieth century would ever have created the idea of the chemical bond had not the concept already been central to the language of structural chemistry.* Thank goodness for the Victorians.

The bond valence method, which has been developed in large part by the author of this book, exploits the essential simplicity of the traditional bonding model in which an atom has a certain bonding capacity (valence) which is shared over the bonds that it forms. By drawing on the wealth of structural data which has become available as a result of the developments in crystallography over the twentieth century it has enabled an empirical relationship to be established between the length of a bond and the number of valence units that the bond contributes. It therefore forms a quantitative theory of chemical structure, which though most

frequently applied to ionic solids, can be applied equally well to covalent compounds and to liquids. The beauty of the method is that it does this without recourse to lengthy calculations.

After a brief historical survey given in Chapter 1, Chapters 2 and 3 examine the theoretical basis of the bond valence method. It is possible to calculate the Madelung or electrostatic field of an ionic crystal, and the collection of all the lines of field joining two charges forms the bond between them. The strength of the bond is characterised by the electrostatic flux. This procedure clearly requires extensive calculation, but fortunately the bond fluxes are generally the same as experimental bond valences ( $S_{ij}$ ), derived from crystallographically determined interatomic distances ( $R_{ij}$ ) using Brown's famous equation:

$$S_{ij} = \exp[(R_0 - R_{ij})/B]$$

$R_0$  and  $B$  are characteristic of a particular bond type; a tabulation is available at [http://www.ccp14.ac.uk/ccp/web-mirrors/i\\_d\\_brown/bond\\_valence\\_parm/](http://www.ccp14.ac.uk/ccp/web-mirrors/i_d_brown/bond_valence_parm/).

Chapter 4 examines the concept of cation and anion bonding strength and the *valence matching principle*, which states that the most stable compounds are formed between cation and anions with similar bonding strengths. Chemists will recognise the similarity of this principle to

Pearson's hard and soft acid and base principle, and the relationship between the two is discussed. The nice thing about bonding strengths is that they are easily calculated and they explain a lot. For example in  $\text{PO}_4^{3-}$  the valence of the central atom is 5, that of oxygen is 2. Each P-O bond must have a valence of  $5/4=1.25$  to satisfy the phosphorus, leaving the oxygen 0.75 valence units (v.u.) for external bonding - for example to a counter-cation. Generally oxygen forms four bonds; one of these is to the phosphorus, and so that each external bond will be worth 0.25 v.u., the anion bonding strength of phosphate. Phosphate is a stronger anion than sulfate, which has a strength of 0.17 v.u. In these few lines lies the explanation for the differences between phosphate and sulfate chemistry. The idea is developed in the following chapter into a discussion of solubilities and the formation of secondary solvation shells in aqueous solution. There is a short, but interesting, section on silicates. Magmas which are rich in magnesium (strength 0.33) tend to crystallise as  $\text{Mg}_2\text{SiO}_4$  because  $\text{SiO}_4^{4-}$  also has a strength of 0.33. Magmas rich in weaker sodium (strength 0.17) tend to form  $\text{Na}_2\text{Si}_2\text{O}_5$  because the strength of the  $\text{Si}_2\text{O}_5^{2-}$  anion is 0.17. The book is full of 'nice' illustrations like this.

Chapter 6 examines the influence of anion-anion repulsion and cation-to-anion bonding strength as factors which determine the co-ordination numbers of cations. A discussion of hydrogen bonds, that is the

structural chemistry of the  $H^+$  cation, is given in Chapter 7, and their somewhat anomalous properties shown, as a development of the material presented in the previous chapter, to be a result of anion-anion repulsions. Madelung fields have been calculated explicitly only for symmetrical structures, and Chapter 8 tackles the problem of distorted structures, and how a local polarisation model can be used to interpret them. For example, cations such as  $Tl^+$  can form stable compounds with anions with varying bonding strengths, and this can be related to the polarisation of its lone pair of electrons. The oddly distorted structures of  $d^0$  transition metal complexes can be addressed with a similar model. Chapter 9 brings the section of the book devoted to fundamental chemical principles to a close with a review of the properties of bonds, such as bond lengths and angles, force constants and their response to temperature.

The next section of the book concentrates on the general theme of the structures of inorganic solids. There is a need to satisfy both chemical and symmetry constraints when compounds form crystals, and the first chapter of this section (10) gives a brief introduction to space group theory. In addition to the two methods described above, bond valences may also be calculated from a bonding graph in the absence of experimental information from the requirement that the sum of the valences of the bonds made to a particular atom must equal

the atomic valence of that atom. Thus, in the case of NaCl, where each cation and anion forms six bonds, each bond must be equivalent to 0.17 valence units. Where symmetry is lower non-equivalent bonds have different valences, and so this constraint is usually not enough to form a tractable set of simultaneous equations. In these cases a valence is considered to be positive in the direction anion to cation, and further equations are added using the constraint that the sum around a closed loop must equal zero. The application of these *theoretical bond valences* to modelling crystal structures will be clear, and the approaches for predicting topologies are described in Chapter 11. The material covered ranges more widely than the immediate application of the bond valence method, and (for example) methods based on simulating annealing for crystal structure prediction are also covered. Structures in which experimentally determined bond valences differ from the theoretical valences just described are termed as being strained, and Chapter 12 examines this topic in detail. The remainder of the book reviews applications of the bond valence method in crystallography, chemistry, physics, mineralogy and biology. A well known crystallographic application is in the assignment of oxidation states, and the calculation of the occupancies of  $Fe^{2+}$  and  $Fe^{3+}$  in the octahedral and tetrahedral metal sites in  $Fe_3O_4$  is given as a specific example. The final chapter

attempts to place the bond valence method into the context of other bonding theories.

Although there are several excellent reviews on the bond valence method in the literature there has long been a need for a dedicated monograph on the subject. This book will appeal to anyone interested in the structure of solids, including crystallographers, structural chemists and materials scientists. Professor Brown has written a highly readable book about a theory that, though it has long found application in inorganic crystal chemistry, deserves to be used more widely. One needs only a pencil and a calculator to use it, and having read the book, readers will be inspired to apply this simple predictive theory to their own work.

Simon Parsons

## STOP PRESS

The Winter Meeting of the Physical Crystallography Group will be entitled, "Complementary Techniques applied to Crystallography". It will be held on Wednesday 11 December, 2002 at the Centre for Science at Extreme Conditions, University of Edinburgh. The local contact is Dr David Allan, [dra@ph.ed.ac.uk](mailto:dra@ph.ed.ac.uk)



## Nucleic Acid Structure and Recognition, From the double helix to the ribosome

**Stephen Neidle**, The Institute of Cancer Research (University of London)

Oxford University Press, 2002

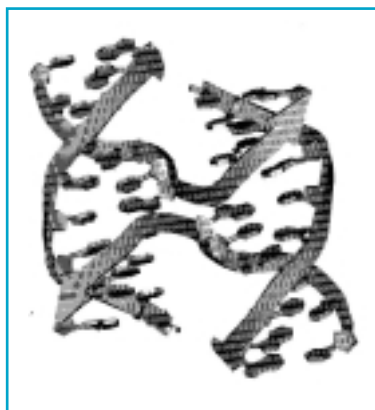
**Price: £29.50 (Paperback)**

ISBN 0-19-850635-X, xi + 187pp

Skipping through Brenda Maddox's new book on Rosalind Franklin is thought-provoking on the history of DNA structure determination. A discarded title for 'The Double Helix' was apparently 'Base Pairs', according to Brenda Maddox a punning self-accusation by Jim Watson that he and Francis Crick had, without her knowledge, made use of Rosalind Franklin's experimental fibre diffraction patterns.

If the fiftieth anniversary of the Watson-Crick model, looming in early 2003, provokes a new wave of interest in nucleic acid structure, alongside the renewed interest in these old controversies, Stephen Neidle's excellent new introductory textbook will prove to be very timely, and provides a calm, balanced and objective study of the major advances. Practising scientists are increasingly too busy for textbook writing, but nothing can replace the perspective that someone of Steve's experience brings to this subject. The book's predecessor, 'DNA Structure and Recognition' was published in 1994, and for the last seven years has been my main introductory recommendation for students of

nucleic acid structure for its clarity, brevity and balance. The new book incorporates all the major advances since then, and has the added bonus of a website ([www.oup.com/na-structure](http://www.oup.com/na-structure)) with free access even if you don't buy the book.



Chapter One describes methods for studying nucleic acid structure, with a short discussion of the X-ray method, and a quick look at n.m.r., molecular modelling methods and databases. Chapter Two is perhaps the most immediately useful for a newcomer, a guide through the complexities of the nomenclature used to describe nucleic acid structure and conformations (slide, roll, twist, pucker, buckle, tilt, and the rest.....), which are very confusing at first. Chapter Three goes back to the original technique used for studying DNA structure, fibre diffraction, and compares these average results with the details available using single crystals. It is striking that the original fibre image remains one of the best known images of science among the general public (along with an even more outdated image, the Bohr orbits!) but this book gives

a short summary of all the work done since then to demonstrate the variability within the familiar A-B- and Z-conformational families. With Chapter Four, we reach the area where there has been much recent excitement, with X-ray structures now available for quadruplex, triplex, and Holliday junction DNA (see picture), all of these structures having resisted years of attempts to demonstrate their crystallographic existence. DNA has the reputation of being difficult to crystallise, because, unlike proteins, it is never globular and always has the negative charge of the phosphates which must be neutralised with cations, but (perhaps so as not to frighten newcomers?) this book makes no direct mention of these problems. It is at this point that the use of the pdb files on the website is particularly encouraged, because unlike the double helix, readers won't be familiar with these recent exotica. (Note – if you try this, the right hand mouse button is the key to unlocking some very pretty and useful ways of viewing the molecules with Chime. Happy viewing!). Chapter Five is an introduction to DNA interactions with small molecules – DNA crystals typically contain at least 50% water, much of which is ordered into well-studied hydration patterns. Drug and cation binding perturb this; a study of these interactions often suggesting modes of DNA-protein interaction, the subject of Chapter Seven.

Chapter Six, though, is an important area which the predecessor book did not cover (hence the change in title) – the RNA Structural World. The compact tertiary structures of RNA are the closest analogues in the nucleic acid field to the folding of globular proteins. We are fortunate that Venki Ramakrishnan has very kindly accepted the BCA's invitation to give the Max Perutz Memorial Lecture at the Spring Meeting in April 2003, when we hope to be treated to a guided tour of the amazing complexity of the ribosome. Meanwhile, this book includes a short and readable description, and the webpage gives quick access to the ribosome coordinate files for an awesome molecular experience (and, yes, you can try this at home, even; I thought the ribosome would crash my PC but it didn't!) – 'the ribosomal RNA framework is likely to be largely invariant throughout the living world', as the penultimate sentence of this excellent short summary puts it. And with that mind-boggling thought, let me congratulate Steve on making this subject so accessible to such a potentially wide audience.

Christine Cardin

### Outline of Crystallography for Biologists

David Blow, Imperial College, London  
Oxford University Press, 2002  
Price: £25.00 (paperback)  
ISBN 0 19 8510519, 236pp

This compact and informative book begins with a quotation from Max Perutz to whom the book is dedicated: 'The X-ray study of proteins is sometimes regarded as an abstruse subject comprehensible only to specialists, but the basic ideas underlying our work are so simple that some physicists find them boring'

A major change in the area of X-ray crystallography has been the invasion of the field by biologists and biochemists who are prepared to have a go at tackling 'their' protein without much formal training. The daily correspondence over the various e-mail bulletin boards provides a lively record of hundreds of intrepid amateurs in laboratories round the world who follow computational recipes and travel far down the sometimes tortuous paths of structure determination. This have-a-go approach should certainly be encouraged and is undoubtedly contributing to the continued exponential growth of protein structures now available - fast approaching the 20,000 mark.

This book is therefore a very timely contribution as it provides newcomers to the field of protein crystallography with a

concise outline of the background physics together with an overview of the practical aspects of protein structure determination by crystallography. David Blow is one of the grand masters of protein crystallography and has made many major contributions to the field; notably in the original development of the theory of molecular replacement and in pioneering work on the structure determination of many key enzymes. I was intrigued to see how someone with such profound insight of the subject would tackle the job of explaining the theory and practice of this arcane art in less than 250 pages in a palatable form suitable for biologists.

The chosen format is to divide the book into two equal halves in which the first more theoretical part discusses crystal symmetry and the physics of diffraction while the second part tackles the more practical steps covering all stages from data collection to structure refinement. It is also claimed that the text is suitable for those with a minimal background in maths. To this end grey-shaded boxes are scattered through the text segregating out algebraic formulae and theoretical explanations. This seems like an excellent idea. To capture the full flavour of the book I read all the grey boxes. In some chapters the approach works well and the thread of the narrative text is maintained. In the chapters on Waves and Diffraction the boxes dominate and this makes for a more patchy read. The second half of the book has

excellent chapters on isomorphous replacement, anomalous scattering and molecular replacement. In all chapters in this section Blow makes good use of well selected historical and recent papers to provide examples of the procedures being described. In such an all encompassing book it is impossible to cover all definitions and there are a few places in the book which may puzzle the true novice where terms like  $s(l)$ ,  $c^*$  and 'phasing power' are introduced in the text without having been defined. Such pedantries should not however spoil enjoyment of the book and I can warmly recommend it to novices and experts alike.

With excitement still high about structural genomics, the future of protein crystallography over the next decade is assured and is set to drift steadily further away from the realms of physics into arms of the biologists. Indeed no crystallography laboratory can exist nowadays without strong biological projects and the editors should perhaps consider a sister volume 'Molecular Biology for Crystallographers and Bored Physicists'

**Malcolm D. Walkinshaw**



### L'Oréal-Royal Institution Science Graduate of the Year 2002 Winner Announced

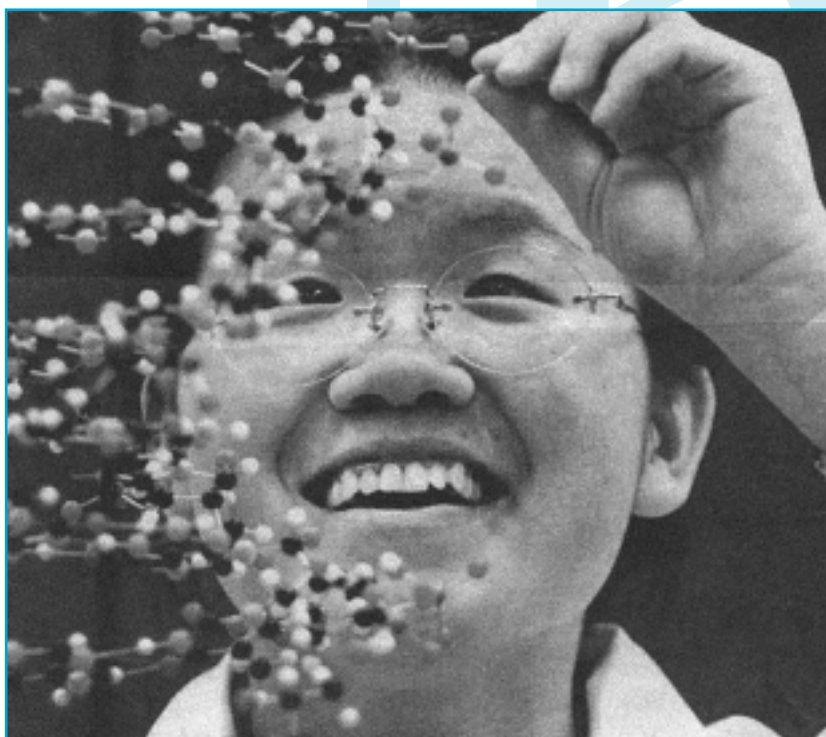
**Chemistry PhD student receives £6,000 to support her work on cancer fighting drugs**

Haimei Chen, a research student from the University of Edinburgh, has been named the **L'Oréal-Royal Institution Science Graduate of the Year 2002**. She receives £6000 and life

membership of the Royal Institution for her groundbreaking work on the design of anticancer drugs. She presented her research in a lecture at the Royal Institution, chaired by the Royal Institution Director Baroness Greenfield.

The jury - whose members included Baroness Greenfield and Professor Richard Catlow, Director, Davy Faraday Laboratory - selected Chen for her research incorporating new design features into ruthenium compounds to target specific genes on the DNA of cancer cells.

While most chemotherapeutic agents have been traditionally based on organic compounds, more recent research shows that nature also uses other elements in human biochemistry, including metals. Chen has developed



Haimei Chen with a DNA model

special organic coats for ruthenium – her new compounds are highly selective in targeting DNA bases using the synergistic effects of both the ruthenium and the coat.

Although Chen's research is still in the early stages, this new approach could lead to the development of a new class of drugs to fight cancer. Her work has already been submitted as a number of patent applications, and she has been published in several leading scientific journals including the prestigious Journal of the American Chemical Society.

Chen, who studied in China before winning a scholarship to the University of Edinburgh in 1999, beat five other finalists who presented their research to the judging panel in May this year. The Award, established by L'Oréal and the Royal Institution, was set up in 2000 to give early recognition to innovative and groundbreaking research by young scientists.

"It is very exciting that a young scientist, especially a young woman scientist, is being acknowledged in this way. I am delighted that the Royal Institution is supporting this important initiative, which recognises innovation and bold scientific research that challenges accepted dogma," said **Baroness Greenfield, Director of the Royal Institution**.

"L'Oréal is founded upon research and innovation and is proud to work in partnership with the Royal Institution in the

encouragement of research. Haimei is a dedicated and brilliant researcher, whose findings are of both clinical and industrial significance - as such she is a very worthy recipient of the Science Graduate of the Year Award," said **Jean-Francois Grollier, Vice-President of Research and Development, L'Oréal**.

*Note from the Editor: This work is typical of much top quality research in that it has a very large crystallographic component hidden in it! Haimei's award is one open to all – last year's winner was Graham Taylor, a research student of the University of Oxford, for his research into animal flight. It is worth noting, however, that L'Oréal's highly prestigious "Women in Science Awards", with a value of US\$ 100 000, are offered in 2003 specifically for work in "Sciences of Condensed Matter". More information is available on the website: <http://www.forwomeninscience.com>*

## Crystal Growth and Design - a New Journal

Dear Colleague,

As Editor-in-Chief for Crystal Growth & Design, I am honoured to inform you that we have been awarded the Best New Journal—Any Category from the Professional and Scholarly Publishing Division of the Association of American Publishers for the year 2001. The Professional and Scholarly Publishing Awards are given annually by the Association of

American Publishers' Professional and Scholarly Publishing Division to acknowledge excellence in book, journal, and electronic publishing in all the disciplines represented by professional, scholarly and reference publishing.

CG&D is published by the ACS and contains articles on the physical, chemical, and biological phenomena and processes related to crystal growth and the design of new materials, and also offers the ability to enhance the presentation of your research, and the reader's comprehension by including web-enhanced objects within your manuscript in the CG&D Web Edition. To view web enhanced objects and a free sample issue of the Web Edition, go to the CG&D homepage at <http://pubs.acs.org/crystal>.

For more information on submitting your research to the journal awarded as the "Best New Journal in 2001," click on "Info for Authors" on the CG&D homepage. And don't forget... for access to the "best new" articles in crystal growth and design, recommend Crystal Growth & Design to your librarian or information specialist today.

Yours sincerely,

**EDITOR**

**ROBIN D. ROGERS**

Department of Chemistry  
The University of Alabama

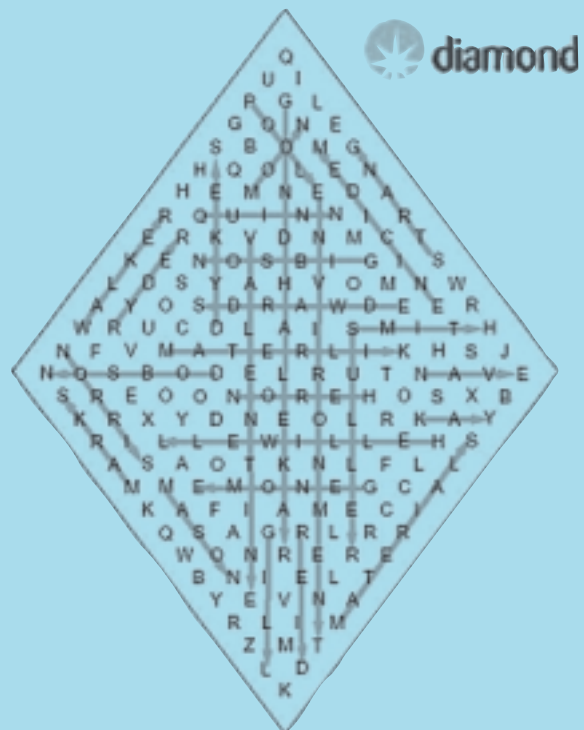
## Puzzle Corner

This month's competition is nice and easy – one might almost call it a soft option, submitted by our roving reporter Mo Skail. It is a simple substitution cryptogram; each letter always represents the same letter throughout the text, and may represent itself. Answers please to the Editor by 18th October, 2002. In case of a tie, extra credit will be given to anyone who can identify the source, which is a well-known textbook! As usual, the prize is a £10 Book Token.

**Urdg af gpnnpidm bplis ai rffpgaruapi eaww  
fjvcjuaij pbuji ai yjaif eaww nrhijfauj pv  
klrvuq, pv rdpih brlduf. Au rdfp bpvnf zm  
uwj dpe hvrsj njurnpvcwafn pb fadagjplf  
spdpnauj, ris urdg fgwafuf rvj ipu ligpnpi.  
Urdg af uwj bavfu najvrd eaww ewagw uwj  
fulsjiu gpnjf aiup gpiurgu.**

Last month's winner is Frances Bernstein, who found all but one of the words in the amazing "word diamond". Congratulations Frances! The solution is shown in the figure. The words included were 4 research topics to be studied at 'diamond' and the surnames of 24 people associated with the project, 23 with the 'diamond' project itself, and the last one the surname of the recently appointed CLRC Director for Synchrotron Radiation.

The names, using Frances's notation, are given alphabetically below, together with her notation, which the enquiring may wish to decode!



The four research topics are:		GIBSON	H10B8	REID	V16D11
		GILL	V14D11	RYDER	R2U12
ENVIRONMENT	V13D3	GONDHALEKAR	V15D2	SMITH	H13F9
GENOME	H20B8	HERON	H16B10	STRANGE	L1U10
MATERIALS	R15U12	KAY	H17F11	SULLER	V19D5
MEDICINE	L2D4	MARKS	L15U6	VALENTINE	V13D4
		MASON	L14D7	WALKER	R1U13
The 23 members of the project are:		MATERLIK	H14F4	And, of course, the recently appointed director is:	
		MOON	R3U5		
		NAVE	H15F12		
DOBSON	H15B6	NORRIS	L14D1		
DYKES	V5U5	POOLE	L3D1	HELLIWELL	H18B12
EDWARDS	H12B10	QUINN	H8F2		

**Queen's Award Success for Bede, one of our Corporate Members**



Bede plc are proud to announce that its UK subsidiary, Bede Scientific Instruments Ltd, has been awarded the Queen's Award for Enterprise: International Trade 2002.

The Award will be formally conferred in a Grant of Appointment ceremony to take place at the company's premises later in the year.

Neil Loxley, Managing Director of Bede Scientific Instruments Ltd and Chief Executive of Bede plc, the Group's parent company, said, "I am delighted that Bede Scientific Instruments Ltd has been successful in receiving its fourth Queen's Award. The award was based on success in international trade during a period of intensive growth for the company culminating in the flotation of Bede plc on the London Stock Exchange in November 2000. The company has achieved good revenue growth in international markets during difficult market conditions, proving that the creation of leading edge technology through investment in R&D, a strong management team and the hard work of dedicated employees can lead to continued success. Bede is definitely growing from strength to strength."

**BACKGROUND NOTES**

Bede Scientific Instruments Ltd, headquartered in Durham, UK has been a global leader in the design and manufacture of non-destructive X-ray metrology tools since it was formed in 1978. The parent company, Bede plc, was floated on the London Stock Exchange in November 2000. The Bede Group also includes offices in Colorado, USA, Shanghai, China and Prague, Czech Republic. Approximately 90% of the company's products were sold overseas in 2001, a typical figure for the level of global sales each year by the company, and a major factor in the granting of the Queen's Award.

The Group's core product line uses X-rays to characterise advanced materials such as semiconductors used in optical and wireless telecommunications and microprocessor devices. By providing customers with information about their materials we are able to help them research and develop new devices and subsequently assess their quality during manufacture, thereby reducing wastage and improving yields.

In March 2001, the Group's long-term strategy of entering the high-volume, silicon based semiconductor manufacturing environment was vindicated when it signed an agreement with a major semiconductor manufacturer to supply up to 20 FAB300™ X-ray tools worth \$18m over a 2 to 3 year period.

The Group is also diversifying into new markets, including life sciences, to reduce its dependence on the cyclical nature of the semiconductor industry. Recently, a major chemical company placed an order with Bede for a novel X-ray diffraction tool for in-line characterisation of pharmaceuticals during manufacturing. This order forms part of a longer term collaboration between the chemical company and Bede, and represents an important step in Bede's overall strategy of developing tools for the pharmaceutical market.

In December 2001 the operations of Bede Scientific Instruments Ltd and the Head Office of Bede plc moved into new 27,000 sq ft custom-built premises in Durham, UK. The new facilities include Class 100,000 and Class 100 clean-room manufacturing areas, sales applications laboratories, development laboratories, meeting rooms and office space.

Bede Scientific Instruments Ltd has been granted three other Queen's Awards in past years. In 1991 the company won two awards, one for international trade and another for innovation. In 1996 the company won the innovation award again for a new X-ray diffractometer.

## Meetings of interest

Further information may be obtained from the website given. If you have news of any meetings to add to list please send them to the BCA Web Master [cockcroft@img.cryst.bbk.ac.uk](mailto:cockcroft@img.cryst.bbk.ac.uk) or to the Editor, [bob@gould.ca](mailto:bob@gould.ca)

### 1-6 September 2002

18th General Meeting of the International Mineralogical Association, Edinburgh, Scotland.

[<http://www.minersoc.org/IMA2002>]

### 4-6 September 2002

Synchrotron Radiation in Polymer Science (European Physical Society Conference on Macromolecular Physics), Sheffield.

[<http://www.polymercentre.org.uk/srps/>]

### 5-6 September 2002

2nd International Workshop on Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation, Argonne National Laboratory, IL, USA.

[<http://www.aps.anl.gov/asd/me/medsi02/>]

### 4-7 September 2002.

40th European High-Pressure Research Group Meeting, Edinburgh.

[<http://www.ph.ed.ac.uk/EHPRG-40/>]

### 4-7 September 2002

6th International Conference on Quasielastic Neutron Scattering, Potsdam (near Berlin), Germany.

[<http://www.hmi.de/qens2002>]

### 8-12 September 2002

Chemistry towards Biology in Portoroz, Slovenia.

[<http://www.portoroz2002.ki.si>]

### 9-13 September 2002

Trends in NanoTechnology International Conference (TNT2002), Santiago de Compostela, Spain.

[<http://www.cmp-cientifica.com/TNT2002.html>]

### 10-14 September 2002

XTOP 2002 6th Biennial Conference on High Resolution X-Ray Diffraction and Topography, Grenoble-Aussois, France.

[<http://www.lmcp.jussieu.fr/lmcp/reunions/xtop2002/>]

### 10-14 September 2002

First Summer School on Polarized Neutron Scattering, Juelich, Germany.

[<http://www.fz-juelich.de/PNCMI2002>]

### 11-12 September 2002

SRS Users Meeting, CLRC, Daresbury Laboratory, Warrington, WA4 4AD

[<http://www.srs.ac.uk/srum/index.html>]

### 11-13 September 2002,

Advances In Thin Film Characterization By X-Rays, Genova, Italy.

[<http://www.ing.unitn.it/~maud/esqui/esqui.html>]

### 12 September 2002

Industrial Aspects of Crystallisation from Solution: Nucleation and Polymorphism: SYMPOCRIST, Marseille, France.

[<http://www.crmc2.univ-mrs.fr/conf/sympocrist/>]

### 13-14 September, 2002

1st Workshop on applications in Biology using a dedicated Petra Storage Ring on the campus Desy in Hamburg, Germany.

[[http://www-hasylab.desy.de/facility/upgrade/upgrade\\_worksh\\_ops.htm](http://www-hasylab.desy.de/facility/upgrade/upgrade_worksh_ops.htm)]

### 16-17 September 2002

1st Users Meeting of the New Synchrotron Facility in Karlsruhe, Forschungszentrum, Karlsruhe, Germany.

[<http://www.fzk.de/anka/>]

### 15-19 September 2002

International workshop on Polarized Neutrons in Condensed Matter Investigations PNCMI 2002, Juelich, Germany.

[<http://www.fz-juelich.de/PNCMI2002>]

## 16-17th September 2002

The eighth workshop to discuss the neutron-beam instrumentation for Australia's Replacement Research Reactor, School of Mechanical and Manufacturing Engineering at the University of New South Wales, Sydney, Australia.  
[<http://www.ansto.gov.au/ansto/neut/workshop7.html>]

## 16-27 September 2002

6th Laboratory Course Neutron Scattering, Juelich, Germany.  
[<http://www.neutronsattering.de/labcourse.html>]

## 23-27 September 2002

Analyse Structurale par Diffraction des Rayons X. Structures absolues, macles, incommensurables, Toulouse, France.  
[[http://www.lcc-toulouse.fr/congres/ecole\\_rx\\_2002/index.html](http://www.lcc-toulouse.fr/congres/ecole_rx_2002/index.html)]

## 24-26 September 2002

Second Virtual Conference on Genomics and Bioinformatics  
[<http://www.ndsu.nodak.edu/virtual-genomics/upcom2.html>]

## 25-28 September 2002

International Conference on Crystal Chemistry of Intermetallic Compounds, Lviv, Ukraine.  
[<http://www.franko.lviv.ua/conference/imc>]

## 6-11 October 2002

XII International Symposium on Supramolecular Chemistry (ISSC-XII), Eilat, Israel.  
[<http://chemsg7.tau.ac.il/~issc/>]

## 7-9 October 2002

29th Annual Stanford Synchrotron Radiation Laboratory Users' Meeting, Menlo Park, CA, USA.  
[<http://www-ssrl.slac.stanford.edu/conferences/ssrl29/>]

## 8-9 October 2002

ISGO Workshop "Automation of X-ray Structure Determination for Structural Genomics", Berlin,  
[<http://www.psf.bessy.de/workshop>]

## 10-12 October 2002

2002 ALS Users' Meeting, Berkeley, CA, USA.  
[<http://www-als.lbl.gov/als/usermtg/>]

## 11 October 2002

35th Annual SRC Users Meeting, Stoughton, WI, USA.  
[<http://www.src.wisc.edu>]

## 17-18 October 2002

2nd International Workshop on Radiation Safety at Synchrotron Radiation Sources, ESRF, Grenoble, France.  
[<http://www.esrf.fr/conferences/Radiation-Safety/index.html>]

## 20-24 October 2002

Surfaces nanostructurées: préparation, caractérisation et application, Centre IGESA, Ile de Porquerolles, France.  
[<http://www.crmc2.univ-mrs.fr/conf/nano2002/index.html>]

## 27-31 October 2003

EMAC '03, 7th European Meeting on Ancient Ceramics (Understanding Man through his Pottery), Lisbon, Portugal.  
[<http://www.itn.pt/EMAC03>]

## 2-5 November 2002

Algerian Crystallography Congress 1, Algiers.  
Email: [alcris@usthb.dz](mailto:alcris@usthb.dz).

## 4-6 November 2002

The fourth NOBUGS Conference, National Institute of Standards and Technology, Gaithersburg, MD, USA.  
[<http://webster.ncnr.nist.gov/events/nobugs2002/>]

## 13 November 13 2002

CCG Autumn Meeting "Dealing with Difficult Data", King's College London.  
[<http://bca.cryst.bbk.ac.uk/BCA/CCG/>]

## 2-4 December 2002

Second International Conference on Structural Biology and Functional Genomics, National University of Singapore.  
[<http://www.dbs.nus.edu.sg/structbio/>]

## 5-6 December 2002

21st BESSY Users' Meeting, Germany.  
[<http://www.bessy.de/announcements/>]

## 8-12 December 2002

The Second Pharmaceutical Powder X-ray Diffraction Symposium PPXR-2, Concordville, Pennsylvania, U.S.A.  
[<http://www.icdd.com/ppxrd>]



## 12-14 December 2002

A workshop on the Perspectives in Single Crystal Neutron spectroscopy (SCNS), Institut Laue - Langevin, Grenoble, France.

[<http://www.ill.fr/Events/ONSITE/SCNS/index.html>]

## 19-21 December 2002

3rd WSEAS International Conference on Mathematics And Computers in Biology and Chemistry (MCBC 2002), Puerto De La Cruz, Tenerife, Canary Islands, Spain.

[<http://www.wseas.org/conferences/2002/tenerife/mcbc>]

## 20-27 January 2003

International school on crystal growth of technologically important electronic materials (ISCGTIEM), Mysore, India.

[<http://www.semiconductors.co.uk/iscg-tiem/>]

## 22-25 January 2003

2nd Workshop on Dynamics in Confinement</A>. Institut Laue Langevin, Grenoble.

[<http://www.ill.fr/Events/ONSITE/confit2003/confit.html>]

## 14-17 April 2003

BCA Annual Meeting, University of York,

[<http://bca.cryst.bbk.ac.uk/BCA/meets/BCAs.html>]

## 4-15 June 2003

High Pressure Crystallography Erice, Italy.

[<http://www.geomin.unibo.it/org/verice/highpres.htm>]

## 22-27 June 2003.

The 12th International Conference on X-ray Absorption Fine Structure (XAFS 12), Malmö, Sweden.

[<http://xafs12.maxlab.lu.se/>]

## 26-31 July 2003

American Crystallographic Association Annual Meeting, ACA 2003, Cincinnati, Ohio, USA.

[<http://www.hwi.buffalo.edu/ACA/ACA-Annual/futuremeetings.html>]

## 10-13 August 2003

Australian Crystallographic Association '03/Crystal-23, Cable Beach Club Resort, Broome, WA, Australia.

[<http://www.crystal.uwa.edu.au/CrystalsDownUnder/>]

## 14-15 August 2003

Workshop on Biological Structure, Cable Beach Club Resort, Broome, WA, Australia.

[<http://www.crystal.uwa.edu.au/CrystalsDownUnder/>]

## 14-19 August 2003

Sagamore Meeting (IUCr Commission on Charge, Spin and Momentum Densities), Cable Beach Club Resort, Broome, WA, Australia.

[<http://www.crystal.uwa.edu.au/CrystalsDownUnder/>]

## 24-30 August 2003

21st European Crystallographic Meeting, Durban, South Africa.

[<http://www.ecm21-africa.co.za/>]

## 2-6 September 2003

ECNS 2003 European Conference on Neutron Scattering, Montpellier, France.

[<http://www.sfn.asso.fr/>]

## 3-7 September 2003

Fifth International Conference On Molecular Structural Biology, Vienna, Austria.

[<http://pharmchem.kfunigraz.ac.at/icmsb2003/>]

## 8-13 September 2003

Aperiodic-2003, Belo Horizonte, Brazil.

[<http://www.fisica.ufmg.br/~ap2003/>]

## 10-21 June 2004

Polymorphism : Solvates and Phase Relationships. Erice, Italy.

[<http://www.geomin.unibo.it/org/verice/bernstei.html>]

## August 2005

XX Congress of the International Union of Crystallography, Florence, Italy.

[Carlo Mealli, email: [mealli@fi.cnr.it](mailto:mealli@fi.cnr.it)]

## *Corporate Members*

Anachem Ltd	International Centre for Diffraction Data
Astex Technology	Oxford Cryosystems
Bede Scientific Instruments Ltd	Oxford Diffraction
Bruker/Nonius	Philips Analytical
Cambridge Crystallographic Data Centre	Rigaku MSC
Hampton Research	

## *BCA Corporate Membership*

The BCA values its close ties with commercial companies involved with crystallography. To enhance these contacts, the BCA is pleased to announce that they are now offering Corporate Membership.

Corporate Membership is available on an annual basis running from 1 January to 31 December and includes the following benefits:

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

*The cost of this membership is £600.00 per annum*

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

BCA Administrative Office  
Northern Networking Ltd  
1 Tennant Avenue, College Milton South  
East Kilbride G74 5NA

Phone 01355 244966  
Fax 01355 249959  
e-mail [bca@glasconf.demon.co.uk](mailto:bca@glasconf.demon.co.uk)

International Centre for Diffraction Data



**More Data** *PDF-4/Full File 2002*  
The Powder Diffraction File

**More Savings**

**More Software**

**More Capability**



*“More with PDF-4”*

The PDF-4 product line offers total pattern analysis with unprecedented power to do full data mining with Boolean searches of all data fields.

**Features**

**Over 136,500 entries (114,500 inorganic & 24,100 organic)**

**Lower cost per pattern**

**Integrated retrieval and full pattern display software**

**Awesome data-mining capability:**

**Search 31 separate diffraction and physical properties**

**56,781 entries with searchable  $I/I_c$  for quantitative analysis**

**Over 49,000 calculated patterns that can be calculated on-the-fly into “total reference patterns”**

**Over 87,000 experimental patterns (with fully digitized patterns)**

**Ambient/non-ambient search capability**

**Empirical formula searches with results sorted in pseudo phase diagram order**

**Pearson Symbol Code sort capability**

**Built-in context-sensitive & indexed HELP documentation**

**Extensive bibliographic references**

**Highest standards for accuracy and quality**



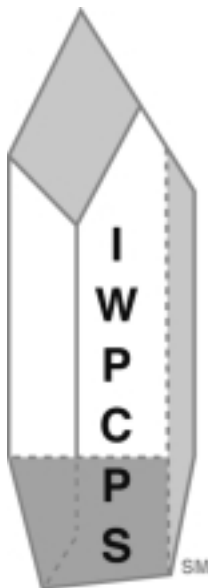
**VISIT US AT**

**[WWW.ICDD.COM/PRODUCTS](http://WWW.ICDD.COM/PRODUCTS)**

**PHONE: 610.325.9814 FAX: 610.325.9823 INFO@ICDD.COM**



The ICDD logo is registered in the U.S. Patent and Trademark Office.  
Powder Diffraction File is a trademark of the JCPDS—International Centre for Diffraction Data.



## Third International Workshop on Physical Characterization of Pharmaceutical Solids<sup>SM</sup>

IWPCPS<sup>SM</sup>-3

[www.assainternational.com](http://www.assainternational.com)

June 9 - 14,  
2002

Leading professionals will present current industry information and explore analytical approaches to characterizing a solid. Workshop participants learn how these approaches can complement each other and be utilized individually or in concert to solve real problems. This is the third year for IWPCPS<sup>SM</sup> and is the only workshop of its nature worldwide. Brand new session topics are geared to keep attendees at the leading edge of solid-state chemistry.

### **The Preliminary Workshop Topics\* include:**

A Modern Pharmaceutical Solids State Laboratory	Polymorphs and Solvates
Solid State NMR Applications	Special XRD Applications
Amorphous Content - Determination And Characterization	Modern Thermal Analysis Applications
Morphology And Surface Characterization	Drug Product Characterization
Characterization And Control Of Dissolution & Bioavailability	Supercritical Fluids (Particle Design)
Expert Systems For Formulation Design (Informatics ñ Particle Engineering)	Regulatory Patent Issues
Novel Technologies for Assessing Bulk Physical Properties	Screening and On-Line Technologies

### **Keynote lectures\* are given by recognized experts including representatives of:**

Aventis Pharma, France	AstraZeneca, Sweden and UK
Boehringer Ingelheim Pharmaceuticals, Inc., USA	Boehringer-Ingelheim, Germany
Bruker-AXS, Germany	CCDC, UK
CRIT Pharma, France	DuPont Pharma, USA
GlaxoSmithkline, UK and USA	Hecus M. Braun, Austria
Merck&Co, USA	Merck Frost, Canada
Monash University of Melbourne, Australia	Pfizer, UK
Purdue Pharma, USA	Threlfall Associates, UK
Toho University, Japan	University of Belfast, Ireland
University of Bradford, UK	University of Leeds, UK
University of Minnesota, USA	UMIST, UK

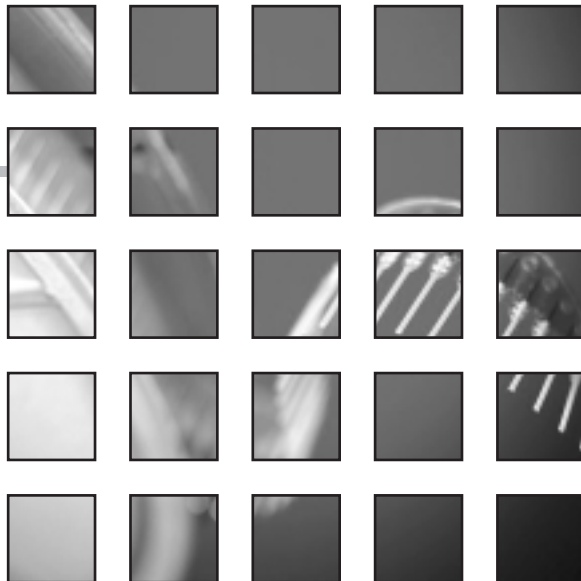
Find more information about the workshop, scheduled speakers and abstract submission as well as online registration at [www.assainternational.com](http://www.assainternational.com) or contact us at [workshops@assainternational.com](mailto:workshops@assainternational.com).

Tel: +1-203-312-0682 or +1-610-942-0261; Fax: +1-203-312-0722 or +1-610-942-0983 \*Topics and lectures subject to change.



TTP LABTECH

## accurate pipetting down to 50 nL



■ with the mosquito automated liquid handling system, crystallographers can now dispense volumes down to 50 nL to set up hanging or sitting drop experiments.

using innovative positive displacement technology, mosquito can pipette proteins and liquors with ease - irrespective of viscosity, surface tension etc. zero cross contamination is guaranteed by mosquito's unique bandolier of disposable pipettes.

to find out more call TTP LabTech on 01763 262626 or email [sales@ttplabtech.com](mailto:sales@ttplabtech.com) ■

TTP LabTech Limited  
Melbourn Science Park  
Cambridge Road  
Melbourn, Royston  
Herts, SG8 6EE, UK

Tel: +44 1763 262626  
Fax: +44 1763 261964  
Email: [sales@ttplabtech.com](mailto:sales@ttplabtech.com)  
Web: [www.ttplabtech.com](http://www.ttplabtech.com)

mosquito. no time washing, no time wasted