ISSN 1467-2790

CRYSTALLOGRAPHY NEWS

British Crystallographic Association

No.84 March 2003

BCA Spring Meeting - York 2003
Software patents and Crystallography
CCP4 Meeting and BSG School

Charging for Crystallography Services
Synchrotron Radiation School
Book Reviews

QUARTERLY





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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 electronically as MSword documents (any version - .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (e.g. awards, honours, retirements etc.), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews. Please ensure that items for inclusion in the **June 2003** issue are sent to the Editor to arrive before **2nd May 2003**.

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President's Remarks

Cover pictures left to right:

Now where on earth can this be?
Apostolic Succession at CCP4
Chemical Crystallographers Coping
Plumbing at Daresbury Laboratory
Waterfront Crystallography in Bristol

Doesn't time pass quickly when you are having fun? When I took over as President nearly three years ago, Mike Glazer warned me that the quarterly 'From the President' column for this newsletter could be a problem especially finding a topic. Now this is my last one, and things have been moving so fast both in crystallography in general, and the BCA in particular that I have had no difficulties with things to talk about.

The Newsletter Editor suggests that I use this last column to look back on my term as President. This is not my style, but there have been a lot of changes in this period. In the past three years we have radically changed the format of this Newsletter to better display our many activities to as wide a public as realistic; we now have Corporate members; the Spring Meeting is changing to be shorter and more concentrated - for better or worse reflecting the busy times we live in. We are a professionally run organisation, something we now take for granted, but Northern Networking provides us with a very high standard of support, something that we also now take for granted.

Crystallography too has not stood still: the explosion of crystal structures arising from developments in technology - CCD detectors, bigger and better synchrotrons etc., developments in structure solution from powders (Who would have thought that we can now solve structure routinely from molecules with over 50 non-hydrogen atoms?), bigger and bigger proteins. It is all very exciting, and I know the BCA and its members have played their part. We will also be getting a UK 4th generation synchrotron. This was not always well handled on the political front, but we should not lose sight of what a boon this will be to UK crystallography.

One thing does need saying, however: it has been a pleasure and privilege to work with the BCA Council, and BCA members. Council is a hardworking, committed bunch of individuals, and we are lucky to have them in the BCA.

Finally, looking forward, in my last column I mentioned the possibility of Foundation Members of the BCA, and asked for comments from members. Uniquely, the result was complete silence.

Crystallographers are not known for their silence. I guess that this signifies some sort of consent. We will discuss it at the AGM at the York Spring Meeting. I trust you will be there?

Chris Gilmore
February, 2003

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

A happy, if somewhat late, New Year to all! This issue looks forward to the Spring Meeting, most of the details of which appeared in December, but the programme, as up-to-date as I could get it, is summarized in the centrespread of this issue. Keep tuned to the website for up-to-date information. As a result of the meeting being so late, we have decided to publish the June edition a little later, so that we can get reports of the meeting in. Unlike last year, there will be changes in the officers of the society, and the two candidates who have so far declared themselves ready to stand (run?) for President have produced election addresses. I should like to take the opportunity of expressing my gratitude to our outgoing President for his excellent leadership. Personally, I thank him both for persuading me to take on the Editorship of Crystallography News, and for being very supportive. The "From the President" column always arrived without fail from one part of the globe or another, and has always been good reading.

I am particularly grateful to those who have reviewed books, and we have another good crop of reviews in this issue. Special mention should be made of the new IUCr pamphlets, reviewed by Marjorie Harding. There are now 22 of these, covering a wide range of topics, and they are essentially free for the printing. There should be more reviews in the next issue, and I hope that readers find these valuable.

Sadly, there are two deaths to report, that of Professor Harold (Hal) Taylor, formerly of the University of Aberdeen, and that of Dr Robertson of the University of Leeds. Obituaries for both of them will appear in the June Issue. As this is the 100th anniversary of the birth of Kathleen Lonsdale, Mike Glazer has agreed to write a memorial article about her, which should also appear in June.

As the President remarks, crystallography is not standing still! Some of the progress brings extra headaches, though. Lachlan Cranswick has submitted an article on the fascinating (and murky!) subject of "idea patents". His full composition is available on the Web, but the brief summary in this issue should show that it is not merely a legal curiosity! Georgina Rosair's survey of how "service" crystallography is done will hopefully get more groups to respond to her questionnaire. Many of our readers will also want to take a look at "Data Overload", by Andrew Bond and John Davies on page 44 of the January edition of *Chemistry in Britain*.

As usual, I hope that more of you will read the note on page 1 encouraging you to write something, preferably before 2nd May 2003. Please do, and please send some pictures if possible, they really help to "make" the magazine. And a final note of warning - my family decided that it was time I got a digital camera at Christmas, and while I don't expect to operate in the Bill Duax league, it will be with me at any meeting I attend!

Bob Gould
March, 2003

Acknowledgements BCA Sponsors

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

The potential power of 'Software Patents' to destroy Crystallographic Software; Crystallographic Software Development; and Crystallography's Future

(The full text of this summary is available on the web at the BCA website via: http://bca.cryst.bbk.ac.uk/bca/cnews/xtlnews.htm or at the CCP14 site via: http://www.ccp14.ac.uk/maths/software-patents/. This short version omits most of the references, and much of Lachlan's inimitable style! *Editor*)

The main principle behind patents is not that of protecting inventors. The original aim was to ensure technological advances and their propagation by encouraging the publication of knowledge. Patents are meant to confer a social benefit by allowing a short-term ownership of an invention, after which it becomes part of the public domain. Protecting the inventors via the use of patents is a means to that end. The problem with the stereotypical Software Patent is that it tries to patent "an idea" rather than "an invention". Such patents give holders the right to restrict your ideas if your ideas too closely resemble theirs. This is different from copyright, which prohibits you from *copying* someone else's ideas, but lets you *express your own.* In principle, Software Patents can apply to any piece of scientific knowledge that is algorithmic in nature (e.g., the ideas as implemented within crystallographic software). This would allow the owners of the ideas within a Software Patent to restrict the spread of "similar" ideas via the legal tool of pursuing patent infringement actions against offenders.

Originally, the US Patent Office did not recognise Software Patents. They were considered "ideas", not "inventions", but by the early 1990's, due apparently to overload and lack of expertise, the Patent Office began to pass them, no matter how trivial or how absurd. In Europe, at present, Software Patents are "officially" considered invalid. The European Patent Office does not recognise "discoveries, scientific theories and mathematical methods" as being patentable. So, until recently, Software Patents were largely irrelevant to European crystallographers. But recently, computer programs have begun to be patented, and there is a move to change patent law to make this practice standard. Meantime, the US Trade Representation Office has sought to get other countries' laws into line with American practice, which might result in our suddenly finding European software and "ideas" infringing against an avalanche of US Software Patents.

One problem is that many of the new patents routinely patent the trivial, but describe their claims in complicated "patent speak". An example, involving software to download music, contains the "innovative" phrase: *"choosing at least one pre-selected portion of the pre-recorded music products from the central host server."* This apparently means *" clicking to say which link to follow."* And put that way, it hardly seems novel!

The main practical rationale behind patents is to help justify and protect the often extremely high costs of research and development for new inventions. In this manner, patents exist to help encourage "innovation". There is a large range of complicated software projects (Operating Systems, Office Suites, Graphics Suites, etc), involving many years and much expense to create, which in general have been able to develop and thrive without the protection of patents (though they have been protected by Copyright and Trademarking).

Software Patents have been causing a goodly amount of mayhem in the non-crystallographic world, with effects that can go beyond their initial US jurisdiction. The litigation is spreading fast. Multi-Tech Systems has just sued the three leading PC makers, Compaq, Dell and Gateway, over patents on transmitting data over a communications line. A St. Louis patent broker is suing Yahoo over a "*method of effecting commerce in a networked computer environment in a computerized system*" - *that is, shopping on line!*

At this point, we will create a hypothetical, "fantasy" example of Software Patents which could be applied to scientific crystallography. Let us look at the Crystals structure refinement suite as developed by the Chemical Crystallography Laboratory of

Oxford University (http://www.xtl.ox.ac.uk/crystals.html). In reality, Crystals is copyrighted “2002, Chemical Crystallography Laboratory, University of Oxford, UK”. Under this copyright, it is a set of ideas as implemented in software - a work of art. There is legally nothing to stop anyone else implementing similar ideas and similar works of art; such as Shelx, NRCVAX, GX, CAOS, Xtal, DS*System, etc. However, what would happen if the ideas based in the Crystals software were protected by Software Patents? Any program doing anything too similar (i.e., crystal structure refinement, which - depending on how the Crystals Patent was written - may or may not be limited to the use of Least Squares, and possibly be inclusive of any diffraction phenomena) would now be potentially infringing the Crystals Patent. The owners of the Crystals Patent could then have the option of acting against this infringement of their intellectual property; and thus let loose the dogs of law on, say, the author of a powder diffraction refinement program. A possible result would be that crystallographers with ideas similar to the Crystals Patent start seeking safer work in different careers, or become bankrupted by the legal proceedings against them. What if any of these software authors ever admitted in their software manuals to using even just one of the ideas of Watkin, Prout, Carruthers, Betteridge or Cooper as implemented in Crystals? Under copyright laws, this is not a legal problem, and it is normally considered laudable to acknowledge sources of ideas. But under patent laws, it would be a naïve, printed confession that will make the jobs of lawyers administering the Crystals Patent much easier.

As a real world example of Crystallographic “Patent Speak”, US Patent 6,192,103 “Fitting of X-ray scattering data using evolutionary algorithms”, issued on February 20, 2001, states::

“The present invention relates to X-ray metrology, and more particularly to the fitting of simulation models to X-ray scattering data for the purpose of determining parameters that characterize the structure of a material being tested.” . . . “Examples of these methods include X-ray absorption, diffraction, fluorescence, reflectivity, scattering, imaging and fringe analysis. In the context of the present invention, the term "X-ray scattering" is employed as a generic term which collectively encompasses any known X-ray technique that is applied to materials characterization.”

It is not unreasonable to expect the Crystals Patent would have been written to be as all encompassing as possible. And there are many real examples relevant to crystallography. For example:

US Patent 5,249,137 (to Xerox Corporation)
US Patent Title: Computer-aided chemical illustration system
Date of Patent: September 28, 1993
Abstract: A computer-aided chemical illustration system is disclosed. Techniques provided include: 1) efficient drawing of bonds; 2) drawing different bond types during a single mode; 3) determining bisect angles for bonds; 4) labeling atoms on the fly; 5) automatic alignment of atom labels; 6) custom alignment of atom labels; 7) changing the type, style, or orientation of an object while it is being drawn; 8) detection of ring structures; and 9) shifting bonds around on a ring.

Have you ever done anything like that? Fourteen further examples of similar patents will be found in the full article. Furthermore, not all patents are used actively; sometimes they are stored up rather like secret weaponry for a suitable occasion! Might your macromolecular software be doing any protein modelling? Then it could be infringing US Patents 5,884,230 and/or 5,557,535, both titled “Method and system for protein modeling”. Might it be generating electron density maps? If so, it might be infringing on US Patent 5,200,910, “Method for modelling the electron density of a crystal”.

Active politicking and activity against software patents of this type has claimed some effect on governmental decision makers. The “Petition for a Software Patent Free Europe” is available via the web (http://www.noepatents.org/) of which the present number of signatures (Sep 2002) are 125,390. People can still sign via the web as well. The other main anti-Software Patents site in Europe is the EuroLinux Alliance (http://eurolinux.ffii.org/).

According to the US Patent Office website, there are options for requesting "reexamination" of a patent in terms of its validity. Be wary that in searching for US Patents, the present default US Patent Office web interface searches the years of 1996-2002. To search all years, you have to click on the list box "Select Years", and select "All years". If you don't do this, patents prior to 1996 will not be found and listed.

While nearly all the above information concentrates on using the US Patent system for patent searching, this would miss other Crystallographic Software Patents issued via the European Patent Office though at present, EPO Software Patents would most likely be found to be invalid if challenged. The European Patent Office website seems to offer the best Internet method for finding out more: (http://ep.espacenet.com/), but personal experience of using the EPO website is that it is very inferior to the US Patent Office web interface in terms of being able to search and find relevant patents. It can often be quite neurotic and return zero matches even if you know the Patent Number, title or authors.

This article asserts the opinion that Software Patents (i.e., the patenting of "ideas") are a "Clear and Present Danger" to Crystallography, and the Crystallographic software that makes it function and progress. The author is not a legal expert, so it would not hurt to validate the above via other means, which is why web links and key words are given at every opportunity.

Given that "forewarned is forearmed", it is the author's option that Software Patents are, at minimum, an issue that crystallographers and anyone using the fruits of the ideas embedded in software need to be aware of.

Lachlan Cranswick

Diamond Update - Small Molecule Single Crystal X-ray Diffraction Beamline Proposal Passes Stage 1

An initial outline proposal for a dedicated small molecule single crystal X-ray diffraction beamline at the Diamond synchrotron was submitted in early November. BCA members and the whole of the single crystal community will be pleased to know that shortly before Christmas the Diamond Scientific Advisory Committee (SAC) announced that the proposal had been selected to go on to the second stage of the selection process, along with eight other proposals covering techniques from infra red microspectroscopy to EXAFS. It is expected that four of these proposals will be selected as Year-3 beamlines with a projected date for their operation of 2008.

The next stage of the selection process involves the submission of a full proposal outlining both the specifications of the beamline and the areas of science to be undertaken. Expressions of interest from the diffraction community have been requested from the Diamond SAC. The deadline for the submission of the full proposal, incorporating the expressions of interest, is 7th March, 2003. The proposal is being co-ordinated by a working group consisting of

Professor Bill Clegg
(Newcastle/Daresbury Laboratory)
Dr Jacqui Cole(Cambridge)
Professor Russell Morris (St. Andrews)
Professor Paul Raithby (Bath)
Dr Simon Teat
(Daresbury Laboratory)
Professor Chick Wilson (RAL)
Dr Claire Wilson (Nottingham)

with the help of the crystallographic community. Areas of science highlighted in the proposal include 'excited state' crystallography, charge density investigations, anomalous dispersion studies, molecular disorder and its relationship to physical properties, dynamic structural changes, and the probing of the structures of materials that give only small weakly diffracting crystals.

The proposals will be considered by the Diamond SAC, and there will be a public presentation of each of the beamline applications at the Rutherford Appleton Laboratory on 20th May. A final decision on the proposals will be announced in July.

The latest details of the progress of the single crystal proposal will be announced at the Diamond Special Interest Group (SIG) Meeting that is scheduled to take place at 12 noon on Thursday 17th April, 2003, at the York BCA Spring Meeting.

Paul Raithby
Co-ordinator BCA Diamond SIG

CCP4 Study Weekend 2003 University of York, 3-4th January 'Experimental Phasing'

This year's meeting was special in several ways. It is 25 years since the foundation of CCP4, with many of the original founders still very active and indeed integral to the success of the project. The Study Weekend has grown over the last few years to a meeting of over 400 people, with the twin functions of introducing the current generation of students to aspects of the programs, and of providing leading edge speakers on the chosen topic. This year the excellent programme of speakers was organised by Airlie McCoy (Cambridge) and Neil Mc Donald (London).

Airlie with Guy Dodson

Neil with Eleanor Dodson

The Chairmanship of CCP4 is an unpaid position held by a leading UK academic, and elected by Working Group One (academic group leaders). The retirement of Neil Isaacs from nine years of service to the community in this capacity was marked by a series of tributes to his excellent leadership, in a period which has seen major growth and changes. The reins were handed over to Jim Naismith, who presented Neil with an engraved quaich and a bottle of the 'Water of Life', a token of our gratitude.

He thanked Neil for his outstanding service to the UK community, leaving us with a debt of gratitude we owe Neil.

Christine Cardin

Bars, the boring sort

That's what Mike Hart called them in his reply to the matter that Howard Flack raised in the last issue (CN 83, p 40), namely how to get those bars into space-group symbols using Microsoft Word. Mike's solution was to use the equation editor, the problem with which is that not all versions have it, and it in effect fills your document with tiny pictures. I also had some adventures with his elegant examples as I moved them from my mail to another document.

A more ingenious method was suggested by Neil Oxtoby. As he puts it:

It is possible to raise any character over any other character without using the equation editor or resulting in unwanted space in front of a symbol.

Unfortunately this method results in increased space above the edited line.To do this in word type the phrase you wish to edit, e.g. P-1. Then select the character you wish to raise and then go to format and font and then character spacing. Change the spacing box to 'condensed' and then the adjacent box to the font size you are using. Also change the position box to 'raised' and then the amount raised needs a little trial and error - I have found about 7pt works well with 12 pt font.

I've tried this, and it works pretty well, providing you use the "long" dash rather than the normal short one. It has the advantage that other symbols than "minus" can be treated this way, but a serious drawback in that it does put a blank space above the line.

Bill Clegg's solution seems to be the best: It uses the "offset overstroke":

It is available as character number 96 in the Symbol font (use Insert-Symbol from the menus, or set it up as a keyboard shortcut). However, it leaves an undesirable space in front of it. To get rid of this, select the previous character (e.g the P in the symbol for space group number 2, "P-bar-1"), and apply Format-Font-Characterspacing; Condensed by 6 pt. Hey presto!

This works well for spacegroup symbols, but is rather clumsy for producing bar-h-bar-k-bar-l, for example. Anyway, I'm not going to show this, because who knows what would happen to any of these things when our printers take them over to their Macs! I think that a general solution to this problem remains in the future. Many thanks to all who expressed an interest in this fascinating topic! To give Mike Hart the last word: "Clumsy, of course, but we expect that from B*ll G*t*s, don't we!?"

The Editor

News Items

Royal Society Fellowships

The Royal Society has secured extra funding from the Government's Spending Review to expand its schemes to help women in science.

1. A Relocation Fellowships scheme will be set up to help excellent scientists to move to a new post, if their spouse or partner is moving their workplace beyond a reasonable commuting distance.These awards, from 2004, will provide salary and research expenses for up to two years.

2. The Society will increase the number of Dorothy Hodgkin fellowships from 2004-5. This scheme, introduced in 1995, is aimed at researchers who have recently completed their PhDs, providing a full salary and research expenses, on flexible terms, to allow career breaks and part-time working, also mentoring. About 80% of applicants have been women.

The Royal Society will receive an extra £31.8m in 2004-5 and £33.2m in 2005-6, an increase in support from Parliamentary Grant-in-Aid from £329.245m in 2003-4 to £332.445m in 2005-6.

For more information, look under Media Release on the Society's home page: http://www.royalsoc.ac.uk

Congratulations

Our congratulations to Professor Dame Louise Johnson, University of Oxford, who was made a D.B.E. in the New Year Honours list for services to biophysics.

Congratulations also to Professor G.R. Desiraju, University of Hyderabad, India who was recently elected as a Fellow of the Third World Academy of Sciences (TWAS). TWAS, with its headquarters in Trieste, is an association for the promotion of scientific excellence for sustainable development in the South. 43 new fellows were elected in October 2002, of which 4 were in the area of chemical sciences.

Director of SRS

Hywel Price, Director of Daresbury Laboratory writes:

Professor John Helliwell has decided to step down from the position of Director, Synchrotron Radiation (SR) at the CCLRC - a post he has held since January 2002, on secondment from the University of Manchester. John Helliwell has made a crucial contribution to the CCLRC and in particular to the programme of the Synchrotron Radiation Source (SRS) at the CCLRC Daresbury Laboratory and to SR matters more widely. During this period the legal, financial and construction planning stages of the new Diamond Light Source have been developed alongside planning for the future operation of the SRS. Similarly, the Quinquennial Review of the CCLRC - which was published in April 2002 - led to a number of key changes in the future operation and development of the CCLRC large-scale research facilities. In these areas John has played an important role in establishing the new management arrangements in consultation with the research communities. John has also laid the foundations for a more extensive engagement of the research communities in the future programme for the SRS and, again, for wider SR matters.

The CCLRC will undoubtedly miss the contribution that John has made to its programme since January 2002. The CCLRC fully understands John Helliwell's personal wish to return to a full-time research position at the University of Manchester - and looks forward to welcoming him back in due course as one of the leading UK users of the CCLRC research facilities. John Helliwell will return to Manchester University immediately.

As an interim arrangement I will take over John Helliwell's management role. I will be assisted by Paul Quinn, Pat Ridley, Tracy Turner and a Chairman of one of the science colleges who will form the SRS senior management team. The CCLRC will be seeking a person to lead the SR science programme immediately.

Award for Rigaku-MSC, one of our Corporate Members

Rigaku/MSC is pleased to announce that ACTOR, the world's first commercial robotic system for automated sample handling, was named winner of a 2002 R&D 100 award, which have been called the Nobel Prizes of applied research. The 40th annual competition saw entries from many of the most prestigious companies, research organizations, and universities in the world.

Rigaku/MSC licensed ACTOR, the proven crystal transport, orientation and retrieval technology, from a major American pharmaceutical company. In conjunction with OSS (the designer of the crystal manipulation robot for NASA and the International Space Station), Rigaku/MSC refined the design and function of ACTOR. With its associated sample manipulation and storage tools and automated sample-evaluation and ranking software, ACTOR is a complete system designed to increase productivity and allow for unattended sample analysis for the high-throughput crystallography (HTC) labs of today. ACTOR eliminates many of the time consuming sample manipulation tasks previously required for routine crystal screening and data collection. HTC, once the wave of the future, is available today from Rigaku/MSC.

Astex Technology, Ltd, a British structure-based drug discovery company pioneering the use of

HTC technology for the rapid identification of novel drug candidates, reported the successful collection and subsequent analysis and interpretation of 53 data sets in 3.5 days in a home laboratory using ACTOR and other instrumentation from Rigaku/MSC. Dr. Andrew J. Sharff of Astex said, "Based on a standard working day/week, this represents an increase in throughput of over 3 fold, compared to manual data collection."

Since its inception in Japan in 1923, Rigaku Corporation has been at the forefront of analytical and industrial instrumentation technology. With hundreds of major innovations to its credit, Rigaku and its subsidiary companies are world leaders in the fields of x-ray spectrometry, diffraction, x-ray optics, as well as small molecule and protein crystallography. Rigaku employs over 800 people in the manufacture and support of its analytical equipment. Its products are in use in more than 70 countries - supporting research, development, and quality assurance activities. Through its U.S. subsidiary, Rigaku/MSC, it continuously promotes partnerships, dialog, and innovation within the global scientific and industrial community.

Paul Swepston

Workshop on Magnetic Rietveld Refinement

So what were the hottest tickets in town over the Christmas 2002 holiday period? Ronan Keating live at Wembley? Frank Bruno's triumphant return with Sooty in "Goldilocks and the Three Bears" at the Southend Pavilion? Jerry Springer the Opera? No, despite stiff competition, the award has to go the the "Magnetic Rietveld Refinement Workshop" organised by Paolo Radaelli and co-sponsored by RAL/IOP/PCG, whose 25 places were snapped up within 24 hours of the course being announced.

The lucky delegates gathered at Cosener's house on the 12th of December for what was advertised as an intensive 2 day course on the theory and practice of magnetic structure determination. Day one was taken up with a mixture of lectures on the Shubnikov groups for describing magnetic symmetry by Paolo Radaelli (RAL) and the theory of magnetic structures, their description and determination by Juan Rodriguez-Carvajal (LLB). These lectures were then backed up by an evening practical session determining the possible magnetic symmetries allowed for simple perovskite structures. On day two, these approaches were generalised by Andrew Wills (UCL) who gave a series of lectures on the application of group theory to understanding magnetic structures. This more general approach both reinforced and complemented the first day's work on Shubnikov groups. The rest of day two was taken up with a series of demonstrations and practical classes involving some of the main software packages required for magnetic structure determination: GSAS, SARAh (AW) and Fullprof (JRC). Hearing about the second two packages directly from their authors was particularly informative.

Following an excellent Christmas dinner the true meaning of the "intensive" nature of the course was brought home to everybody, with post-dinner "games" including "Flip the Spin", "Prime the Symmetry Operator" and "Reduce the Representation". It was clear from the number of participants (and tutors) still working away at magnetic refinements at midnight, that people were enjoying the course greatly.

The final morning was taken up with computer-based exercises giving people the opportunity to tackle both test examples and real data they had brought along. This was a rare and valuable opportunity to learn directly from the experts about an area of condensed matter science that is topical, important, and perhaps poorly understood by many. The fight for places on the course and the wide variety of nationalities represented (attendees came from, *inter alia*, the UK, Spain, Finland, Sweden, Japan, Greece, France, Germany) clearly showed the huge demand for a forum such as this. We can only hope that Paolo, Andrew and Juan can be persuaded to make this the first in a regular series of workshops.

John Evans

BCA Biological Structures Group, Winter Meeting 2002 Structural Studies of Macromolecular Assemblies University of Warwick, 13th December 2002

The BSG winter meeting focussed on studies of macromolecular assemblies using X-ray crystallography and cryo-electron microscopy as primary techniques. A wide range of systems, including protein/protein, protein/nucleic acid and membrane protein complexes were covered. More than 70 delegates attended the meeting and we received financial support from 6 sponsors.

The meeting was divided into three sessions. In the first session (session chair: David Roper) Dale Wigley (Cancer Research UK) described both the full length and truncated version of the DNA repair protein Rad52. Whereas the full-length protein had a heptameric, the truncated form showed an undecameric circular structure. In both cases, protein/protein interactions were identical and the DNA could be modelled into the highly positively charged groove around the surface of the complex. Chris Oubridge (MRC-LMB, Cambridge) presented his research on the ternary complex of the bacterial signal recognition particle (srp). He suggested that the initial binding of srp19 to the top of the helices of 6 and 8 facilitated the binding of srp54 to helix 8 of the RNA. Robert Robinson (Uppsala University) described the structure of gelsolin and arp2/3 protein complexes and their highly complicated interaction during the filament formation and protein capping, crucial for cell motility. His presentation featured a number of molecular movies.

After lunch (session chair: Corinne Smith), David Leys (University of Leicester) presented the ternary complex of trimethylamine dehydrogenase bound to two molecules of electron transfer flavoproteins (ETF). The FAD domain of ETF is highly flexible and its role was implicated in electron transfer. Neil Isaacs (University of Glasgow) described the structure of a photosynthetic bacterial core complex. He indicated that protein PufX has a role in exchange of ubiquinone within the oxidised and reduced forms of the reaction centre - light harvesting protein 1, and in the supra-organisation of the complex. So Iwata (Imperial College) gave a comprehensive presentation about the evolution of respiratory membrane proteins. Using the combination of site-directed mutagenesis and crystallography of succinate dehydrogenase, they identified the quinone-binding site to be primarily responsible for electron leakage, causing increased level of superoxide radicals and consequently premature ageing.

After coffee, which included an exhibition and a mini poster session, we enjoyed three talks about larger and lower resolution (cryo-EM) complexes (session chair: Vilmos Fülöp). Ben Berks (University of Oxford) described their ongoing work on the twin-arginine transporter system responsible for transporting fully folded proteins into the periplasm of a gram negative bacterium. Corinne Smith (University of Warwick) talked about using cryo-electron microscopy of clathrin cage complexes to investigate clathrin coat structure to elucidate the structure and mechanism of action of the molecular chaperone, Hsc70 and its co-factor auxilin during vesicle uncoating. The last speaker of the meeting, Robert Gilbert (University of Oxford) described how they used messenger RNA lacking a stop codon to stall the end product release of translation. Using a 13Å resolution electron density map of the working ribosome, they showed that nascent protein started forming at the L1 stalk of the tunnel.

All the talks were extremely interesting and well received by the delegates.

Vilmos Fülöp with contributions from Warwick Protein Structure Group

Report of the 2002 CCG Autumn meeting

The autumn meeting of the CCG was held in the Great Hall of King's College London on 13th November 2002. The topic for the day was "Dealing with difficult data", and the large number of delegates indicates it was a popular choice of topic.

The first speaker was Simon Parsons of the University of Edinburgh who spoke on "Difficult Refinements: an Overview". He highlighted the most common problems that may beset a crystal structure including poor data to parameter ratio due to weak or incomplete data, disorder, pseudosymmetry, twinning, poorly defined parameters and incommensurate phases. The particular problems of twinning, poorly defined absolute structure and incomplete data were highlighted. Non-merohedral twinning may arise when extra symmetry occurs in a supercell and there may be overlap of diffraction spots in some regions of the diffraction pattern. The program ROTAX may be used to determine a twin law. An example of a multi-domain twin model used for the structure of $V(NEt_3)_4$ was described, where the final model was of a 3 domain twin, and the accuracy of the twin model used was confirmed by noting that the predicted spots of the three matrices overlap with all measured diffraction spots. The Flack parameter is a twin scale factor for an inversion twin. Flack requires a standard uncertainty of 0.1 before any conclusion can be drawn regarding the absolute configuration; this is, however, difficult to attain for structures containing only light atoms. Simon described using multiwavelength (Mo + Cu + Cr) refinements to try to improve the precision of the Flack parameter. This was found to give only a marginal improvement due to incompatible absorption corrections. By measuring Friedel opposites at different wavelengths in such a way that the absorption effects are the same, and applying restraints, they were able to obtain meaningful Flack parameters for light atom structures. Poor completeness of high pressure data sets was introduced with reference to Alice Dawson's talk later in the day.

Simon Coles, of the EPSRC National Crystallography Service based at the University of Southampton, spoke on "Getting Good Data from Bad Crystals", and focussed on sample preparation and handling, data collection instrumentation and processing. Clues that a crystal is imperfect may come from optical microscopy, where inclusions or external twins are visible, while polarising light may reveal internal twinning, and also from the diffraction pattern. For instance crystals with anisotropic mosaicity will show streaking in their diffraction, while split crystals will have irregular groupings of diffraction spots and irregular spacings on lattice lines. The presence of disorder can be indicated by weak diffraction at high angle and diffuse scattering at low angle. Tails on spots, satellites, bizarre groupings or irregular spacings of reflections on the same lattice line may indicate twinning. External twins or clusters of crystals can be cut up while the crystal is viewed in polarised light. Simon stressed that the best approach is often to try to obtain a better sample by recrystallisation. Hints for successful recrystallisation included using H-bond acceptor solvents, taking your time, and operating on a small scale. Other methods for crystal growth were also discussed, such as using thermal gradients, diffusion and cocrystallisation. He referenced websites with advice for crystal growing: www.chem.wisc.edu/~powell/xtalgrow.html; www.cryst.chem-uu.nl/growing.html; www.xray.ncsu.edu/GrowXtal.html. He also stressed the importance of ensuring that your diffractometer is properly aligned and the use of advanced software for dealing with multi-component systems such as Ndirax.

Adrian Parkins of King's College described "A Poor Man's CCD". Stan Nyburg at King's College has taken a 1960's vintage Picker four-circle diffractometer and replaced the scintillator detector system by a Photonics Science CCD. A monochromator has not been fitted, Zr-filtered Mo radiation is used. Crystal rotation and shutter control is via a simple Quickbasic programme.

The first speaker after lunch was David Watkin from the

A few adjustments had to be made...

University of Oxford on "Weak Data can still be Good Data". David started by noting that CCD detectors have revolutionised small molecule crystallography. Crystal size is no longer such an issue and absoption/scaling programs such as SADABS can cope well with large crystals. He described a series of data sets from a tetraphenylene crystal that were collected at the recommended exposure time, a slow exposure time, a fast and a very fast exposure time. It was found that there was very little difference between the structures obtained for the slow, recommended and fast exposure times. For the very fast data collection, where observed data was only marginally stronger than absent data, the structure was solved by cutting off the weakest data. There was very little difference of chemical relevance between the structures derived from the very fast data set and the stronger data sets; however, as the speed of the data collection increases Ueq increases. David suggested that we could be doing 10-12 data sets a day, but people aren't doing this as they don't have the capacity to process the data. He went on to describe trashing the very fast data set by randomly perturbing the data, computing new observed intensities, or deleting half the data. In each case, the relevant results of the refined structures (*e.g.* C-C bond lengths) were good. He concluded that random errors were less damaging to a refinement than systematic errors and that having high redundancy is a good safeguard against errors.

Sandy Blake of the University of Nottingham spoke next on the topic "Are Difficult Structures Difficult to Publish?". Limitations of the crystal can propagate into a refined structure, so how can we convince people that the structure is worth publishing? There may be a number of problems such as missing hydrogen atoms, disorder and partial occupancies, twinning, large residuals and significant voids. In reporting the problem, it is important to identify it, describe the action taken, and describe the outcome. While crystallographic and chemical journals have different requirements for reporting structures, we should ensure that any one who reads the paper is aware that there was a problem.

The University of Durham's Mike Probert presented a case study "To Collect or Not to Collect - That is the Question". Mike was faced with crystals of (S)-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1-(N,N-diisopropyl) ferrocene carboximide which failed to index under normal conditions, despite their good appearance. After examining seven crystals on a Friday night

...but the food was outstanding!

he collected the data. Split diffraction peaks revealed twinning, and Mike described his successful disentangling of the twinning using the Gemini program, and the subsequent solution and refinement.

Afternoon tea was followed by Jonathon Charmant of the University of Bristol presenting "Small Molecule Crystallography on a Big Molecule Diffractometer". A diffractometer fitted with a rotating Cu anode generator, beam focusing optics and a large format CCD area detector has recently been installed at Bristol. Results show that small molecule samples that might otherwise be earmarked for synchrotron study can be successfully studied on a machine of this type. Jonathon described a number of hydrogen bonded network structures of anionic coordination complexes and organic cations where only very small crystals (eg 60 x 60 x 20 microns) were obtained, but could be studied successfully with this diffractometer.

The final speaker was Alice Dawson of the University of Edinburgh, whose topic was

"Difficulties in High Pressure Data Refinement". Diamond anvil cells may be used to put crystals under up to 150kbar of pressure; they make data processing and refinement very challenging, however. The diamonds used to apply the pressure diffract strongly, in addition to the beryllium used as X-ray windows, making the obtained diffraction pattern a mixture of that of the sample, diamond and beryllium. Also, access to reciprocal space is severely limited by the steel body, a problem exacerbated by the low symmetry of the majority of samples under study. The high pressure structures of acetic acid and $Ti(OiPr)_4$ were presented, and problems with peak overlap, data to parameter ratios and ADP's blowing up were highlighted.

This has been the largest attendance at a CCG Autumn meeting to date, and many people must be thanked for their contributions to a highly enjoyable, informative and successful day. Thanks must go to the local organisers Jon Steed and Jamshed Anwar, ably assisted on the day by Dave Turner and Carl Wallis, the session chairs Paul Raithby, Sandy Blake and Jon Steed, all the speakers and to the organising committee. Extra thanks must also go to Bruker-Nonius for generous sponsorship and to Pfizer Ltd for sponsorship that allowed for free registration of all student participants.

Michaele Hardie

PCG Autumn Meeting

This autumn's PCG meeting was held on December 11th at the University of Edinburgh on the topic of "Complementary Methods for Crystallography". Thanks to generous sponsorship from the Edinburgh Physics department and the PCG this has to qualify as the best value meeting of 2002 - combining free food, free registration and an excellent programme of scientific presentations.

Dave Allan and Pam Thomas had put together an impressive line up of speakers, with each talk emphasising a different experimental technique that can provide information additional to diffraction data, information which can often be crucial in solving otherwise intractable structural problems. Stewart Clark from Durham started the session off with a presentation entitled "Calculating the Structural and Electronic Properties of Materials", taking the audience from "primary school" quantum mechanics through to state-of-the-art DFT calculations for periodic systems. Stewart stressed the importance of generating a "Crystallographic Computational Toolbox" especially as computers become cheaper year on year while experiments become more expensive! It was instructive to hear both the strengths and limitations of such calculations, and the importance of basic structural information in guiding the theorist. The rapid progress of this type of calculation from problems containing 10's of atoms a few years ago to 100's of atoms of today, and the promise of tackling still bigger problems in the future was particularly impressive.

Paul McMillan's (UCL/RI) presentation on the high pressure structures of Ga_3N_4 followed on naturally from Stewart's introduction, emphasising the dual role of theoretical calculations and experimentation in understanding the pressure-temperature behaviour of these exciting materials. Paul showed how an elegant combination of high pressure synchrotron X-ray and Raman studies have been crucial in unravelling the key structural changes in the system. The complementarity of different techniques was brought home by the fact that the number of Raman lines seen for the high pressure form of this material showed immediately that the true unit cell had to be larger than was observed by X-ray diffraction studies, in this case revealing a subtle incommensurate superstructure.

The different length-scales of different techniques were also addressed by Mark Smith (Warwick), Stephen Blundell (Oxford) and Ian Reaney (Sheffield). Mark emphasised how the local structural probe provided by solid-state NMR studies provides a wonderful tool to study both crystalline and disordered materials. He gave an extremely clear overview of the information NMR can bring to bear on structural studies and how improvements in sample spinning speed and magnetic

field strength mean that even difficult nuclei such as titanium can now be studied. Particularly impressive was a recent ^{17}O DOR study on Ferrierite by Bull and co-workers in which the 10 crystallographically unique, though chemically similar, O environments in the structure could all be resolved (L.M. Bull *et al.*, *J. Am. Chem. Soc.*, **2000**, *122*, 4948).

Stephen Blundell gave an excellent overview of a different local probe - the muon. Although each us of apparently receives up to 10 muons per minute hitting our fingernails from cosmic rays, muon spin rotation spectroscopists require slightly higher fluxes, and frequent pulsed neutron sources such as ISIS where approximately 1% of the proton beam is used to produce muons (that's where all the neutrons get lost!). In contrast to scattering techniques, muons are implanted in a material (one plays darts rather than squash) where their precession round magnetic moments and the resulting anisotropy of positron emission gives an extremely sensitive magnetometer capable of measuring local fields. The consequent ability of muons to differentiate, for example, a uniformly weak magnetic sample from a non-magnetic material with small magnetic impurities, and to detect phase segregation in manganites provide wonderful examples of the muon's ability to provide otherwise inaccessible information.

Ian Reaney's talk on the applications of electron diffraction emphasised again the importance of probing different experimental length-scales to those observed using X-ray or neutron diffraction. In the perovskite materials Ian discussed, short range order and defects are often of crucial importance in determining the functional properties of the material. His example of the composition dependence of the structure of $Ca_{1-x}Sr_xTiO_3$ materials showed the importance of complementing bulk powder diffraction measurements with the local probe provided by electron diffraction.

Mike Glazer took length-scales to the other extreme, and spoke about one of the "forgotten" or "ignored" areas of crystallography - birefringence studies, which were the mainstay of crystallographers before X-rays. Mike showed how modern CCD based birefringence equipment, computationally-coupled to elegant false-colour images of the data, can give wonderful insight into many aspects of crystallography ranging from phase transitions in minerals through to the quality of protein crystals and strain in diamond samples. The ability to "see" a whole phase diagram in a single set of optical measurements on a single sample with a compositional gradient was particularly impressive.

Overall, this was an excellent and instructive meeting, with the speakers not only highlighting the individual techniques they'd been asked to address, but also showing how their technique interacts with many of the others. It was clear from the meeting that the best structural science will only result from applying a battery of modern techniques. The meeting was very well attended and the PCG's thanks go to Dave Allan for the local organisation, the Edinburgh Department of Physics for sponsorship, and the speakers for an excellent afternoon of talks.

John Evans

CCG Autumn Meeting 2003

The next CCG Autumn Meeting will take place at Accelrys Ltd, Cambridge Science Park, Cambridge on Wednesday 12 November 2003. The title of the Meeting is "Beyond Refinement - What Happens Next?" It will deal with issues such as validation and the dissemination of results. The following have so far agreed to speak at the Meeting:

Kirsty Anderson (RSC)

Richard Cooper (Oxford)

John Davies (Cambridge)

Tony Linden (Zurich)

Peter Murray-Rust (Cambridge)

More details will appear at http://bca.cryst.bbk.ac.uk/BCA/ccg/ccg.html and in Crystallography News. If you have any enquiries about the Meeting e-mail A.J.Blake@Nottingham.ac.uk.

BSG Protein Crystallography Summer School

The date was Sunday 1 September, and forty postgraduate macromolecular crystallographers were flocking to Clifton Hill House, their home for the next five nights in Bristol, for the 9th BCA Protein Crystallography Summer School. The mood was one of excitement juxtaposed with trepidation. Excitement because of what we were attending and the new friends we would all meet and trepidation for that evening we were all due to present a five minute summary on our research and answer questions.

Before this however, was the first dinner and for most of us our first glimpse at the six course tutors. They were introduced as Mark Banfield, Leo Brady, Jon Cooper, Elspeth Garman, Airlie McCoy and Martin Noble, a veritable feast of knowledge that we were all to benefit from over the next six days. Unfortunately, dinner was all too brief and it was time for the presentations to begin.

In reality, these were pain free with each attendee realising that we all knew similar amounts, albeit in different areas within the field. People began to relax and the drink started to flow, as it continued to do for the rest of the week.

The lectures began bright and early Monday morning, after what for most people proved to be a cold shower and a battle with wasps that seemed, rather unfortunately, to love the warm damp conditions in the bathrooms. Notwithstanding, the lectures began with a short introduction by Leo, who enthralled us all with his comments that the week was very intensive and not to worry if we didn't understand it all.

This was how the week proved to be, with the macromolecular crystallography processes explained from beginning, with the expression of protein, to the end, with structure deposition. Though the lectures were intensive, each proved very informative and most, interesting. One highlight had to be the attempt (successful … I think) by Airlie McCoy to describe maximum likelihood using real and imaginary, any numbered side die you would like to imagine.

Though the week was meant to inform, a suitable amount of alcohol was consumed during a social program that ran alongside the lectures. The Monday evening saw a cruise around the Bristol harbour, which included just a few stops at pubs. Wednesday afternoon was free time, enjoyed, by those rather too energetic and health conscious, with a game of softball, followed by some very strong cider to wash any benefits of the exercise away. Finally, the Thursday evening saw the conference dinner, where wine flowed, some interesting structures were built and destroyed, once again instigated by Airlie McCoy, and a guest speaker, Professor Judith Howard FRS spoke. The talk was motivational indeed. Speaking of her one-time supervisor Dorothy Hodgkin, Professor Howard concluded with a comment of hers on those who stay in science, "Some people will live greatly and achieve modest things but I hope some of you will live modestly and

achieve great things".
It was now Friday 6 September, and forty postgraduate macromolecular crystallographers were flocking from Clifton Hill House, their home for last five nights in Bristol, informed and enthralled by what they had heard. The mood was one of happiness and excitement. Happiness for new friends made and new challenges to be met, and excitement for new challenges to be met and for the British crystallographic community of which we all now felt a part.

Finally, on behalf of everyone that attended the school I would like to thank the course tutors for such an informative and highly enjoyable week.

Ben Gale

Summer School in Synchrotron Radiation Science

27 participants gathered in Chester at the end of August for a 10-day course covering both theoretical and practical aspects of SR and its applications. 'Students' (actually ranging from new postgraduates to academic and central facilities staff) were drawn from many different countries, mainly in Europe, but also including Canada. The course was sponsored by some of the UK research councils (particularly by EPSRC and CCLRC) and the European Union, enabling many students to attend with reduced or no cost.

The hard work is done! Relaxing at the closing dinner.

The school began with a week in Chester, during which a variety of speakers gave informal lectures and seminars on SR basics (theory, instrumentation and operations), theory and practice of scientific techniques, and wider applications. The topics included a guide to 'SR-speak', historical developments and future prospects; properties of SR, storage rings, optics and detectors; a range of diffraction and spectroscopic methods, microscopy, polarisation and magnetic effects; applications in chemistry, earth and environmental sciences, physics, biology, medicine, and engineering. Daresbury Laboratory provided many of the speakers, particularly on the basic SR topics, but major users of SR from British universities were also well represented, especially in describing many of the scientific applications.

Discussions continued well beyond the timetabled sessions, through meal-times and other breaks, and into the evening social programme, which also provided welcome relaxation; activities included exploration of some of Chester's rich history, a boat trip, a refreshingly informal reception by the Lord Mayor, and some excellent meals. The students showed their engagement and enthusiasm for the whole school programme right from the beginning, with virtually full attendance at every session (scientific and social). In fact, many of the most interesting questions came from those in disciplines lying outside the particular session topic; it was very encouraging to hear students of biological science, for example, say how interesting they had found the explanation of engineering strain measurements, and to have favourable comments on medical imaging and biological spectroscopy presentations from physicists.

Seeing real-life SR work on one of the experimental stations at Daresbury Laboratory.

Chester College was, overall, a very good venue for the first week. The lecture facilities were excellent, and there was plenty of choice of activities for the social programme. The college's food was good and generous, and the accommodation perfectly adequate and convenient. Sharing the site with some other residential parties added to the variety, though the behaviour of a visiting group of young Canadian football players left much to be desired; our Canadian school participants disclaimed all responsibility, of course!

A free day at the end of this first week was used in various ways; some visited Liverpool (with transport provided), others ventured into North Wales or stayed in Chester. Following this, we reconvened, this time at Daresbury Laboratory, for three days of practical work. Groups of 2-6 students spent half-day periods working on several of the experimental stations of the SRS, sampling the delights of diffraction and spectroscopic techniques as well as having a general tour of the facility and seeing how it was operated. We were enormously helped by the dedication and hard work of the

station scientists and other Daresbury Laboratory staff. Accommodation was conveniently at the hostel, where the breakfast was voted a great success, especially compared with the evening meal at the site restaurant (regular SRS users won't be surprised to read this!); buffet lunches and a final dinner at a nearby Chinese restaurant meant that we weren't entirely reliant on the usual catering, however. A final seminar was given by Gerd Materlik, Chief Executive of the Diamond project, the new UK synchrotron radiation source.

Anonymous questionnaires showed that the students very much enjoyed and benefited from the school. Some very helpful comments were received, that will help in the planning of the next event, currently earmarked for the late summer of 2004, when we expect to run a similar school. Many of the students will be at the BCA Spring Meeting in York, when it is expected there will also be a brief presentation about the school at the Education SIG session.

The joint directors of the SR Summer School were Bob Cernik (Daresbury Laboratory) and Bill Clegg (Newcastle University and Daresbury), but a great deal of the really hard work was done by Alison Mutch (Daresbury), for whom there was a particularly hearty round of applause at the closing dinner. We thank her, and other colleagues, very much for making this such a resounding success.

Bill Clegg

2003 Annual General Meeting of the BCA

The Annual General Meeting of the British Crystallographic Association will be held at 16.30 on Wednesday 16 April 2003, in the University of York

Agenda

1. Approval of Agenda
2. Apologies for absence
3. Minutes of the last AGM (published in this issue of Crystallography News).
4. Secretary's Report to Council (published in this issue of Crystallography News).
5. Northern Networking's Report.
6. Report of the Treasurer to include Presentation of the Accounts for 2002 and the Examining Accountant's Report.
7. Acceptance of the Accounts
8. Elections to Council
   President (manifestos in this issue of Crystallography News)
   Treasurer
   Ordinary Members (3)
8. Appointment of Examining Accountant for 2003.
9. Any other business

Christine Cardin
Secretary to Council

British Crystallographic Association

Minutes of Annual General Meeting held on Wednesday, 27th March 2002 at 1600 in room C16, Pope Building, University of Nottingham. The President (Chris Gilmore) in the Chair.

85 members were present. One minute's silence was observed in memory of Max Perutz, Helen Megaw and Charles Taylor.

1. **Approval of agenda.** The agenda was approved

2. **Apologies for absence.** Apologies for absence had been received from Margaret Adams.

3. **Minutes of the previous AGM**. These had been published in the December 2001 issue of Crystallography News. Chick Wilson wished to record that he had been present and certainly had not apologised for absence. Paul Raithby proposed that the Minutes be approved, seconded Paul Fewster.

4. **Secretary's Report.** The secretary, Christine Cardin, presented her report, which had been published in the March 2002 issue of Crystallography News.

5. **Northern Networking report.** This report was presented orally. Gill Houston said that there were now 948 members, broken down into 746 ordinary members, 68 retired, 134 students, 31 life and 9 honorary. In terms of groups, there were 284 BSG members, 264 CCG members, 119 PCG members, 153 IG members and 128 members with no specified adherence. The

work of the office was carried out by Euan Woodward (Spring Meeting), assisted by Yvonne, Kirsty (bursaries) and Mark. There were no questions for Gill. She was thanked by Chris Gilmore .

6. **Treasurer's report.** The Treasurer, David Taylor, presented a detailed report, which is published separately. Points highlighted were, under expenditure, that £3 of each BCA membership subscription goes to the International Union of Crystallography, as we are the single national organisation representing crystallography in these islands. This is a large fraction of the current subscription, which the Treasurer is reluctant increase for administrative reasons. Second, at the Reading Spring Meeting there had been a big overspend on speakers' expenses, largely due to the provision of complete expenses for all speakers without a requirement that they stay for the whole meeting, leading to unnecessary wastage on unused accommodation etc. The Treasurer recommended a much stricter policy in future.

7. **Acceptance of the accounts** A general point highlighted was the complexity of presenting an overall financial picture given that there are separate Group accounts. In questions, David was asked whether in future he could present an overview of Group finances alongside the detailed breakdown he had just presented. Members would like an overview of the whole financial picture. David said that the Group accounts had full details for all the Groups. Chris Gilmore thanked David for his tireless work on behalf of members, and Sheila Gould proposed that the accounts be accepted. This was seconded by Harry Powell.

8. **Appointment of Examining Accountant for 2002.** David Taylor said that The Young Company had been proposed as accountants for 2002, with a fee of £1600. Paul Raithby proposed that we accept this, seconded by Richard Pauptit.

9. **AOB.** The future of the Spring Meeting was discussed, against a background of concern about the cost of the meeting (for which there is no major financial subsidy), the length of the meeting, and the low attendance by the biological community, worrying because this is the largest Group within the BCA. Points raised included:

Pierre Rizkallah - is it cheaper to have the meeting after Easter?

Claire Wilson - would it be cheaper to have the meeting in a fixed venue? Would it be better to have a 2.5 day meeting? If so, should there be more parallel sessions? Should there be an overall theme?

Roy Copley - Would exhibitors be happy with a shorter meeting? Would industrialists prefer this?

Richard Pauptit - the meeting should be better advertised. Who should be responsible for this?

Student bursaries should be properly publicised and new students made aware that by joining at the start of their courses they would be eligible for Spring Meeting bursaries the following spring.

Chick Wilson - some of the meeting proceeds should be published and negotiations were underway with Taylor and Francis publishers.

The idea of having a Chartered Crystallographer grade of BCA membership was discussed. The majority felt this was attractive but unworkable in practice.

There being no further business the meeting closed at 1650.

Secretary's Annual Report to the AGM 2003

First, the composition of Council. This year has been one of stability for Council - there were no elections in Nottingham, and so the list of Council members for the year looks very like last year.

Chris Gilmore (President), Paul Fewster (Vice-President), David Taylor (Treasurer), Christine Cardin (Secretary) - the Officers

Margaret Adams, Jeremy Cockcroft, Paul Raithby - Ordinary Members

Harry Powell (CCG), John Evans (PCG), Chris Frampton (IG), Andrea Hadfield (BSG) - the Group Representatives

Chick Wilson and Paul Barnes (co-opted)

Bob Gould and Kate Crennell (*ex officio* as Editor of Crystallography News and as Education Officer)

We are grateful to Richard Pauptit, Peter Moody, Nick Keep and Eleanor Dodson, who have helped to represent the BSG during Andrea's maternity leave. As the largest subject group, we must have strong representation on Council from BSG. There will be big changes after the York meeting - the President, Treasurer and three Ordinary Members all reach the end of their terms of office in 2003, and we thank them for all their hard work on behalf of members. Nominations for all positions close two weeks before the AGM (see the separate Announcement of Elections).

Council met twice, in Nottingham after the Spring Meeting and in Birkbeck (London) in September. On both occasions, there was a long agenda, and there is never enough time for detailed debate. Issues which continue to concern Council, and which should be discussed at the AGM, include the possible introduction of Foundation Membership, the large task of maintaining a quasi-professional website, and whether we have now got it right with the Spring Meeting format. The Northern Networking contract comes up for renewal in June 2003, and Council will have to take decisions in that area in York. A contract has been agreed for the publication of part of the Spring Meeting proceedings in the journal Crystallography Reviews. Chick Wilson is Guest Editor of the inaugural BCA Review Symposium issue.

On membership, we now have about 1000 members, but this number could be even higher. Chick Wilson has designed an excellent poster, and by now your lab should have several copies, including one with this issue of Crystallography News. If not, please contact the Administrative Office. It is a particular concern that non-members do not receive Crystallography News and therefore miss the main publicity for the Spring Meeting. A suitable poster design would help here. September is the best time of year to add new memberships, at the start of the academic year. So far there are no plans for top-up fees to members, as the Treasurer points out that the cost of administering a membership fee increase is too high. Membership subscription therefore remains a bargain, and cost cannot be a reason not to join.

Four excellent issues of 'Crystallography News have appeared thanks to the hard work of the new Editor, Bob Gould. This is now a professional publication with a wide readership, which is now seen is a magazine members are happy to display as representing their interests. We thank both Bob and the previous Editor, Jo Jutson, for their sterling services.

All four Groups held meetings, already reported in 'Crystallography News'.Themes were 'Sample preparation' (IG), 'Dealing with Difficult Data' (CCG), 'Complementary Techniques applied to Crystallography' (PCG), and 'Structural Studies of Macromolecular Assemblies' (BSG). The Protein Crystallography School was held in Bristol, organised by Leo Brady. The last Spring meeting in Nottingham, under the local organisation of Sandy Blake and Claire Wilson, was a financial and scientific success, and we thank them very much for their hard work in cooperation with Euan Woodward of Northern networking. We look forward to the York meeting, 15-17th April 2003.

We have three new Honorary Life Members, Professors Michael Woolfson, Andrew Lang and Jane Brown, and we welcome nominations for more. Constitutionally, we are allowed to have 20 such members.

It is a pleasure to report that a Damehood was conferred on Professor Louise Johnson in the New Year Honours list. More sadly, we lost two members with the deaths of Harold ('Hal') Taylor and John Robertson.

Finally, we are a voluntary organisation which nevertheless presents itself to the outside world as a professional body. UK crystallographers underpin more disciplines than ever each year. The BCA is the single body which represents UK crystallography internationally and to the wider scientific community, and must continue to be a coherent and representative umbrella organisation for us all. This is currently achieved with the minimum of professional administrative support and with the maximum of cheerful volunteer labour. So, thank you to all who have helped. It always feels that the whole is greater than the sum of the parts.

Christine Cardin
Secretary to Council

News from the Biological Structure Group

Biological Structure Group Logo

Following the competition last year, a new logo (see head of article) has been adopted by the Biological Structure Group.

Biological Structures Group Winter Meeting 2002

The Winter Meeting of the British Crystallographic Association, Biological Structures Group: "Structural Studies of Macromolecular Assemblies" was held at the University of Warwick on 13th December 2002. A wide range of systems, including protein/protein, protein/nucleic acid and membrane protein complexes were covered. A meeting report in this issue of crystallography news describes the sessions in more detail.

Biological Structures Group Sessions at BCA Spring Meeting

York 15th-17th April 2003
This year the Spring meeting has been reorganised into a condensed format, to keep delegate costs down and to take up less of your Easter holiday. This is particularly in response to feedback from the biological crystallographic community. Another new feature this year is one-day registration. Whilst the whole meeting has sessions which should be of interest to crystallographers of all descriptions, the sessions organised by the BSG are centred around the Wednesday when the BSG AGM will be held, as well as the conference dinner. We look forward to seeing a lot of you there.

BSG sessions organiser, to whom scientific enquiries/comments should be addressed:
Dr. Gideon Davies E-mail:
davies@ysbl.york.ac.uk

Late registration (including day registration) is still available for this meeting after the deadline of March 10th. For details, see the BCA Website.

Tuesday 15th April. Plenary Session: High Throughput, Databases and Data mining
The meeting starts with an afternoon of plenary lectures, one from each special interest group within the BCA. These are designed to be of broad appeal across the crystallographic community. Christian Cambillua will be talking about structural genomics in a medium sized laboratory. After tea BSG will hold an oral poster session. There will also be a meeting of the Education Special Interest Group before a wine reception.

Wednesday 16th April
Parallel Sessions
This year under the umbrella title of High throughput, Databases and Data mining the talks organised by the BSG will cover topics including crystallisation (Julie Wilson, Marek Brzozowski), phase determination (George Sheldrick), automated building of protein models (Victor Lamzin). There will also talks about structural genomics (Yeast, Herman van Tilbeurgh), information management for high throughput structural biology (Robert Esnouf) and Data Mining (Tom Oldfield, European Bioinformatics Institute).

On Wednesday we will also hold the **BSG Annual General Meeting** at lunchtime, and the **BCA AGM** after tea. The **Max Perutz Memorial Lecture** will be given in the early evening by Venki Ramakrishnan, followed by the **Conference Dinner**.

Thursday 17th April
After last year's successful workshop there will be a **CCP4 workshop** on Thursday morning including recent developments and overview of CCP4 software. This will be followed by a session of general interest on **Synchrotron Radiation** highlighting the cutting-edge science which takes place at synchrotrons in fields from biology through physics and chemistry to science, and a meeting of the **DIAMOND Special Interest Group** to get an update on the development of beamlines of interest to the crystallographic community.

Biological Structure Group AGM

This will be held at the BCA Spring Meeting as usual. A provisional agenda is published below. The chairman, secretary/treasurer and vice chairman posts are all due for re-election this year. Committee posts will also be becoming vacant. Please send nominations for any of these posts to Andrea Hadfield along with additional agenda items to the Secretary by 31st March (a.t.hadfield@bris.ac.uk).

Twentyfirst Annual General Meeting
to be held on Wednesday 16th March at 12:00 during the BCA 2003 Spring Meeting at York University

Provisional Agenda

1. Minutes of 2002 annual meeting (Nottingham)
2. Matters arising on the minutes
3. Chairman's Report - Dr. Richard Pauptit
4. Secretary/Treasurer's report - Dr. Andrea Hadfield
5. Committee Membership and Officers (2003-2004)
6. Any Other Business

Current Officers and Committee
Chairman
Dr. Richard Pauptit (2000-2003)
Vice-Chairman
Dr. Jim Naismith (2000-2003)
Secretary/Treasurer
Dr. Andrea Hadfield (2000-2003)
Webmaster
Dr. Martin Noble (1998-2005)
Dr. Andrew Leslie
Dr. Nick Keep
Dr. Harry Powell
Dr. Jon Cooper
Dr. Vilmos Fulop
Dr. Katy Brown

Biological Structures Group Winter Meeting 2003

The BSG winter meeting will be held in London this year in December, on a topic to be finalised. Details will follow.

Bursary Report 2002 - From the Treasurer

Several generous donations have boosted the Arnold Beevers Bursary fund by over £1200 this year. A GIFT AID refund of £708 has also been allocated to the fund.

The Nottingham Spring Meeting saw the award of bursaries totalling £5,400 to 30 students from 13 Universities. For the first time 17 of these Bursaries were commercially sponsored. The BCA is grateful to the following organisations for this valuable support: Bede, Bruker, Hampton, ICDD, PANalytical, Mar, Oxford Cryosystems and Syngenta.

Through the year there were 18 applications for **Arnold Beevers Bursaries**. Two were rejected, one on membership grounds and the other because of previous awards. 16 bursaries were awarded totalling £4,000.

Conference details:

- XIX - IUCr Congress, Geneva.
- Pneumococcal - 3rd International Symposium on Pneumococci and Pneumococcal Diseases, Alaska, USA.
- 223rd ACS - 223rd American Chemical Society Spring Meeting, Florida, USA
- CRYSTENG - Crystal Engineering Communications Discussion Meeting, Bristol
- IMA - International Mineralogical Association Conference, Edinburgh.

Through the year "good works" have benefited from BCA funding.

£500.00 Schools Crystal Growing Competition. Details of the Bursary scheme can be found under Membership on the BCA web site.

Surname	Institution	Conference	Award
Mr T S Lyford	University of Warwick	XIX IUCr	£250.00
Mr E A Collier*	UMIST	XIX IUCr	£250.00
Dr G M Rosair*	Heriot Watt University	XIX IUCr	£350.00
Miss J E Saunders	Dept of Biological Sciences	XIX IUCr	£250.00
Mr J W Murray*	Oxford University	XIX IUCr	£250.00
Dr I R Evans	University of Durham	XIX IUCr	£350.00
Mr G M Day	UCL	XIX IUCr	£250.00
Miss K M Heslop	University of Bristol	XIX IUCr	£250.00
Mr A Angeloni	University of Bristol	XIX IUCr	£250.00
Miss R A Baber	University of Bristol	XIX IUCr	£250.00
Mr P A Crawford	University of Bristol	XIX IUCr	£250.00
Mr B D Salt	University of Bristol	XIX IUCr	£250.00
Mr C Bent*	University of Glasgow	Pneumococcal	£200.00
Dr N Blagden	University of Bradford	223rd ACS	£200.00
Dr A L Gillon*	UMIST	CRYSTENG	£200.00
Dr A R Oganov*	University College	IMA	£200.00

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

BCA Spring Meeting 2003 - York Timetable

March 2003

08.30 hrs	BCA Council Meeting 09.30 hrs - 10.30 hrs	Parallel Session **High Throughput, Databases and Data Mining in Chemistry and Biology**	Parallel Session **High Energy Diffraction**		Parallel Session : **Phase Identification principles**
10.00 hrs		**Coffee/Exhibition**			
10.30 hrs .....1 .00 hrs	**Plenary Session : High Throughput, Databases and Data**	Parallel Session **High Throughput, Databases and Data Mining in Chemistry and Industry**	Parallel Session **High Energy Diffraction**	Parallel Session **High Throughput, Databases and Data Mining in Biology**	
12.00 hrs			**AGM** Physical Crystallography Group	**AGM** Biological Structures Group	
12.30 hrs	**Lunch/Exhibition**	**Lunch/Exhibition**			
13.00 hrs					
3.30 hrs	**Plenary Session : Mining** **High Throughput, Databases and Data** **John Faber** **Christian Cambillua**	Parallel Session **High Throughput, Databases and Data Mining in Chemistry**	Parallel Session **Discussion on the Rietveld Method**	Parallel Session **Phasing and Model building in Biology**	Parallel Session : **Phase Identification practice**
		AGM Chemical Crystallography Group			**AGM** Industrial Group
15.00 hrs	**Tea/Exhibition**	**Tea/Exhibition**			
15.30 hrs	**Introduction to powder diffraction**	**Prize lectures PCG & CCG**		Parallel Session **BSG Session**	Parallel Session : **Phase Identification Workshop with PCs**
	Oral posters PCG, IG and CCG and BSG				
16.30 hrs			**BCA AGM**	**16.30 hrs - 17.15 hrs**	
17.00 hrs	Education **SIG**	**17.30 hrs-18.30 hrs Max Perutz Memorial Lecture** **Venk Ramakrishnan**			introduced by David Blow
18.00 hrs	**Dinner**				
	19:00hrs **Poster/Exhibitors Wine Reception**	**19:30 hrs Conference Dinner**			

Parallel Session **Crystallograpgy for Technology**	Parallel Session **Structures with Z'>1**	Parallel Session **Quantitative Phase Analysis**	**CCP4** Workshop
Coffee/Exhibition			
Parallel Session **Crystallography for Technology**	Parallel Session **Synchrotron Radiation**	Parallel Session **Quantitative Phase Analysis**	
12:00 to 12:45 hrs DIAMOND SIG			
Lunch/Exhibition			
Parallel Session **Structure Solution from Powders**	Parallel Session **CRYSTALS Workshop with PCs**	Parallel Session **Quantitative Phase Analysis**	
Tea			
Parallel Session **Structure Solution from Powders**	Parallel Session **CRYSTALS Workshop with PCs**		
BCA Council Meeting 17.00 hrs - 19.00 hrs			

Commercial Exhibition

A record breaking commercial exhibition is an important feature of the Spring Meeting. At York we have 14 exhibitors confirmed with some exhibiting for the first time. Prime positions have seating areas overlooking a lake and feature some of the largest display spaces ever seen at our meetings.

Exhibitors include:

Anachem

Bede Scientific

Beevers Miniature Models

Bruker AXS

CCDC

deCODE genetics

ICDD

IUCr

Molecular Dimensions

Oxford Cryosystems

Oxford Diffraction

PANalytical

Rigaku/MSC

Roentec GmbH

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

Check out the Spring Meeting WEB pages for the latest information and to download an Exhibition Plan. With one day registrations on offer, can you afford to miss this exhibition? The excellent scientific sessions are the bonus that warrant the full three days of your time!

Did you know?

- The membership section of the BCA website has been updated to include downloadable forms for Membership, Gift Aid, Donations, Bursaries and individual ECA membership.
- You can keep the BCA informed of changes to your membership details by filling out an online form.
- The extra numbers on the address label of this edition are your Membership Number.
- You can check if you are registered for the BCA Gift Aid scheme by checking your membership number against a list linked form the Gift Aid section.
- You can now calculate the value of gift aid to the BCA using a JavaScript routine.
- Gift Aid has added almost £1400 to the Bursary fund in the last two years and only 20% of members are registered.

David Taylor

Chemical Crystallography Group AGM

The Annual General Meeting of the Chemical Crystallography Group will be held on Wednesday 16th April during the BCA Spring Meeting at York, starting at 14:30. Final details of the agenda and venue will appear on the CCG website (http://bca.crystal.bbk.ac.uk/BCA/CCG/agm03.html). Items for inclusion in the agenda are invited and should be sent to the Secretary of the CCG to be received no later than Wednesday 9th April 2003.

Call for nominations
Elections will be held for the positions of Chairman, Deputy Chairman and one ordinary member of Committee. The present incumbents (Chairman: Professor Paul Raithby; Deputy Chairman: Dr Sandy Blake; Member of Committee: Dr Jon Steed) will each have served a full term and are not eligible for re-election to the same posts (see rules 12 and 15 of the Constitution). The deadline for nominations is Wednesday 9th April 2003, i.e. 7 days before the AGM. Nominations may be made by e-mail; they must be supported by no fewer than two members of the Group and should be accompanied by the written consent of the nominee.

Current Officers and Committee (term of office)

Chairman:
Professor Paul Raithby (2001 - 2003)

Deputy Chairman:
Dr Sandy Blake (2001 - 2003)

Secretary/Treasurer:
Dr Harry Powell (2000 - 2004)

Committee:
Dr Simon J. Coles (2001 - 2004)
Dr Richard Cooper (2002 - 2005)
Dr Michaele J. Hardie (2002 - 2005)
Dr Georgina M. Rosair (2002 - 2005)
Dr. Jonathan W. Steed (2000 - 2003)
Dr Simon J. Teat (2002 - 2005)
Mr Duncan M. Tooke (co-opted Student Representative) (2001 - 2003)

Harry Powell

No crystallography in UK secondary schools!

Last December I went to a meeting at the Institute of Physics (IoP) to learn more about their project to provide CD based Resources for physics teaching in the lower forms of secondary schools with pupils in the age range 11 to 14. Apparently most physics graduates find more attractive employment than school teaching. This means that the physics content of the National Curriculum is often taught by teachers who have not studied physics at University. They may not understand the concepts very well themselves and are understandably nervous about presenting these topics to the students. To help these teachers, the IoP is funding the production of CDs based on topics such as 'Electricity and Magnetism' or 'Light'. They are to be made by experienced physics teachers and will include sections on 'Common misconceptions' , 'Frequently Asked Questions (FAQs)' as well as draft overheads for presenting the topics, worksheets for the pupils and pages to show pupils the relevance of the topic to their everyday lives. Workshops will be held to show the teachers how the CDs can be used as an additional resource in their teaching.

This seemed to be an excellent project. I was about to volunteer to make a CD on the relevance of crystallography to modern technology when I discovered that this project cannot try to cover any topic from the whole of physics. With its limited funding it is ***only making CDs for topics which are in the National Curriculum for physics.*** Unfortunately this does not include crystallography, nor any mention of condensed matter and materials science. So all our efforts to interest younger children in primary schools in crystal growing will be wasted because there is no obvious way to maintain their interest through the secondary schools and on to university. One teacher at the IoP meeting thought that 'materials' might be covered by the chemistry topics of the National Curriculum, but he was not sure, and thought there was no crystallography.

How can the BCA get crystallography into the National Curriculum?

Come to the Education Session at the BCA Annual meeting in York to suggest what the BCA might do to foster an interest in crystallography at all levels of the UK educational system.

Kate Crennell

From the Secretary - Announcement of Elections to Council

Old hands will know that we elect our Officers and Council members by secret ballot at our AGM during the Spring Meeting. This year is the Big One in this sense - we will elect a new President. The President serves for three years, and should be a person that members feel can represent a broad swathe of crystallographic interests. But we cannot afford to elect a figurehead; the president has to chair the Council meetings and play a leading role in developing the BCA still further. Our very distinguished and hard working past Presidents have been -

1982-1984
Professor David Phillips

1984-1988
Professor David Blow

1988-1990
Professor Michael Woolfson

1990-1992
Dr Bob Diamond

1992-1996
Professor Judith Howard

1996-2000
Professor Michael Glazer

Despite these dates, the President is elected for a single three year term, as is shown by the following extract from the Statutes

Elections shall take place as follows:

a. *Elections of Officers and Ordinary Members shall take place at an Annual General Meeting of the Association.*

b. *Each elected member of Council shall serve from the end of the Annual General Meeting at which the election took place until the end of the third Annual General Meeting following the election.*

c. *The President shall normally serve for one three-year term only.*

d. No person shall serve more than two consecutive three-year terms in the same capacity.

e. No person shall serve more than three consecutive three-year terms in any elected capacity.

Other Council vacancies this year are for Treasurer and for three Ordinary Members.

Please send your properly seconded nominations to me as soon as possible. I will accept nominations until two weeks before the date of the AGM on 15th April 2003. If you nominate someone, it is your responsibility to make sure that the person you nominate is willing to stand for election.

Two nominations have been received so far for the office of President, and statements from each of them follow:

Professor John Helliwell, Professor of Structural Chemistry, University of Manchester. Nominated by Professor Paul Raithby and seconded by Dr Naomi Chayen.

Professor Chick Wilson, Head of the Crystallography Group, ISIS neutron sources at the Rutherford Appleton Laboratory. Nominated by Professor Chris Gilmore and seconded by Dr Christine Cardin.

Christine Cardin

Statement by Professor John R Helliwell

I am keen to offer myself to serve the BCA as its next President.

I have been involved with the BCA from its inception in 1982. This has included being an active participant at many BCA Conferences, as a Council member including as the BCA's Vice President from 1989 to 1993, and as a local organiser of the BCA Spring Meeting Conference in 1993. My students and staff have also essentially attended all of the BCA Spring Meeting Conferences, and various Autumn Group Meetings, year-on-year. They offer terrific value for money and a great educational experience, in breadth and depth, in crystallography.

In recent years I have gained experience in the global scene including as IUCr's Editor-in-Chief of Acta Cryst since 1996, and as EinC thereby also a member of IUCr's Finance Committee. I was also a JSR Main Editor between 1994 and 2000. Since 1999 I also have served as the ECA's Founding Chair of its Instrumentation and Experimental Techniques (IET) SIG. I was joint organiser of the ACA Transactions Symposium in Buffalo in 1999. I led the UK delegation to the IUPAB General Assembly in New Delhi, India in 1999.

My science interests are broad but encompass especially biological crystallography and methods. Specifically my research work has involved crystal structure studies of enzymes, lectins and of the carotenoid binding protein crustacyanin. My methods development research has involved the SR, and now neutron, Laue method and the use of SR anomalous scattering in macromolecular crystallography.

As a specific proposition I am keen to share my thoughts on the setting up of what I would call for the moment BCA 'Methods Groups', which I envisage would cut across and underpin our BCA core Groups (BSG, CCG, PCG and ICG), and complement the new diamond and Education SIGs. Thus Methods Groups could be convened on eg:

1. Software and Databases.
2. Instrumentation and Experimental Techniques.
3. Time-resolved and Perturbation Structural Studies including non-crystalline techniques such as the various spectroscopies. [Involving other structural techniques such as NMR in the BCA is perhaps a bold step but witness the success of the recent RSC Faraday Discussion Meeting on Time-resolved chemistry organised by Prof Chick Wilson and myself and also the BCA CCG Manchester Autumn meeting of 2 years ago, also in Hulme Hall, on Complementary techniques organised by Dr Madeleine Helliwell.]

At each BCA Spring Meeting these Methods Groups would meet. They should/would include people who have not so far committed time to BCA events.
Overall I know I have much to build on from the leadership and work of all the previous BCA Presidents. I hope then that you would give me the chance to make my contribution to the BCA from 2003 to 2006 as its next President.

Statement by Professor C C Wilson

It is an honour to be nominated for election as BCA President. As a longstanding active member of the BCA I believe that I have its interests at heart and would put my energy and enthusiasm into helping the organisation move on from its present strong position. There has been an increasing professionalism to the BCA, introduced during the tenures of recent presidents, which is essential to our continued good health as a major scientific association in the 2000s. The consolidation of our previously part-time organisation into the hands of the professionals at Northern Networking has been a positive experience, and it is our responsibility to work with our professional organisers to continue to develop the BCA in an appropriate manner for a 1000-member organisation.

In spite of our healthy position, both in terms of our international standing and influence and our finances (stemming largely from the success of the Glasgow IUCr meeting), I see there are still issues we must address. There is still a sense of fragmentation within the BCA that is unhealthy, and our flagship event, the Spring meeting, is still not attracting the level of attendance I feel it deserves.

Special interest groups

As a means of mitigating against fragmentation, particularly within the Spring meeting, I believe that the formation of further cross-subject group Special Interest Groups is important for the future of the BCA, and will work for their introduction if elected as President. The cross-disciplinary nature of much of Crystallography makes this step appealing. Examples of possible SIG areas might include: Supramolecular chemistry (CCG/BSG): Structural solid state chemistry (PCG/CCG); Drug design and interactions (BSG/CCG/IG); High resolution diffraction (PCG/IG); Structure solution from powders (PCG/IG/CCG); Crystallisation and polymorphism (BSG/CCG/IG). There will be many more ideas, and SIGs that embrace partnerships with related organisations (e.g. CCP4, IoP & RSC groups, BACG) can also be encouraged. The combination of these cross-group SIGs in stimulating the Spring meeting, with the successful role of the existing subject groups in organising more specialist meetings, workshops and teaching events, represents to me a healthy way forward.

Spring meetings

Related to the above, I believe the impact of (and attendance at) our Spring meetings can be substantially enhanced. Over the past couple of years there has been a major discussion over the future directions of the BCA Spring meeting, centred around cost and duration on the one hand and scientific programme on the other. In the former, we will be exploring at York a new structure for the meeting, while on the latter there has been an attempt to give increasing emphasis on joint sessions between the subject groups. However, I still feel that there should be significantly increased competition for scientific slots at the Spring meeting. The formation of SIGs would give added impetus to this and offer to the Programme Committee a wider choice of proposed sessions with which to seek an exciting and balanced programme. With the Spring meeting being the key forum for the BCA as a whole, it is vital we get both the science and practicalities right, and make our meeting attractive to BCA members and also to our colleagues in associated fields. The introduction of the publication of the BCA Review Symposium is another step towards increasing the impact of the meeting. With our membership base there is no reason why the Spring meeting should not regularly attract attendances of 400+ to a vibrant and scientifically competitive programme.

Diamond

The BCA can have a significant role in canvassing and representing the needs of the UK crystallography community in the development and exploitation of the Diamond synchrotron. The new source will be of high relevance to all interest groups within the BCA, and for this reason we have inaugurated the Diamond SIG. The work of this SIG should develop as the plans for the source develop and act as a focus for informing, lobbying and representing the community.

CCW

My own background is as a crystallographer and chemical physicist using X-ray and neutron diffraction, largely single crystal but also powder diffraction, in the study of organic and related structures. I currently head the Crystallography Group at the ISIS neutron sources at the Rutherford Appleton Laboratory, where I also head the Centre for Molecular Structure & Dynamics, and am Visiting Professor in Chemistry at the University of Durham. My role at the central facility gives me the opportunity to see a wide range of Structural Science, and to track the trends in a range of areas - my recent appointment as Co-editor of Acta Cryst B will consolidate this. Within the BCA, of which I have been a member since 1986, I have been a member of the Committees of both the CCG and PCG (the latter as Secretary/Treasurer), and have been a member of Council since 1997. I am currently UK Councillor to the European Crystallographic Association. Since1998 I have organised the Abstract submission and Conference book for BCA meetings, and in 1999 led the Abstracts Team for the Glasgow IUCr Congress. More recently, I have been involved in the restructuring of the Spring meeting and am Guest Editor of the inaugural BCA Review Symposium issue of Crystallography Reviews.

If elected I shall work hard to advance the best interests of the BCA and all its constituent parts.

Industrial Group AGM 2003

The 20th ANNUAL GENERAL MEETING of the Industrial Group will be held at the University of York on 16thApril 2003 at 2:30pm.

Nominations are sought for Secretary/Treasurer and **four** committee members to serve for three years from April 2003.

Nominations, which shall be proposed by not less than two members of the Group and shall be accompanied by the written consent of the nominee, shall be sent to reach the Honorary Secretary of the Group not later than seven days before the Annual General Meeting.

Phil Holdway
Hon. Secretary/Treasurer

Physical Crystallography Group AGM 2003

The Annual General Meeting of the Physical Crystallography Group (also the Structural Condensed Matter Physics Group of the IoP) will be held on Wednesday 16th April during the BCA Spring Meeting at York, starting at 12:00. Final details of the agenda and venue will appear on the PCG website (http://bca.crystal.bbk.ac.uk/bca/pcg/welcome.html). Items for inclusion in the agenda are invited and should be sent to the Honorary Secretary of the PCG (john.evans@durham.ac.uk) to be received no later than Wednesday 9th April 2003.

Elections will be held for Ordinary Members of the committee. Nominations (with name of seconder and note of acceptance from the nominee) for these positions should be sent to the Hon. Sec. by April 9th, or communicated to him in person at the 2003 BCA Spring Meeting.

Current Committee
Chair: Pam Thomas (2002-2004)
Deputy Chair: Paolo Radaelli (2002-2004)
Honorary Secretary/Treasurer: John Evans (2002-2004)
Committee Members: Dave Allan, Jeremy Cockcroft, Steve Collins, Jon Goff, Sue Kilcoyne, Jonathan Wasse

John Evans
(Hon. Secretary/Treasurer)

Book Reviews

Fundamentals of Crystallography

C. Giacovazzo, H.L. Monaco, G. Artioli, D. Viterbo, G. Ferraris, G. Gilli, G. Zanotti and M. Catti
IUCr Monographs on Crystallography, Oxford University Press, Second Edition, 2002
Price: £75.00 (hardback) , £39.50 (paperback)
ISBN 0-19-850957-X (hardback) ; 0-19-850958-8(paperback) + xxi + 825 pages and CD.

This is an impressive book, not only in its size but also as the possible inheritor of the reputation garnered by the first edition published in 1992. The authors acknowledge the extensive advances in crystallography over the past decade and set themselves the task of augmenting and updating the material in the first edition: for example, a new Chapter 4 draws together pre-existing and new material on non-ideal crystals. The book is organised into ten chapters, most penned by a single author. The majority of chapters have appendices containing supplementary material on specialist and mathematical topics, and the authors have included a CD with browser-based software to facilitate the teaching and learning of the crystallographic concepts described in Chapters 1-3.

The first Chapter (CG) is entitled "Symmetry in crystals" and covers the concepts required for the remainder of the book: these include symmetry elements, lattices, point groups, symmetry and Laue classes, crystal systems, Bravais lattices and of course space groups. The definitions, properties and consequences of all these are illustrated by well-chosen examples. This chapter has a substantial set of appendices to which the more advanced material is relegated, making the main text more accessible.

The second chapter (CG) entitled "Crystallographic Computing" covers a wide range of procedures implicitly or explicitly used in routine crystallographic calculations. These include metric aspects, reciprocal lattice calculations, relationships between parameters, basis transformations and orthogonalisation. Next, a number of simple but fundamental calculations are described: these involve torsion angles, least-squares mean planes and Niggli reduced cells. Electron density and structure factor calculations are dealt with, before beginning a major section on least squares refinement. The least squares problem is outlined in principle and the properties of both linear and non-linear refinement are explored. Their application to a wide range of crystallographic procedures is described, with particular emphasis on two areas, namely Rietveld refinement against powder data and structure refinement against observed structure factor moduli, the latter being most commonly associated with single crystal data. The treatment of key parameters such as atomic coordinates, atomic displacement parameters and overall scale, occupancy, absolute structure and extinction parameters is followed by a valuable section dealing with practical aspects of refinement such as the computing time required, different refinement approximations, possible problems, and the features to be expected in an effective least squares program. The sources and consequences of a range of systematic errors and the role of constraints and restraints are then discussed, before brief descriptions of maximum likelihood and gradient methods as alternative refinement methods. The next section is a substantial exposition of Rietveld refinement, beginning with descriptions of the main steps leading to the point where refinement can begin followed by the basis of the method, including the establishment of the optimum peak shape function, and ending with an informative enumeration of some practical aspects. The next two sections cover related topics, the analysis of thermal motion and its effects on molecular geometry. A final section addresses the question of the accuracy of refined parameters.

Chapter 3 (CG) introduces the diffraction of X-rays by crystals, giving an account of the properties of X-rays and how they are scattered, and demonstrating Bragg's Law. A section on symmetry deals inter alia with Friedel's Law, systematic absences, space group

identification and the phase problem. The aim here is to allow an understanding of diffraction effects by modelling the radiation, the crystal and their interaction. The description of Thomson scattering includes a derivation and explanation of the polarisation factor. There is a good explanation of atomic temperature factors, both isotropic and anisotropic, along with some of the assumptions and dependences involved. A major section is devoted to factors which affect diffraction intensities, including mosaic structure, various crystal defects, and primary and secondary extinction. Anomalous dispersion is considered, from its origins in resonance between bound electrons and an incident X-ray beam with similar frequency, through real and imaginary dispersion corrections and the effects on Friedel's Law. The appendices include a concise outline of neutron scattering which could equally well be associated with Chapter 5 (experimental methods), but some generalisations about the need for large crystals and deuterium substitution should be qualified. Other appendices cover charge density and electron diffraction studies.

Chapter 4 (CG) entitled 'Beyond Ideal Crystals' provides a useful introduction to eight topics ranging progressively further from the ideal crystalline state, starting with crystalline twins and finishing with gases. No attempt is made to give a comprehensive coverage of these topics, rather an overview of the area with key definitions is provided, and references are given to reviews and other more specialised texts in each of the areas covered. The areas included in this chapter are crystalline twins, diffuse scattering, modulated structures, quasicrystals, liquid crystals, the paracrystal concept, and amorphous and liquid states and gases, including a section on small angle scattering. The approach is more mathematical than some of the other chapters, but there are some good illustrations particularly for quasicrystals, and some useful tables, especially in the twinning section. Appendices include further practical information about twins including some examples taken from a paper by Herbst-Irmer and Sheldrick. The sections are illustrated by examples drawn from many areas of science - from minerals to biological materials - and overall it helps to illustrate the breadth of crystallography.

Chapter 5 (HLM & GA) gives an extensive and thoroughly updated review of 'Experimental methods in X-ray and neutron crystallography'. The chapter takes the reader from the production and definition of the radiation beam, through methods of detection and data collection strategies, to data reduction for both types of radiation and for both single crystals and polycrystalline materials - all in a very readable style. It includes information on laboratory and synchrotron X-ray sources, including a mention of the microsource, and of both reactor and pulsed neutron sources, with discussion of the optics and types of detector used. A wide range of camera and diffractometer geometries for both single crystal and powder diffraction is discussed and there is also a section on *in situ* measurements under non-ambient conditions. Data reduction covers commonly applied corrections such as Lorentz, polarisation (for both conventional and synchrotron X-ray sources), absorption and radiation damage corrections.

Entitled 'Solution and refinement of crystal structures', Chapter 6 (DV) is very skilfully written to make the material impressively accessible. The chapter opens with a description of statistical analysis of structure-factor amplitudes, and then moves on to give a description of the Patterson function and its uses in very clearly written text. This is followed by a discussion of the heavy atom method for structure solution with several worked examples in different space groups, and in one case with more than one heavy atom. Direct methods is then covered in a similarly lucid manner. The final sections of this chapter deal with completing and refining the structure and are largely concerned with the least-squares method. More mathematical detail of some of these topics is given in the appendices.

There then follow two complementary Chapters covering inorganic (GF) and molecular (GG) crystals, respectively. Chapter 7, whose full title is "Mineral and inorganic crystals" begins with an attempt to distinguish these

from organic materials, but some of the wording is slightly unhelpful: stating that "almost the totality of minerals is based on elements other than H, C, N and O" could easily be read to mean the exclusion of these from mineral compositions, hardly what was intended! An extensive section then considers bonding aspects and how bond types (ionic, covalent, metallic, etc) affect properties such as hardness, conductivity, appearance, melting behaviour, cleavage and morphology. Ionic radii and their consequences for the structures of simple solids are explored, as are fundamental aspects such as the packing of spheres, coordination polyhedra and interstitial sites. The applications of the charge distribution method and the effective coordination number in order to rationalise structural features are explored. There follows one short section on polymorphism and the possible mechanisms of polymorphic transitions, and one on substitution and solid solutions. A survey of structural types includes closest-packed and close-packed structures (with and without the filling of interstitial sites), layer structures and structures containing complex anions, the most extensive, diverse and significant of the last being the silicates. The chapter ends with an account of modular structures, polytypism, order/disorder and modulated structures, and the phenomena which impinge on ideal crystals to produce real ones.

Chapter 8 'Molecules and molecular crystals' covers some of the key aspects of the analysis of the structures of small molecules, in particular of organic compounds. It is divided into an introduction and four main sections. The first of these sections is entitled 'the nature of molecular crystals' and discusses intermolecular forces including hydrogen bonding and how these lead into crystal structure predictions. The second section presents elements of classical stereochemistry providing useful definitions of some key aspects of conformation and configurations of structures, including a discussion of isomerism and analysis of ring conformation. The third main section, 'Molecular structure and chemical bond', presents various approaches to classifying or interpreting observed molecular geometries in terms of theories of chemical bonding, covering some of the most widely used methods. These include a short section on quantum-mechanical methods and some more qualitative approaches only applicable to particular types of structures such as VSEPR, ligand field theory and molecular mechanics. The final section is devoted to the interpretation of molecular structures, or what is often described as the study of structure-property relationships. Unsurprisingly, given the author's interests, this section also includes classifications of hydrogen bonds: one minor reservation concerning this section is that it possibly fails to indicate the level of controversy in classifying hydrogen bonds, and the examples chosen are less wide-ranging than they could have been.

Chapter 9 (GZ) provides a detailed description of protein (more precisely, macromolecular) crystallography, starting with an outline of some of the advances in the field since the first such structures were determined 40 years ago. Many of the advances, for example in computing hardware and software or the utilisation of area detectors, have parallels in chemical crystallography, but others such as isomorphous replacement are largely confined to macromolecules. One result of these advances is seen in the rapid increase in the annual number of additions to the Protein Data Bank. After an introduction to protein structure and function, the author embarks on the methodology, starting with the techniques of the key stage of protein crystallisation: extreme conditions much be avoided lest the protein degrade or the resulting structure be too different from that found in vivo, but variation of pH, salt concentration, organic solvent and precipitant, are possible. Although there are simpler methods, the most widely used today (such as hanging drop) are based on vapour diffusion. While cooling protein crystals can greatly extend their lifetime under irradiation, their high solvent content requires the use of a cryoprotectant regime to prevent icing: flash cooling then also confers many of the advantages seen for simpler compounds. The text describes the preparation and exploitation of isomorphous heavy-atom derivatives in solving novel protein structures via the

location of the heavy atoms by single isomorphous replacement (SIR), multiple isomorphous replacement (MIR) and anomalous scattering, including multiple anomalous dispersion (MAD) experiments using tuneable sources. After optimisation of the heavy atom positions, the next step is to improve the electron density maps. Alternative methods of solving macromolecular structures include molecular replacement and, in special cases, direct methods. Model building proceeds by using molecular graphics which allow segments of protein chain to be fitted to the electron density. The complexity and limited resolution of typical structures require that refinement must employ extensive constraints and restraints but, even so, significant manual adjustments to the model may be needed. Useful geometric indicators include the Ramachandran plot, which flags amino acids with suspicious chain conformations. This chapter ends with a discussion of solvent regions, a cautionary sub-section on the relevance of crystal structure to *in vivo* structure, and finally a discussion of the challenging but promising field of dynamical biological crystallography.

Chapter 10 (MC) discusses the physical properties of crystals. This final chapter concerns crystal physics, which it considers as a bridging discipline between crystallography and solid state physics. The chapter is divided into two main areas: the first presents the effects of crystal anisotropy and symmetry on the physical properties of matter. An initial introduction is given into crystal anisotropy and tensors and this framework is used to present a number of physical properties broadly presented as electrical and mechanical properties with the example of piezoelectricity given which bridges these two areas. The presentation is somewhat dry for this section, but it is coherent, and the examples are carefully chosen to illustrate certain types of properties and use of tensors. Theoretical methods used to model these behaviours are also presented. The second part of the chapter is devoted to crystal defects and the necessity of considering them in explaining some very important phenomena of real crystalline solids, e.g. mechanical behaviour and all transport processes in crystals, e.g. diffusion and electrical conductivity. This section is more readable, and covers several types of defects: point defects, planar defects such as stacking faults, line defects or dislocations, and the effect of these deviations from an ideal crystalline state on the properties of the crystal. It also presents the use of X-ray topography in these studies.

One minor complaint is that some of the text would have benefited from some careful editing of the English, because in some cases it is not as clear or correct as it might have been. The authors have decided, possibly on grounds of space, to include only scant coverage of crystallographic databases such as the CSD and ICSD. In general, however, this is an extensive and thoroughly updated textbook gathering together a great of deal of information: it succeeds as an introduction to many areas of the field and provides a valuable indication of the breadth of our subject.

Sandy Blake and Claire Wilson

Super Materials

Wendy Madgwick
Hodder Wayland (Science Starters series), 2002
Price: £4.99 (paperback)
ISBN 0-7502 4142 X , 32 pages

This booklet is intended to be used by adults to try to interest children in the differences between materials. It is aimed at children just starting primary school aged roughly between 5 and 7. Simple activities and experiments for the children are described in colourful pages with large print which some of the older children may be able to read for themselves. There are guidance notes for the adults, including pages of 'Materials you will need', 'Hints for helpers', a glossary of terms illustrated by simple colour drawings and an index. The materials are all common objects which could be found in most family homes, and the activities are ones which do not need batteries, so the book could be useful to any parents faced with the plaintive cry 'What can I do now?' from a child cooped up in the house on a rainy day towards the end of school holidays. The booklet attempts to answer such questions as "Where do metals come from? or 'How are crystals formed?. They suggest growing crystals from washing soda.

Find out more by looking at the publishers website: *http://www.hodderheadline.co.uk* or by following up the suggestions in the 'Further Reading' section: **Materials Around us** Steve Blackman 1999 Scholastic, **My World of Science: Materials** Angela Royston 2001 Heinemann Library, **Ways into Science: Materials** Peter Riley 2001 Franklin Watts, **Hands on Science: Matter and Materials** Peter Mellet 2001 Kingfisher. This booklet is very good value for money, and should provide hours of scientific activity.

Kate Crennell

Elements of Synchrotron Light for Biology, Chemistry and Medical Research

Giorgio Margaritondo, *École Polytechnique Fédérale de Lausanne, Switzerland.*
Oxford University Press, 2002
Price: £49.95 (hardback) , £24.95 (paperback)
ISBN 0-19-850931-X (hardback) ; 0-19-850931-6(paperback) + x + 260 pages.

Let me say right away that I have very mixed feelings about this book. It has much to commend it, and I was very favourably impressed as I started to read it. However, this was tempered by numerous shortcomings that emerged as I proceeded. It is, therefore, only a qualified recommendation that I finally make for it.

The book sets out "to present a simple, practical and broad picture of synchrotron light sources and of the corresponding experimental techniques." It is aimed particularly at readers who have little or no practical experience of synchrotron radiation (SR), particularly new graduate students. One of its main tasks, then, is to explain some of the jargon that has grown up with the development of SR over several decades.

The most positive aspects are the opening chapters, providing information about the basics of SR: its nature and properties, and the production and conditioning of radiation suitable for various experimental purposes. Explanations are given at two levels, a relatively qualitative one in the main text, and a more rigorously mathematical treatment in a series of clearly marked "Insets". The simpler explanation will satisfy many readers, while the deeper level is available for those who want more detail. I found these sections (skipping the Insets initially) easy to read and generally useful, and the informal style of writing helps. The different magnetic components of modern storage rings, responsible for generating SR with a range of characteristics, are well explained, together with some of the experimental arrangements and ways of operating SR facilities, and important properties such as coherence and polarisation. In this way, I reached the end of two of the book's five chapters (70 out of about 250 pages) with a generally very positive impression.

However, these sections are not without their problems, which include errors in some of the equations and incorrect units for physical quantities, and these are scattered throughout the book. Further flaws in later sections include the reversal of the definitions of cations and anions, errors such as the name potassium for the element with symbol P, and some symbols in equations that are confusingly different from those commonly used (such as *f* for structure factors and *F* for molecular scattering factors in the treatment of Fourier transforms in crystallography). The English is odd in places, which does not promote comprehension, and some of the descriptions of storage ring operations seem distinctly out of date and may be a legacy of material adapted from the author's previous and shorter text of 1985 (described in the Preface).

The longest chapter (more than half the book) is devoted to a description of applications of SR, divided into sections on imaging, spectroscopy, microscopy, EXAFS specifically, scattering and diffraction, and microfabrication techniques. The treatment here seems to me to be very variable, reflecting the author's own specialist interests. There is a clear bias towards biological and medical applications, which appear to be the best treatments, while applications in the physical sciences and engineering are less convincingly covered. The majority of examples in some of these areas are biological and medical, including a major emphasis on

macromolecular rather than chemical crystallography, on medical imaging, and on biological spectroscopy. Since this is a review for *Crystallography News*, I should say that I found many of the explanations and arguments in the crystallography section far from convincing and clear, especially regarding the phase problem, Patterson functions (particularly confusing), structure factors, and convolution. These are topics that are not specifically SR-related, and they seem to betray a lack of expertise in this area for the author. This is certainly not a primary reference for the basics of the experimental techniques! You should go elsewhere for that.

The book reverts to its initial style and attractiveness in dealing with some advanced topics at the end, particularly in the treatment of free electron lasers.

In conclusion, the book (much less expensive, as a paperback, than some of OUP's other recent publications) is a useful introduction to synchrotron radiation for those who know little about it and its uses, but it needs to be read in conjunction with better descriptions of some of the scientific applications. It's a pity about some of the serious errors. It would be worth having a copy for research groups making (or considering making) limited use of synchrotron facilities as non-experts.

Bill Clegg

Three New IUCr Teaching Pamphlets

International Union of Crystallography, 2002, available free on their website

Many years ago, the International Union of Crystallography produced two series of 'Teaching Pamphlets' on various aspects of crystallography, written by experts in the fields. The original versions were sold by the IUCr, as hardcopy versions. These have now been made available through the internet, and three new ones have been added to the series. They may be found, below the heading Publications, on the IUCr main website (http://www.iucr.ac.uk/) and it should be possible to view each and explore it with a web browser; some may be downloaded in pdf format and printed. (There are still some hitches!)

No. 20 : Crystals - A Handbook for School Teachers
Elizabeth A. Wood
28 A4 pages.

No. 20 is a 'reprint' of a delightful booklet by Elizabeth A. Wood, first published in 1972. The author, aware that many school teachers may not themselves have had much introduction to crystals, provides a series of experiments/activities which can be carried out by children, with simple explanations and comments. As she says in the introduction, 'the essence of science is by observation and wonder, curiosity and the effort to satisfy that curiosity' and she provides an excellent guide for children to do just that, at school or at home.

There is an introductory section on aims, and then equipment and materials. The text of the main sections is suitable for children to use directly. They are about growing and examining crystals from solution (salt, borax, sugar, alum, copper sulphate, and magnesium sulphate), crystals from a melt (ice, phenyl salicylate, bismuth), crystals from vapour (ice, naphthalene), observations with polarised light, other crystals that can be observed (rocks and minerals in museums or in open country, crystals in building stone, in jewellery, etc.). The practical instructions are clear and simple and leave me with the strong expectation that they will work; the comments lead in to the ideas of characteristic crystal shape, crystal faces, cleavage, and the underlying structure. The equipment used is mostly very simple (measuring cup, teaspoon, microscope slide or upturned glass, polaroid film, etc.). The suggested procedures appear to be safe, and with cautions where appropriate, though a modern teacher would also check C.O.S.H.H. rules. The level looks appropriate for early years of secondary school, or upwards. All this should enable a young person to 'observe, wonder and ask questions ', the stated aims of the author; she also states that the booklet is 'for all schools, everywhere in the world', and in commendable support of this aim, the IUCr has provided translations in Arabic,

Czech, Polish, Russian and Spanish in addition to the original English version.

The illustrations are the simple free-hand drawings of the 1972 original booklet, not as sophisticated as modern computer drawn figures, but completely clear and adequate. In republishing the booklet on the web the IUCr is quite right not to change this. It might, however, have been helpful to replace, or add to, the original three references given for further study; the latter were all published before 1965 and are not likely to be accessible. This is a very minor criticism, and the pamphlet can be very strongly recommended to all involved with encouraging young people to take an interest in crystals.

No. 21 : Crystal Packing
Angelo Gavezzotti
20 + 4 A5 pages

No. 21, Crystal Packing, is new. It is a simply and quite clearly presented introduction to the important factors in crystal packing, containing sections headed thermodynamics, the forces, crystal symmetry, symmetry elements, crystal structure descriptors, polymorphism (thermodynamics versus kinetics), chirality, experiments, and suggestions for the future. There is a simple description of intermolecular forces in ionic and molecular crystals, and formulae for the calculation of potential are presented. Hydrogen bonds are included, though there is little indication of the strength of these relative to ionic or covalent bonds or van der Waals interactions. The effectiveness of different symmetry elements for the packing of organic molecules in a crystal is then examined, and their combination in space groups. These are the factors which determine which packing arrangement is adopted in the crystal, and their consideration leads to an understanding of the observed distribution of space groups for these crystals.

Throughout, it is assumed that the reader is familiar with space group symmetry, and with the determination of crystal structures by X-ray diffraction, as well as with thermodynamic principles (free energy, enthalpy and entropy, G,H and S). In the general description of the series of teaching pamphlets the IUCr states that each is prefaced by a statement of aims, level, necessary background etc. Unfortunately no such statement is given here, nor does the material appear to live up to the IUCr's usual standards (as in their peer-reviewed journals) of presentation, quality of illustrations, accuracy and completeness of technical information. For example, in the section on crystal symmetry the author appears to say that the only symmetry elements which may contribute to the packing of organic molecules in crystals are the inversion centre, the 2-fold screw axis and the glide plane; while undoubtedly these are the commonest, others certainly do occur (3-, 4- and 6-fold screw axes, and pure rotation axes). Likewise, in Table 2 the heading should state that the space groups listed are the most commonly occurring ones, and that many others do occur, in smaller numbers. The blank entries in column 4 would be much more helpfully shown as (100%), and the heading of column 5 should be 'Point group symmetry of molecules in special positions'. Solvent molecules often play an important part in crystal packing, but there is no mention of them here. Finally, there is a brief statement that crystallisation from a racemic solution sometimes produces chiral crystals, in which only one isomer at a time appears, and that in these cases spontaneous resolution has been achieved. This appears to suggest that spontaneous resolution can occur, giving only crystals of one optical isomer; if it ever occurs, it is rare and unusual, and further evidence should be given. It would be helpful to state that the normal result of such a crystallisation is either racemic crystals, or equal amounts of chiral crystals of opposite chirality.

Despite these criticisms, a student with reasonable familiarity with crystallography could use this pamphlet to make a simple start on the topic of crystal packing, and perhaps go further with the set of references provided.

No. 22 : Matrices, Mappings and Crystallographic Symmetry
Hans Wondratschek
82 A5 pages

No. 22 is based on material

provided for a summer school in Egypt in 1997. The first part is concerned with points and vectors, and with matrices and determinants. It gives careful definitions and examples, including instructions for inverting 2x2 and 3x3 matrices. This material provides the mathematical tools and concepts which are applied in the main section (representing six lectures and 3 problem sessions) to crystallographic topics - space group operations, crystallographic groups, a detailed explanation of the form of the space group tables in International Tables Volume A, followed by the use of matrices to express crystallographic symmetry operations. There are examples, and three problems involving coordinate transformations, with solutions (and reasoning) provided. The explanations are mostly full and clear, and there are a good Table of Contents and a good index.

Regrettably, this pamphlet does not state the kind of crystallographic applications for which the author hoped to prepare the summer school students, or the expected entry level. The careful, painstaking definitions and explanations might be helpful to some research students, but some of the treatment of symmetry is over-elaborate for students in chemical or biological crystallography; it may be important in solid state chemistry or in the consideration of phase transitions. For example the author distinguishes 'space groups' and 'space group types': according to the mappings which it describes, there are an infinite number of space groups, and 230 space group types (p40). However, since matrices and crystal symmetry are topics which many people working in crystallography find difficult to understand and use, and since this pamphlet is so readily available, it makes good sense that such people should look at it and see if they find the approach useful.

Final Comments: The continuation of the teaching pamphlet series by IUCr is to be welcomed, but there are still a few technical limitations or hitches in the presentation. No 20, Crystals - A Handbook for School Teachers, is not yet available in pdf format; in the html version some tools for navigation would help - for example allowing each section to be entered from a table of contents. No 21, Crystal Packing, can be found in html or pdf format if Internet Explorer is used, but Netscape (v 4.7) finds neither ! For No. 22, Matrices, Mappings and Crystallographic Symmetry, there appears to be no html version yet, and the Adobe Acrobat reader is launched automatically. Also, the pdf versions of No. 21 and No. 22 appear as A5 pages, each centred within an otherwise blank A4 page - thus printing is not at all economical !

Marjorie Harding

Cohesion, a Scientific History of Intermolecular Forces

J.S. Rowlinson,
Cambridge University Press, 2002
Price: £65 (hardback)
ISBN 0-521-81008-6 (hardback); x + 342 pages.

The problem of cohesion - why matter hangs together in its non-gaseous forms - is the fundamental problem of condensed matter physics, and has held the attention of scientists continuously since the dawn of the modern scientific enterprise. John Rowlinson, a distinguished liquid-state theorist, has written a fascinating and well-documented account of this history.

Having pointed out that some of the ablest scientific minds have worked on the puzzle of cohesion (Chapter 1), Rowlinson organised the main, and most detailed, parts of his study (Chapters 2 to 4) round three 'big names': Newton, Laplace and van der Waals. Newton's commitment to a corpuscular theory of matter and his theory of universal gravitation led rather naturally to speculations on the nature of inter-corpuscular forces. Since the direct study of these forces did not become possible until well into the twentieth century, scientists during earlier periods had to *infer* information about them from macroscopic phenomena, principally (in Rowlinson's account) capillarity (Laplace, Young and others), crystalline elasticity (Poisson,

Navier, Cauchy, and others) and condensation (Andrews, van der Waals, and others). Studies of other phenomena, e.g. viscosity, also contributed. As we now know, a proper understanding of cohesion requires quantum mechanics to describe intermolecular forces, and statistical mechanics to relate them to bulk properties. These 20th-century developments are treated more briefly in Chapter 5.

The chief strengths of this book are two. First, Rowlinson's grasp of the science enables him to guide the reader firmly through the sometimes-obscure reasoning of previous generations of scientists. (This does mean, however, that the book is technically demanding.) Secondly, the book is a bibliographic treasure trove, with more than 1000 references to original publications spread over all the main European languages as well as Latin. There are also short biographical notes on all but the most well known of the scientists involved.

I have two *scientific* reservations. First, Rowlinson does not appear to distinguish between cohesion and rigidity. On p. 1, he asks: 'Why do gases condense to form liquids, liquids freeze to solids or, as it has been put more vividly, why, when we lift one end of a stick, does the other end come up too?' Condensation is indeed a matter of cohesion and attractive intermolecular forces. But freezing is about the emergence of rigidity - crystals have finite zero-frequency shear moduli because they are *symmetry-broken* states. Moreover, as Rowlinson knows (pp. 285f), hard spheres crystallise at high density - attraction is *not* essential. A clearer distinction between these two issues is called for. Secondly, the final chapter is strangely silent on ionic and metallic systems. While, as Rowlinson himself has pointed out, a comprehensive treatment of 20th-century sources would require a book of its own, brief comments on these important classes of (charged) condensed systems would have given a more well-rounded finale.

To conclude, I should point out that reading this book, one gets a good sense of the fitful, untidy way in which science develops. Professional historians and philosophers, who have often lamented the tidily linear 'history' presented in science text books, should be impressed! On the other hand, I am not convinced by Rowlinson's claim that 'sociological, political, religious and economic' factors have had little effect on the development of the 'specialised' subject of cohesion. I have little doubt that future studies will show how the study of cohesion was as integrated with its social milieu as were any other areas of science. This fine volume by Rowlinson has laid a firm foundation for such studies.

Wilson C K Poon, The University of Edinburgh

Single Crystal Neutron Diffraction from Molecular Materials

Chick C. Wilson, *CLRC Rutherford Appleton Laboratory.*
Series on Neutron Techniques and Applications, World Scientific Publishing, Singapore, 2000.
Price: £44.00 (hardback)
ISBN 981-02-3776-6, xiii + 370 pages.

The book is the second in a monograph series on Neutron Techniques and Applications, edited by J. L. Finney and D. L. Worcester. The author, Chick Wilson, is Group Leader in Crystallography and beamline scientist at the ISIS spallation neutron facility at the CLRC Rutherford Laboratory in the UK.

As its title suggests, the monograph focuses on single crystal neutron diffraction, though on molecular crystals rather than materials *per se*. There is clearly scope for a book such as this, aimed at chemists and chemical crystallographers, which makes it clear what single crystal neutron diffraction has accomplished and may in future be able to accomplish. The book effectively comprises two parts, the first (chapters 1-3) in which an introduction to crystallography, neutron scattering and single crystal neutron diffraction is provided, and the second, longer section (chapters 4-7) in which studies conducted up to 1999 are reviewed. The book concludes with a brief look forward (chapter 8) at the potential for the technique in the future. This

organisational style reminded me of Dunitz's classic book on "X-ray Analysis and the Structure of Organic Molecules" in which again there is a similar division between providing information on the fundamentals of the technique and demonstrating its chemical applications.

The book opens with a very brief introduction to crystallography in chapter 1. The majority of chapter 1, however, is devoted to outlining the areas that are covered in greater detail later in the book. Chapter 2 concentrates on neutron scattering, including very useful sections on different types of sources and detectors. The opening component on the properties of neutrons pertinent to scattering provides the necessary information but avoids the physics needed to understand the observed scattering lengths. Chapter 3 focuses on techniques, and takes the reader stepwise through aspects of a single crystal diffraction experiment that are specific to using neutrons rather than X-rays. These chapters are probably the strongest part of the book and reflect the author's many years of experience in single crystal neutron diffraction. However, while this section covers virtually all the important points, readers who are looking for more than an overview will probably need to seek an alternative source.

The next and largest section of the book is devoted to applications of single crystal neutron diffraction. The chapters on "The Accurate Location of Atoms," "Hydrogen Bonding," "Vibrations and Disorder" and "Materials Properties and Design." necessarily have some overlap, but most of the major areas of application to molecular crystals are covered. The main omissions are discussion of magnetic scattering and significant consideration of atoms other than hydrogen/deuterium.

Chapter 4 covers cases in which neutron diffraction can clarify structural ambiguities or inaccuracies in hydrogen atom position, e.g. tautomer identification, accurate bond length determination, structures of metal complexes with hydride and related ligands, and applications to structures of biological macromolecules, especially in characterising the water structure. This latter component is perhaps the best part of the chapter and provides valuable insight into an area that clearly has potential for important further development. Unfortunately, the major (25-page) component on hydride and related ligands is the weakest part of the book. The narrative works its way through studies of numerous compounds with 5-10 line descriptions, which read somewhat like a list. Too often, the chemical importance of the neutron diffraction study does not really come through, other than the common fact that neutron diffraction was necessary for accurate location of the hydride ligands. Given that there are comprehensive reviews on this specific topic in the literature, the most recent by Bau in 1997, a more valuable approach would have been to select a smaller number of case studies for more in-depth description. Such an approach could have been used to emphasise the importance of the neutron diffraction study and to bring out fully the chemical significance in each case. There are also a number of examples of incorrect chemical nomenclature and unclear wording, as well as misinterpretations or misunderstanding of the pertinent chemistry.
Chapter 5 provides a good overview of different types of hydrogen bonds (strong, weak, inter- and intramolecular, bifurcated, different donor and acceptor atoms, etc.) and different aspects of hydrogen bonding that have been studied by single crystal neutron diffraction. However, this is again an area in which there are many reviews available and more comprehensive coverage is likely to be found elsewhere. The narrative style improves upon Chapter 4, in that more extensive descriptions are provided for most examples presented. The chapter, however, does suffer from a number of inconsistencies and unclear statements, the worst offender being the overuse of the description "normal" or "as predicted", mostly without a frame of reference these terms. Section 5.2, entitled '*Normal*' *hydrogen bonds* does define such interactions to be, in the author's view, hydrogen bonds of medium length and moderate strength. However, within the same section, for example, dialuric acid is described as having a "normal, strong hydrogen bond."
Diagrams are generally clearly presented in this chapter and throughout the book, the exception being figures 5.8, 5.9, 5.12 and 5.13 in which hydrogen

bonds are inconsistently drawn as different types of dashed or solid lines, leading to confusion with covalent bonds.

Chapter 6 turns our attention from atomic positions to atomic and molecular motions. There is a good introduction to such motions, both harmonic and anharmonic and to crystallographic models used to describe them. Special attention is given to hydrogen atom motions, where neutron diffraction has its greatest advantage over X-ray methods. The chapter then concludes with a few examples of disorder and phase transitions as studied by neutron diffraction.

Chapter 7, on "Materials, Properties and Design", is inevitably a difficult one to write given that the impact of neutron diffraction in this area does not primarily involve the study of molecular crystals. The chapter includes brief sections, with examples, on structure determinations of bioactive small molecules, hydrogen-bonded NLO molecular materials, organic conductors, and on X-H…p hydrogen bonds studied in the context of crystal engineering.

The final chapter looks ahead to what improvements in instrumentation and sources might be attainable and what might be achieved with access to such facilities. Improvements in flux at the source and in utilization of those neutrons through multiple detector instruments are noted as exciting developments already in progress. The main area of study cited for major future development is in the study of biological macromolecules, while the core area of small molecule structural studies is expected to see increases in the rate of data collection and use of smaller crystals. Perhaps surprisingly omitted, is mention of magnetic scattering by neutrons, both here and throughout most of the book. Given the current high-profile work in molecular magnets based upon coordination networks, and the related area of single-molecule magnets, one might anticipate a valuable future role for polarised neutron single crystal diffraction studies.

In summary, this monograph should provide a valuable reference for chemists and chemical crystallographers seeking an overview of the technique of single crystal neutron diffraction and a perspective on its application to studies of molecular crystals. There is not an abundance of texts on neutron diffraction, and some of those most used were written many years ago. This monograph provides an up-to-date look at the practical aspects and applications of the technique and has an extensive list of references following each chapter. However, it is not without its problems, primarily in descriptions and interpretations of the chemical significance of results in parts of Chapters 4 and 5. It should nevertheless be a useful addition to Chemistry library holdings and, priced at *ca.* £40, to some personal collections.

Lee Brammer

Meetings of interest

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

3-7 March 2003
2003 American Physical Society March Meeting. Focus on High Pressure Research. Austin Convention Center; Austin, TX USA. [http://www.aps.org/meet/MAR03/index.html]

6-8 March 2003.
Workshop: "Structural Analysis of Aperiodic Crystals" University of Bayreuth (Germany) [http://www.uni-bayreuth.de/departments/crystal/inc-workshop2003/index.html]

10-13 March 2003
Second French-German Crystal Growth Meeting organized jointly by "Groupe Français de Croissance Cristalline (GFCC)" and "Deutsche Gesellschaft für Kristallwachstum und Kristallzächtung (DGKK)" Nancy, France. [http://www.lcm3b.u-nancy.fr/FGCGM2003/]

12-16 March 2003
The NICEST JINS Workshop: Neutrons in Solid-State Chemistry and the Earth Sciences Today and Tomorrow (NICEST) Oak Ridge, Tennessee, USA. [http://www.sns.gov/jins/NICEST2003/]

17 March 2003
1st Annual Biomaterials Workshop, Department of Materials & Medical Sciences, Cranfield University, Shrivenham
E-mail: S.E.Etok@rmcs.cranfield.ac.uk

6-11 April 2003
EGS-AGU-EUG Joint Assembly, Nice, France
[http://www.copernicus.org/egsagueug/]

7- 9 April 2003
Infrared and Raman Spectroscopy for Pharmaceutical Applications, Stamford, Connecticut, USA
[http://www.assainternational.com]

7-15 April 2003
9th BCA/CCG Intensive Course in X-ray Structure Analysis, Durham
[http://bca.cryst.bbk.ac.uk/BCA/CCG/du03rg.pdf]

9-11 April 2003
International workshop on hard synchrotron X-rays for texture and strain analysis, HASYLAB, Hamburg
[http://www-hasylab.desy.de/conferences/workshop/]

14-17 April 2003
BCA Annual Meeting, University of York
[http://bca.cryst.bbk.ac.uk/BCA/meets/BCAs.html]

28 April - 2 May 2003
Practical X-ray Fluorescence Spectrometry, ICDD clinic, Newtown Square PA, USA
[http://www.icdd.com/]

29 April - 1 May 2003
12th Users Meeting for the Advanced Photon Source. Argonne, IL, USA
[http://www.aps.anl.gov/conferences/12um/]

12-16 May 2003
2003 Particle Accelerator Conference - PAC2003, Portland, OR, USA
[http://www.conf.slac.stanford.edu/pac03/]

12-17 May 2003
Charge Density Workshop, Chemistry Department, State University of New York, Buffalo, USA
[http://harker.chem.buffalo.edu/group/announcement/xd.html]

19-21 May 2003
2003 NSLS Users' Meeting, Upton, NY, USA
[http://nslsweb.nsls.bnl.gov/nsls/users/meeting/Default.htm]

19-23 May 2003
Third National Crystal Chemical Conference, Crystal Chemical Section of the Scientific Council on Chemical Structure and Reactivity of the Russian Academy of Sciences, Moscow, Russia
[http://www.icp.ac.ru/Conference/NCCC3/]

25-30 May 2003
The Seventh International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors (M2S-HTSC-VII), Rio de Janeiro, Brazil
[http://www.m2srio.cbpf.br]

25 May - 1 June 2003.
Fourth European Workshop in Drug Design, Certosa di Pontignano (Siena), Italy
[http://www.unisi.it/4EWDD.]

1-5 June 2003
6th Multinational Congress on Microscopy, Pula,Croatia
[http://www.6mcm.kbsm.hr/]

2-6 June 2003
Fundamentals of X-ray Powder Diffraction ICDD clinic, Newtown Square, PA, USA
[http://www.icdd.com]

4-15 June 2003
High Pressure Crystallography Erice, Italy
[http://www.geomin.unibo.it/orgv/erice/highpres.htm]

7-11 June 2003
The Clay Minerals Society 40th Annual Meeting jointly with the Mineralogical Society of America, Athens, Georgia, USA
[http://cms.lanl.gov]

9-13 June 2003
Advanced Methods in X-ray Powder Diffraction, ICDD clinic, Newtown Square PA, USA
[http://www.icdd.com]

15-20 June 2003
The 4th International Workshop on Physical Characterization of Pharmaceutical Solids, Danbury, CT USA
[http://www.assainternational.com]

20-25 June 2003
LERM 2003, International Symposium on the Role of Light Elements in Rock-forming Minerals Nové Mestona, Czech Republic
[http://sci.muni.cz/~lerm/index.htm/]

21-25 June 2003
5th EMU School: Ultra-high pressure metamorphism, Budapest, Hungary
[http://www.univie.ac.at/Mineralogie/EMU/]

22-25 June 2003
XIIth International Workshop on Quantum Atomic and Molecular Tunnelling in Solids, University of Florida in Gainesville, USA
[http://www.clas.ufl.edu/QAMTS]

22-26 June 2003
Euroclay 2003, Modena, Italy
[http://www.unimo.it/euroclay2003/]

22-27 June 2003.
The 12th International Conference on X-ray Absorption Fine Structure (XAFS 12), Malmö Sweden
[http://xafs12.maxlab.lu.se/]

22-27 June 2003
8th International Kimberlite Conference, Victoria, BC, Canada
[http://www.venuewest.com/]

22-27 June 2003
Gordon Research Conference on Thin Film and Crystal Growth Mechanisms Mount Holyoke College, South Hadley, MA, USA
[http://www.chem.cornell.edu/ThinFilm/]

29 June - 3 July 2003
11th Annual International Conference of Intelligent Systems for Molecular Biology, Brisbane, Australia
[http://www.iscb.org/ismb2003]

7-10 juillet 2003
Le colloque de l'Association Francaise de Cristallographie , Caen, France
[http://www.crismat.ismra.fr/afc2003/index.html/]

20-24 July 2003
The Fifteenth American Conference on Crystal Growth and Epitaxy (ACCGE-15)
Keystone, CO, USA
[http://www.crystalgrowth.org/conferences/ACCGE15/index.html]

24-26 July 2003
2003 Current Trends in Microcalorimetry, Boston Marriott Copley Plaza, Boston, MA, USA
[http://www.microcalorimetry.com/seminars/2003Conference2.html]

26-31 July 2003
American Crystallographic Association Annual Meeting, ACA 2003, Cincinnati, Ohio, USA,
[http://www.hwi.buffalo.edu/ACA/ACA-Annual/futuremeetings.html]

4-6 August 2003
Polarised Neutrons and Synchrotrons X-rays for Magnetism, Venice
[http://venice.infm.it]

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/]

16-22 August, 2003
Symmetry 2003, Budapest, Hungary
[http://www.conferences.hu/symmetry2003/]

24-30 August 2003
21st European Crystallographic Meeting, Durban, South Africa,
[http://www.ecm21-africa.co.za/]

25-29 August 2003
Eighth International Conference on Synchrotron Radiation Instrumentation, San Francisco, CA, USA
[http://www.sri2003.lbl.gov/]

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/]

7-12 September 2003
13th V.M. Goldschmidt Conference, Kurashiki, Japan
[http://www.ics-inc.co.jp/gold2003]

8-13 September 2003
Aperiodic-2003, Belo Horizonte, Brazil
[http://www.fisica.ufmg.br/~ap2003/]

8-18 September 2003
8th Oxford School on Neutron Scattering, University of Oxford, Mansfield College
[http://www.isis.rl.ac.uk/conferences/osns2003/]

14-19 September 2003
Structure Solution from Powder Diffraction Data, Stara Lesna, Slovak Republic
[http://www.sspd-03.sav.sk]

22-26 September 2003
XVII International Congress on X-ray Optics and Microanalysis", Chamonix Mont Blanc, France
[http://www.esrf.fr/Conferences/ICXOM]

6-10 October 2003
Introduction & Advanced X-Ray Diffraction For Pharmaceutical Applications, Danbury, CT, USA
[http://www.assainternational.com]

15-17 October 2003
Polymorph Screening - Techniques & Applications, Stamford, Connecticut, USA
[http://www.assainternational.com]

24-31 October 2003
International Symposium on Radiation Physics. Cape Town, South Africa
[http://www.medrad.tlabs.ac.za/isrp9.htm/]

10-21 June 2004
Polymorphism : Solvates and Phase Relationships. Erice, Italy
[http://www.geomin.unibo.it/orgv/erice/bernstei.html]

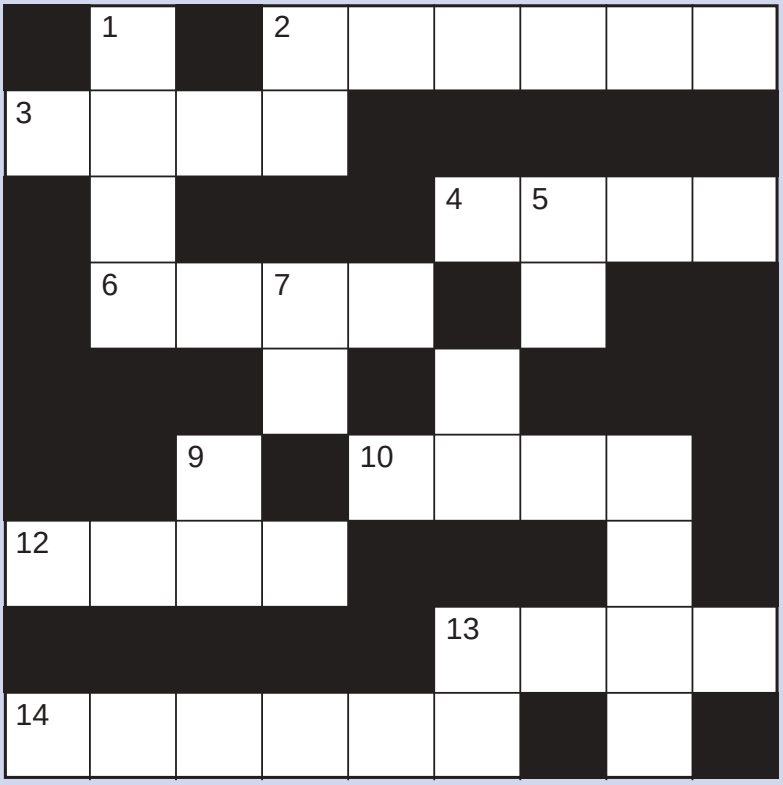
20-28 August 2004
32nd International Geological Congress, Florence, Italy
[http://www.32igc.org/]

August 2005
XX Congress of the International Union of Crystallography, Florence, Italy
[Carlo Mealli, email: mealli@fi.cnr.it]

28 November - 2 December 2005
The dates for the 2005 International Conference on Neutron Scattering, Sydney, Australia. A website will be up and running shortly.

Puzzle Corner

This month's puzzle is a cross"word" - in fact all of the answers are valid space-group symbols, although not all are standard settings! The convention is that a number, including one with a subscript or a "bar", occupies one space. A solidus or a letter also occupies one space. Following the Windows, rather than the Unix convention, we are case insensitive! The usual £10 book token is offered for the first correct solution submitted to the Editor before 1 May 2003.



Across

2. Graphite
3. non-polar, but no special positions
4. add centre to 3-across
6. contains recently rebranded glide
10. Non-standard setting of this could be Muslim cleric!
12. garnet - and the end of all things
13. non-standard 4 across
14. Body centred cubic gets stretched along edge!

Down

1. Top of the pops for molecules
2. Number 2 for chiral molecules
5. "First setting" of C2
7. Beware of Marshing!
8. Non-standard and nickname for God (Exodus 3.14)?
9. Face centred cubic gets stretched along diagonal
11. Sub-group of 6 across

Sadly, last month's puzzle did not get any replies. Maybe people had better things to meditate about over Christmas. My analysis of the Chartres labyrinth is as follows.

Fixed constants:
number of "teeth" on the border.
number of leaves in the centre.

Variable parameters:
Overall scale factor
Diameter of central circle
Width of border
Ratio of "track" width to "wall" width
Width of extra wall at turning points

I think that that about does it, but I'm happy to share "my" prize with anyone else who has a better analysis!

The winner of the previous competition, who not only solved the cryptogram but said where it came from was Dr E.J.W. Whittaker, to whom congratulations and apologies.

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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.
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From the Vice President.

Notice of proposed changes to the Statutes and By-Laws of the British Crystallographic Association

Introduction

A new class of BCA membership has been discussed by Council for consideration at the 2003 AGM in York. Council propose that two new grades of membership (Fellow and Life Fellow) are adopted for introduction in the 2004 membership year.

These new grades of Membership require the following changes (underlined) to Statute B Membership.

Clause 2. There shall be **seven** classes of membership, as follows:

a. Ordinary Members

b. Joint Members

c. Corporate Members

d. Founder Members

e. Honorary Members.

f. *Fellows*

g. *Life Fellows*

Two additional clauses to be added before the final clause:

Fellows - shall be those persons whose application for membership satisfies eligibility criteria set by Council, is approved by Council and pay an annual subscription. This subscription shall be double the full membership fee paid by Ordinary Members. In all other contexts the expression Ordinary Members shall include Fellows.

Life Fellows - shall be Fellows of 10 or more years standing who are over 65 years of age. The Officers of the Association shall from time to time recommend the name(s) of person(s) deserving of Life Fellowship of the Association, and such recommendations must be ratified by Council. Life Fellows shall be absolved from paying annual subscriptions but in all other contexts the expression Ordinary Members shall include Life Fellows.

The final clause becomes:

The rights and privileges of Ordinary and Joint Members, *Fellows and Life Fellows* and of Corporate Members are as prescribed in Statute F, Statute H, and the By-Laws.

If this proposal is ratified by the membership then it is also proposed that the 28 existing 'life members' will be made 'life fellows'.

The ability to award 'life fellowship' is deemed necessary to allow council flexibility in the next few years to accommodate long standing members who fall short of 10 years 'fellowship' at 65 years of age.