ISSN 1467-2790

CRYSTALLOGRAPHY NEWS

British Crystallographic Association

No.80

March 2002

Agendas for BCA Spring Meerting 2002

The Chatt Lecture, 2002

Educational Models and Crystal Growth in Schools

CCP4 at York

Quarterly





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

NEXT ISSUE OF CRYSTALLOGRAPHY NEWS

CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association. Text should preferably be sent as MSword documents (any version - .doc files) or else as .rtf on a PC disk or electronically. Diagrams and figures are most welcome, but, if possible, please send them separately from text as .jpg, .gif, .tif or .bmp files. Items may include technical articles, news about people (e.g. awards, honours, retirements etc.), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews. Please ensure that items for inclusion in the **June 2002** issue are sent to the Editor to arrive before **19th April 2002**.

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

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

Contents

President's Remarks

Cover pictures left to right:

Sir Tom Blundell at the Chatt Lecture

Snowflake? See Puzzles page!

Prizes for Edinburgh Primary School Crystal Growers

Ian Langton receives the Industrial Group Award

Dr Richard Walker, new Technical Director of Diamond

First, a warm welcome to Bob Gould who is our new newsletter editor. Bob needs no introduction to most of you, and I am sure that he will stamp his crystallographic knowledge and humour on this publication in a very personal way. At the same time I would like to record a great 'thank you' to Jo Jutson, who has overseen the major changes in the newsletter that have taken place in the past year. The new format is now one year old, and will be reviewed at our next Council meeting. Most people seem to prefer it. Although it is more expensive to produce than the old A5 format with a lot more colour, it is proving very popular with advertisers. It has always been profitable (with thanks to Northern Networking for their help with this), but profitability is rising, and we are having to increase the number of pages devoted to advertisements. I also note with some pleasure that it sits on reception desks in a lot of places I visit, and looks good. I feel that it is a very positive reflection on the BCA and all its work.

We continue to grow: We now have over a thousand personal members and ten corporate ones making us easily the largest crystallographic association in Europe and second only to the ACA worldwide.

Why all these statistics? Well, the BCA is 20 years old this year, and it seems to me that crystallography, and the UK community has amply fulfilled the vision of its founders. I am writing this at the ESRF; who could have forseen such developments in radiation sources; the rise of macromolecular crystallography; new detectors and the ability to study materials that are less and less crystalline. And in the next 20 years we should have the free electron laser working at hard X-ray wavelengths, and with it diffraction from single particles and even cells.

What better way to celebrate our twenty years than at the Nottingham Spring Meeting? It is an exceptional programme - very interdisciplinary with central themes running over several days, and enough to interest everyone, and maintain that interest throughout the meeting. A lot has been done to make it affordable to students. It is a pleasant campus as well - I look forward to seeing you there.

Chris Gilmore
February 2002

BCA Council Members 2001 - 2002

President (2003)
Prof. Chris J.Gilmore
Department of Chemistry
University of Glasgow
GLASGOW G12 8QQ
tel: 0141 330 3716
chris@chem.gla.ac.uk

Vice President (2004)
Prof. Paul Fewster
Philips Analytical Research Centre
Cross Oak Lane
Redhill RH1 5HA
tel: 01293 815714
paul.fewster@philips.com

Secretary (2004)
Dr. Christine Cardin
University of Reading
Dept of Chemistry
Whiteknights
Reading RG6 6AD
tel: 0118 9318215
c.j.cardin@reading.ac.uk

Treasurer (2003)
Mr. David J.Taylor
35 Birchley Road,
Billinge
WIGAN
Lancs WN5 7QJ
tel: 01744 893108
djtaylor@lineone.net

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

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

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

GROUP REPRESENTATIVES

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

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

Industrial
Prof. Christopher S. Frampton
Department of Chemistry
University of Southampton
Highfield
Southampton SO17 1BJ
tel: 02380 594167
chrisf@soton.ac.uk

Physical Crystallography
Dr C.C.Wilson,
Rutherford Appleton Laboratory,
ISIS Facility,
CHILTON,
Oxon OX11 0QX
tel: 01235 82 1900 ext 5137 or 01235 44 5137,
C.C.Wilson@rl.ac.uk

Co-opted Members
Prof. P.Barnes,
Department of Crystallography,
Birkbeck College,
Malet Street,
LONDON, WC1E 7HX
tel: 020 7631 6817
barnes@img.cryst.bbk.ac.uk

Prof. M.M.Woolfson FRS (2002)
University of York
Department of Physics
Heslington
York, Y01 5DD
tel: 01904 432 238
MMW1@unix.york.ac.uk

Ex-officio Members

Editor "Crystallography News"
Dr Robert Gould
33 Charterhall Road
Edinburgh EH9 3HS
Tel: 0131 667 7230
bob@gould.ca

Education Officer
Mrs K.M.Crennell
'Fortran Friends'
P.O.Box 64
Didcot
Oxon OX11 0TH,
tel: 01235 834 357
BCA@ISISE.RL.AC.UK

GROUP CHAIRMEN

Biological Structures Group
Dr. Richard Pauptit
Protein Structure Lab
AstraZeneca,
Mereside,
Alderley Park,
Macclesfield
SK10 4TG,
tel: 01625 516135
richard.pauptit@astrazeneca.com

Chemical Crystallography Group
Prof. Paul R. Raithby
Department of Chemistry
University of Bath
Claverton Down
BATH BA2 7AY
tel: 01225 323183
p.r.raithby@bath.ac.uk

Industrial Group
Prof. Christopher S. Frampton
Department of Chemistry
University of Southampton
Highfield
Southampton SO17 1BJ
tel: 02380 594167
chrisf@soton.ac.uk

Physical Crystallography Group
Professor J.L. Finney
Department of Physics & Astronomy
University College London,
tel: 0171 380 7850
j.finney@ucl.ac.uk

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

If you are reading this, it implies that the fifth issue of Crystallography News in A4 format, and issue number 80 overall has seen the light of day! I am grateful to the Council of the BCA for having offered me the post of Editor, and I look forward to getting to know more of you better in this role. I have been a member of the BCA from the beginning, and in the busy life that goes under the name of "retirement" hope to serve in the post for at least two years. Jo Jutson, who edited the News last year, and oversaw the big changes in format and organization, has been most kind in helping me to learn the ropes. She will, however, not be an easy act to follow!

I gladly acknowledge the help of group secretaries and others in submitting reports without too much arm-twisting. In particular, this issue would not have been possible but for the stalwart work done by our Education Officer Kate Crennell in rooting out items of interest from all sorts of places. Thank you Kate!

The contents of the Nottingham meeting were given almost in entirety in a pull-out section in the December issue, so they are not repeated here. The summary program, in its form at the time of going to press, is, however, in the middle of this issue, together with agendas for the meetings of the BCA and the four groups.

In this issue, in addition to reports of some lively group meetings, there is an account of what was clearly a very useful CCP4 study weekend in York and the Chatt Lecture given by Sir Tom Blundell.

Our sister organization, the Mineralogical Society, is hosting the quadrennial meeting of the International Mineralogical Society in Edinburgh from September 1–6 this year. These meetings contain a lot of crystallography, and I can recommend them highly as lively and interesting. See http://www.minersoc.org/IMA2002.

In addition to getting news about two meetings devoted to the properties of ice [in Indianapolis in March and Newfoundland in July(!) – see meetings' list for websites], we have received an E-mail from Dr. Marina A. Balakshina in Russia. She is coordinating an ISTC project studying a large range of properties of ice. She is looking for international collaborators, and would gladly hear from anyone interested at bal@niik.vniief.ru.

Despite the help I have had, I have doubtless missed some things that should have been included. Please, all of you, send me your E-mails about anything that you think would be interesting. In addition, I would welcome suggestions of any sort for new features or improvements. The Puzzle corner has been revived, and I hope that that will generate some interest. Its success will depend of your reactions. On a more basic level, we will soon have exhausted all the reasonable colours for the front cover of the News and will need a new design. Suggestions for replacements for the diffraction pattern currently used as a background would be thus be gratefully received.

Bob Gould
February, 2002

Acknowledgements
BCA Sponsors

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

News from ISIS

New Technical Director for Diamond

On 13 November 2001 the CLRC Press release announced the appointment of the Technical Director for Diamond, the synchrotron due to be built at the CLRC Rutherford Appleton Laboratory. He is Dr Richard Walker, who started his new job on 7 January 2002. The appointment has been made jointly by the OST, the Wellcome Trust and the French Government. Dr Walker has been at Sincrotron Trieste in Italy since 1988 where he was Director of the Light Sources Division. Prior to his employment in Italy Dr Walker spent 13 years in the Accelerator Physics Section at Daresbury Laboratory in Warrington, location of the UK's Synchrotron Radiation Source (SRS).

BTM Willis Prize awarded to Chick Wilson

Congratulations to Chick Wilson; he has been awarded the first BTM Willis Prize, given by the Neutron Scattering Group of the Institute of Physics and the Royal Society of Chemistry, for outstanding contributions to neutron scattering science.

He delivered his prize lecture, entitled 'Beyond the Thermal Ellipsoid in Molecular Crystal Structures', at the Neutron and Muon Users Meeting recently in Grenoble at the ILL.

The Willis Prize and Lectureship is now an annual award in honour of Terry Willis, a founding father of the neutron scattering group. It is expected that normally the recipient of the lectureship will be under 40 years old and employed at a British University, Institution or Research Facility (including the Institut Laue Langevin, Grenoble). A detailed nomination must be made to the Chairman of the Neutron Scattering Group and must be accompanied by three letters of support from appropriate authorities in the field, of which at least two must be from outside the nominee's institution. For further information, see http://www.isis.rl.ac.uk/NSG

New! Diamond Web discussion group

Members of the diamond user community are invited to contribute to our newly launched web discussions group. From here you can search the archives , post a message and look at messages gathered by the month of posting.

The discussion area is available at http://www.diamond.ac.uk/Activity/ACTIVITY=Discussions;
This discussion area is only available to registered users. To register, fill in the application form located at the link above.

Philip Leverhulme Prizes for 2002

"This could be of interest to some of our younger readers"!

Kate Crennell

The prizes, which are awarded annually, are intended to recognise the achievement and to facilitate the work of outstanding researchers, normally under the age of 36, in a specified number of fields. Each prize has a value of £50,000 and the prize holder may spend the award on a research purpose of his or her own choosing.

Nominations are invited in the following subject areas:

* Biochemistry and Molecular Biology
* Earth, Ocean and Atmospheric Sciences
* Economics
* Software Technology for Information and Communications Systems
* History since 1800

It is expected that 25 prizes will be awarded across the sum of the five disciplines. No more than 2 prizes will be awarded to any university in any one discipline.

Further details are as follows:

Prizes:

Each Prize carries an award of £50,000. This will be paid in 2 equal instalments to the Prize holder. The 1st will be made when the holder takes up the Prize with the 2nd made 12 months later.

Use:

Expenditure from the award may be used for any purpose related to the advancement of the research of the Prize holder, provided that the items of expenditure fall within the categories classically eligible for the support of the Leverhulme Trust. e.g. research assistance, teaching replacement, travel and subsistence, consumables, technical and clerical support or computing and software. The award may not be used to fund capital equipment, augmentation of the Prize holder's salary or institutional overheads.

Eligibility:

Candidates must hold a post in a UK institution of HE and should normally be under 36 on 15 May 2002. Account will be taken of the circumstances of candidates who have begun their academic careers late or who have experienced career changes or breaks. Nominators should make an explicit statement of such circumstances where nominees are over 36.

Nominations:

Nominations should be made be the nominee's head of department, but must be endorsed by the head of the institution. No more than two Prizes will be granted in any one discipline to any one university.

Awards:

Prize holders will be asked to give brief details of the broad area of research for which they agree to accept the Prize, and to provide a brief interim and final report with details of their achievements and with an indication of how funds have been spent.

Timing:

The closing date for receipt of nominations at the Leverhulme Trust is 15 May 2002. As applications must be submitted through your own institution, it will normally have a somewhat earlier deadline.

Application Materials are available from the Leverhulme Trust (1 Pemberton Row, London EC4A 3BG) direct or from their website: http://www.leverhulme.org.uk

Biological Structure Group News

Andrea Hadfield
Secretary/Treasurer
a.t.hadfield@bris.ac.uk

Biological Structure Group - Logo Competition Update

There were three entries for the BSG logo competition: A, B and C.

A vote was held at the Winter meeting (200 attendees) with the following results:

A) 12 votes

B) 9 votes

C) 15 votes.

Logo C was therefore the winner by 3 votes (J. Cooper, Southampton). However, we have since discovered that there are other logos incorporating the three strands motif (e.g. Birkbeck Centre for Structural Biology) - D and we are looking for a logo to create a separate, easily recognisable (and potentially protectable) identity. The committee has taken professional advice and, bearing in mind this advice, along with the suggestions and votes from the competition, will produce a logo in time for the Spring meeting at Reading.

Logo A

Logo B

Logo C

Logo D

Biological Structures Group Winter Meeting 2001

The Winter Meeting of the British Crystallographic Association, Biological Structures Group: "Membrane proteins: Challenges to Structural Biology", held on Monday 17 December 2001 at Imperial College, London attracted a record number of attendees (>200). The meeting focussed on the recent results in membrane protein research, including expression, crystallisation and structural studies and covered a wide range of methodologies including kinetic crystallography, electron microscopy and single-molecule observation. A meeting report is on page 12.

Biological Structures Group Sessions at BCA Spring Meeting

Nottingham 25th - 28th March 2002

BSG sessions organiser, to whom scientific enquiries/comments should be addressed:
Dr. Peter Moody
E-mail: pcem1@leicester.ac.uk

Late registration is still available for this meeting. For details, see the BCA Website.

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

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

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

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

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

CCP4 Workshop
Software demonstration including recent developments and overview of CCP4 software.

Biological Structures Group Winter Meeting 2002

The BSG winter meeting will be held in Warwick in 2002, organised by Vilmos Fulop. The suggested topic is "Macromolecular Complexes". Subject and speaker suggestions will be welcomed by Vilmos.

Chemical Crystallography Group News

Harry Powell
(hrp1000@cus.cam.ac.uk)
Secretary/Treasurer

Autumn Meeting 2002

The next CCG Autumn Meeting will be held at King's College London on Wednesday 13 November 2002. The local organisers are Jon Steed and Jamshed Anwar. The title of the Meeting is "Dealing with Difficult Data" and so far the following have agreed to speak:

Simon Parsons (Edinburgh)
Simon Teat (Daresbury)
Simon Coles (Southampton)
David Watkin (Oxford)

As usual, there will be the opportunity for short presentations, and anyone wishing to offer one should contact the CCG Deputy Chairman, Sandy Blake (email: A.J.Blake@nottingham.ac.uk). Further details will appear in later issues of Crystallography News.

Industrial Group News

Phil Holdway
(pholdway@QinetiQ.com)
Secretary/Treasurer

Change in Program for BCA Spring Meeting: Title for Chris Frampton's talk in the polymorphism and structural change session is "A Beginners Guide to Polymorphism".

Physical Crystallography Group News

Chick Wilson
(c.c.wilson@rl.ac.uk)
Secretary/Treasurer

PCG/ISIS Workshop: Introduction to the Principles and Practice of Rietveld Refinement

The workshop will take place immediately prior to the Nottingham BCA meeting, on Sunday 24 and Monday 25 March, 2002, in Room A63a in the Economics & Geography Building.
This meeting is intended to begin a series of tutorial workshops organised by the PCG on powder diffraction profile refinement methods. This technique, much used and a vital component of much of physical crystallography, is very powerful but if improperly used can lead to problems both in the refinement process itself and in the resulting structural models. The aim of these workshops is to provide a general introduction to the method and its applications. They are aimed both at those new to the technique, particularly research students and post-docs, and at those who feel the need for a refresher. The first of these workshops will introduce the basics of profile refinement using the Rietveld method. The workshop will include introductory lectures, demonstrations and hands-on examples. Topics will include:

- principles of Rietveld refinement, including minimisation;
- crystal structure refinement and what it achieves, including the use of constraints and restraints;
- data collection strategies, including angle- and energy-dispersive techniques with both X-ray and neutrons;
- basic refinement strategies - how to give yourself the best chance to get the right result;
- an introduction to some of the software suites available.

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

http://www.isis.rl.ac.uk/crystallography/rietveldworkshop.htm or http://bca.cryst.bbk.ac.uk/bca/pcg/riet2002.htm

Otherwise contact the organiser, **Chick Wilson** (c.c.wilson@rl.ac.uk), for further details.

PCG/SCMPG Bursaries

The PCG welcomes bursary applications from BCA or IoP members who are affiliated to the PCG or to the Structural Condensed Matter Physics Group of the IoP. These are intended mainly to help young scientists (students and post-docs) to attend meetings and conferences relevant to PCG/SCMPG areas of

interest. Bursaries can be applied for at any time, through the PCG/SCMPG Secretary (C.C.Wilson@rl.ac.uk) and will be considered by the Group Committee. However, each year we expect to target selected meetings as highly relevant for the award of bursaries. The IUCr XIX Congress in Geneva, August 2002, is the next targeted meeting.

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

Bursary Report 2001 - From the Treasurer

The Bursary fund was renamed the Arnold Beevers Bursary Fund in March of this year and £20,000 of funding was allocated from the IUCr windfall. Several generous donations have boosted the fund by almost £500. The GIFT AID refund of £668 has also been allocated to the fund.

The Reading Spring Meeting saw 40 bursaries of £50 awarded to students from 15 Universities.

Through the year **Arnold Beevers Bursaries** were awarded to all 7 applicants.

Applicant	Institution	Conference*	Award
Miss C K Broder	Durham University	ICC Sicily	£200.00
Mr S T M Allard	St Andrews	ACA - USA	£200.00
Mr A R Oganov	U College London	ECM20 - Poland	£200.00
Miss N Martin	Univ of Newcastle	ECM20 - Poland	£200.00
Mr T S Lyford	Univ of Warwick	ECM20 - Poland	£200.00
Dr E Ferrari	UMIST	ISPC -USA	£200.00
Mr V L Jennings	Univ of Warwick	IMF 10 - Madrid	£200.00

Conference details:

- ICC - International Course in Crystallography, 32nd Course, Erice, Sicily.
- ACA - American Crystallographic Association Annual Meeting, Los Angeles,
- ECM20 - 20th European Crystallography Meeting, Krakow, Poland
- ISPC - 3rd International Symposium: Polymorphism & Crystallisation, San Francisco, USA.
- IMF 10 - International Meeting on Ferroelectrics, Madrid, Spain.

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

£800.00 Neutron Summer School, Oxford
£500.00 Schools Crystal Growing Competition

Did you know that the BCA has fewer than 150 Student Members and no University has more than 10 student members? There must be lots more students out there who should be members and are missing out on the chance of a Bursary (you must be a member for 6 months before applying). Please inform potential student members of the benefits of the £6.00 - £7.50 membership fee.

David Taylor

2002 Annual General Meeting of the BCA

Notice is hereby given that the Annual General Meeting of the British Crystallographic Association will be held on Wednesday 27th March 2002 at 4.00 p.m. in room C16 of the Pope Building in the University of Nottingham.

The current Council members and Officers of the society are all due to continue in post until 2003 or 2004, so there will be no election at this meeting.

Agenda

1. Approval of Agenda
2. Apologies for absence
3. Minutes of the last AGM (published in the December, 2001 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 2001 and the Examining Accountant's Report.
7. Acceptance of the Accounts
8. Election of Officers and Ordinary Members of Council.
9. Appointment of Examining Accountant for 2002.
10. Any other business.

(It would be helpful if items for inclusion under 2 and 10 could be notified to the Secretary before the meeting)

Christine Cardin (Hon Secretary)

From the Secretary

The present membership of Council is as follows -

President
Professor Christopher Gilmore

Vice-President
Dr Paul Fewster

Secretary
Dr Christine Cardin

Treasurer
Mr David Taylor

Members
Dr Margaret Adams
Dr Jeremy Cockcroft
Professor Paul Raithby

Group Representatives
Dr Andrea Hadfield (BSG)
Dr Harry Powell (CCG)
Dr Chick Wilson (PCG)
Professor Christopher Frampton (IG)

Co-opted
Professor Paul Barnes
Professor Michael Woolfson (retires 2002)

Ex Officio
Dr Robert Gould (Editor, Crystallography News)
Mrs Kate Crennell (Education Officer)

Annual Report to the Council (2001)

Northern Networking now run much of the administration of the BCA. In addition they have been closely involved in the organisation of the Spring Meetings, at Reading in 2001, Nottingham in 2002, and forthcoming at York in 2003.

The Council has met twice during the year: during the Spring Meeting at The University of Reading, and at Birkbeck College, London in October 2001. At the AGM in Reading, Professor Paul Fewster was elected as Vice President, Dr Christine Cardin was elected as Secretary.

In 2001 the newsletter appeared in its new A4 format under the Editorship of Jo Jutson. Four excellent issues have appeared, and Council is very grateful both to Kate Crennell, for all her hard work in creating the conditions for the successful transfer to the new format, and to Jo Jutson for her effort in managing the transition to the new arrangements. Publication of the newsletter remains a very important activity for the BCA, with the website the main medium for current details of meetings and committee membership changes.

During the year there were several meetings and workshops. All four Groups have held meetings, including ones on 'Membrane proteins: Challenges to Structural Biology', attended by about 200 people (Imperial College, London),

'Mesomolecular Structures' in Aston University, 'Applications of High Pressure in Structural Studies' at the Daresbury Laboratory, and 'Crystallography in Industry' at Pilkington plc. The Eighth Intensive Course in X-Ray Structural Analysis in Crystallography was held in Trevelyan College, University of Durham.

Membership is approaching 1000, and a campaign is currently underway to increase membership both among students and among the biological structure community (which has grown considerably in recent years). Many young crystallographers have received BCA bursaries to attend meetings and conferences, both in the UK and worldwide. The Nottingham Spring Meeting will have free registration to students presenting posters, and efforts are currently being made to provide more student bursaries through named industrial bursaries as well as those from the Arnold Beevers Bursary Fund. The future of the Spring Meetings depends on the success of these efforts, as numbers attending have been steadily falling.

It is a pleasure to record that in 2001 Richard Nelmes was made an OBE, that Andrew Leslie and George Sheldrick have been elected Fellows of the Royal Society, and that Julia Higgins was made a Dame in the Queen's Birthday Honours. Jack Dunitz was made a Honorary fellow of the Royal Society of Chemistry, Jane Brown was awarded the 2001 Walter Hälg Prize, and Chick Wilson the first ever B.T.M. Willis Prize. Dorothy Hodgkin was honoured by the presentation of a Royal Society of Chemistry Landmark in Oxford. All these events and others have been recorded in Crystallography News.

We are looking forward to the BCA Spring Meeting in Nottingham. The Plenary Session is on 'New Methods of Structure Solution and Phasing' and the local organisers are Sandy Blake and Claire Wilson.

The next BCA Spring meeting will be held in York, April 14-17, 2003.

Christine Cardin (Hon Secretary)

Biological Structure Group AGM 2002

This will be held at the BCA Spring Meeting as usual. There are no posts vacant on the committee this year. A provisional agenda is published below. Additional agenda items to the Secretary by 10th March. TWENTIETH ANNUAL GENERAL MEETING to be held on Wednesday 27th March at 12:30 during the BCA 2002 Spring Meeting at Nottingham University

PROVISIONAL AGENDA

1. Minutes of 2001 annual meeting (Reading)
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 (2002-2003)
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

Dr Andrea Hadfield
(Hon. Secretary/Treasurer)
(a.t.hadfield@bristol.ac.uk)

Chemical Crystallography Group AGM 2002

The Annual General Meeting of the Chemical Crystallography Group will be held on Tuesday 26th March 2002 during the BCA Spring Meeting in Nottingham, starting at 12:30 pm. Final details of the agenda and venue will appear on the CCG website (http://bca.crystal.bbk.ac.uk/BCA/CCG/agm02.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 Monday 18th March 2002.

Nominations are invited for four ordinary members of the CCG Committee.

Nominations must include the names of a proposer and seconder, and written consent (by e-mail or otherwise) from the nominee that he or she is willing to stand. Nominations must be received by the Secretary of the CCG not later than Monday 15th March 2002.

Three members of the Committee are retiring (Dr Christine Cardin, Dr Simon Parsons and Dr Claire Wilson) and a further vacancy has been created by the early retirement from the Committee of Dr Jamshed Anwar. All other officers and Committee members continue in office.

Dr Harry Powell
(Hon. Secretary/Treasurer)
(hrp1000@cam.ac.uk)

Industrial Group AGM 2002

The 18th ANNUAL GENERAL MEETING of the Industrial Group will be held at the University of Nottingham on 28th March 2002. Nominations are sought for one committee member to serve for three years from March 2002. 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.

Dr Phil Holdway
(Hon. Secretary/Treasurer)
(p.holdway@QinetiQ.com)

Physical Crystallography Group AGM 2002

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

DRAFT AGENDA

1. Apologies for Absence
2. Minutes of the 58th AGM, held at Reading University, 8 April 2001
3. Matters Arising
4. Chairman's Report
5. Secretary/Treasurer's Report
   (a) Reports from BCA Council and IoP
   (b) Presentation of accounts
6. Elections to Committee
   Appointment of representative to CMMP Division of the IoP
7. Future Meetings/Activities
8. Any Other Business

Elections to the Committee
There will be elections for Chair, vice-Chair, Secretary/Treasurer and also vacancies for Ordinary Members. Nominations (with name of proposer and seconder and note of acceptance from the nominee) for any of these positions should be sent to the HonSec by March 22nd, or communicated to him in person at the 2002 BCA Spring Meeting, prior to the AGM.

Professor Chick C Wilson
(Hon. Secretary/Treasurer)
(C.C.Wilson@rl.ac.uk)

BCA Biological Structures Group, Winter Meeting 2001

Membrane Proteins: Challenges to Structural Biology

Imperial College, London,
17 December 2001

The BSG winter meeting focused on recent results in membrane protein research, including expression, crystallisation and structural studies. A wide range of methodologies was covered at the meeting, including kinetic crystallography, electron microscopy and single-molecule observation. More than 200 delegates attended the meeting (including scientists from as far afield as Japan and the United States) making it the largest ever BSG winter meeting. We also received financial support from 10 sponsors. This level of interest clearly indicates that the area of membrane protein structural biology is an expanding one.

The meeting was divided into three sessions; 1) New structures (session chair: Paul Freemont), 2) Expression of membrane proteins for structural studies (session chair: Bernadette Byrne) and 3) New techniques to study membrane protein structure (session chair: So Iwata). These three sessions were arranged to cover the hottest topics in the structural biology of membrane proteins.

In the first session, three exciting new membrane protein structures were presented. So Iwata reported the structure of formate dehydrognase-N at 1.6 Å, the highest resolution for a membrane protein complex obtained so far. The next speaker, Petra Fromme (Berlin) presented the beautiful structure of photosystem I. This membrane protein is incredibly complicated, incorporating more than 100 co-factors. Petra also included a progress report on the structural study of the related photosystem II at 3.6 Å resolution. The last speaker in the session Jade Li (MRC, Cambridge) revealed the structure of bovine Rhodopsin from a new crystal form. The high resolution and lack of twinning for these new crystals have allowed a more detailed study of this photoreceptor than has been previously possible.

After lunch, which included an exhibition and mini poster session, we focused on the expression of membrane proteins, a current bottleneck of the structural studies on the membrane proteins. Chris Tate (MRC, Cambridge) gave an elegant presentation describing the expression and 2-D crystallisation of the small multi-drug bacterial transporter, EmrE. Oliver Dolly (Imperial College) then showed how his group has been able to overexpress eukaryotic K+ channels from mammalian brain using the Semliki Forest virus system. It is still extremely difficult to work on eukaryotic membranes due to the difficulties in expression and purification and solving the problems associated with these processes seems key to the future application of membrane protein structural biology to medicine and pharmacology. The last speaker in the session, Peter Henderson (Leeds) gave a beautiful presentation on his heroic efforts to express bacterial membrane transporters. Peter described the spectacular successes he and his group have had in this area and how 3-D crystallisation attempts are the next area to be tackled.

After coffee, we enjoyed three inspiring talks on novel techniques. Bonnie Wallace (Birkbeck College) gave a very clear talk on circular dichroism spectroscopy of membrane proteins with a particular emphasis on using synchrotron radiation. Richard Neutze (Göteborg, Sweden) presented an "almost" movie of the molecular mechanism of proton pumping by bacteriorhodopsin based on the cutting edge technology of kinetic crystallography. The talk of Masasuke Yoshida (Tokyo Institute of Technology, Japan) fascinated the whole audience. He has been able to visualise the rotation of ATP synthase using the state-of-the-art, single molecule observation technique. His single molecule manipulation technique is so elegant that it is even possible to control the rotation of a single ATP synthase molecule using a magnetic field.

We conclude that the meeting was a success and was thoroughly enjoyed by all the delegates and sponsors alike. There is still no magic solution to obtaining crystal structures of membrane proteins. However, we clearly feel major progress is being made towards this goal. As more membrane protein structures are solved, so the body of knowledge grows, inviting the development of novel techniques as well as encouraging scientists into this challenging but extremely rewarding area of research. Structural studies on membrane proteins requires expertise in a number of areas from molecular biology to physics, and this meeting highlighted the importance of the collaboration of crystallographers and researchers in other fields including biochemistry, molecular biology and biophysics.

So Iwata and Bernadette Byrne

BCA Chemical Crystalloraphy Group, Autumn Meeting 2001

Mesomolecular Crystallography

Aston University, Birmingham, 14 November, 2001

The CCG Autumn meeting was attended by 71 people, including 17 new members. The local organiser was Carl Schwalbe, and the Meeting was sponsored by Bruker-Nonius. The topic of the meeting was 'Mesomolecular Crystallography', and was concerned with the structures of and bonding in large molecular (up to 200 unique non-hydrogen atoms) and supramolecular materials. The eight speakers recounted some of their experiences in the area, describing methods of structure solution and analysis, and outlining the chemistry relating to these large systems. The Chairman of the CCG, Paul Raithby, opened the meeting by welcoming the audience, and chairing the first session.

Martin Schröder (Nottingham) in his lecture entitled "Construction of Framework Polymers: Catenates, Helicates and Porous Materials", discussed structures based on n-connected nets which can arise as a result of metal-metal interactions between organic chains. Initially, he concentrated on ligands based on bipyridyl with different linkers between the two aromatic rings, showing that Ag-Ag interactions can give a helical arrangement of Ag ions with the organic chains extending outward, i.e. producing a chiral polymer starting from non-chiral components.

Three-connected nets can be formed from reactions of Cu(I) salts with 180° building blocks, such as di-trans-bipyridyl species, to produce "polycatenating ladders". By an appropriate choice of solvent, these ladders can be either interpenetrating or non-interpenetrating.

Three-dimensional four-connected nets can give rise to "adamantoid frameworks"; again, the voids are filled by interpenetration. Perhaps more interesting are the five-connected interpenetrated nets, which have been called "metallorganic" zeolite analogues. However, this analogy is somewhat limited because of the thermal instability of the metal-containing materials above ~200°C.

With phenylene as the organic linker group, hexagonal channels are formed which can act as a host for organic 'guest' molecules. For example, the bipyridyl molecule can be washed out with CH_2Cl_2. These materials are stable up to ~150°C and are better described as clays rather than zeolites; e.g. N_2 absorption gives a typical clay isotherm.

He rounded off the talk by showing examples of lanthanide complexes with unusual network topologies, with 6-, 7- and 8-connected nets.

Andrew Burrows (Bath) followed with "Co-ordination and Hydrogen Bond Interplay in Supramolecular Network Formation"; he concentrated on aspects of "crystal engineering" by outlining the two main categories, (i) co-ordination bonding and (ii) hydrogen bonding. He described studies relating to the second type, and used di-imines in combination with trans-aromatic carboxylic acids to make polymeric structures via DD:AA interactions.

He chose to use Zn (because of its d^{10} configuration) as the metal, water as a competitive solvent and thiosemicarbazide compounds to stabilise the metal-ligand bonding. This chemistry gave rise to co-ordination polymers, rather than H-bonded networks. In water, 1D chains are formed which run through the structure; this approach also works for other metals e.g. Ni.

Borrowing an idea from synthetic organic chemistry, he used the idea of "combinatorial crystallography" to produce an array of different products by changing dicarboxylate or adding thiosemicarbazide in a systematic way. Changing the carboxylate group showed that the chemistry is largely determined by solubility. If the thiosemicarbazide is deprotonated, self-assembly into chains occurs. This can be tuned to a certain extent, for example, thiourea mainly gives polymers, methylthiourea gives a mixture

dominated by polymers but containing molecular species, and dimethylthiourea gives a 50:50 mix. In the case where trimethylthiosemicarbazide was used, the product was found to depend crucially on the carboxylate.

Kathryn Holmes (Loughborough) finished the morning session with her talk on "Hydrogen bonding in Sulfimides and their Complexes". This work developed from the study of S_4N_4 and its derivatives which are explosive. Fortunately, sulfimides do not have this property. The compounds display strong hydrogen bonding and a number of ligand structures have been solved which show stacked hydrogen bond linked ladder arrangements which are hydrated. Reaction with $CuSO_4$ eliminates SO_4^{2-}, and gives 1D chains, with coplanar CuX_4 with 90° between adjacent units; specific examples were that fumarate gives a 2D ladder, benzene dicarboxylic acids give a linear structure with 1D chains running in 2 directions, whereas Na terephthalate gives H-bonding bridges.

After lunch, following an introduction by the CCG Deputy Chairman, Sandy Blake, **Richard Winpenny (Manchester)** gave us an insight into "Studies of High Nuclearity 3D-Metal Cages with Unusual Magnetic Properties", in particular the so-called "single molecule magnets", which are paramagnetic in the absence of magnetic fields. These magnetic properties have been observed in a number of species involving transition metal clusters. The main synthetic challenge is how to make the polymetallic cages. Two types of ligand have been investigated with this in mind, i.e. carboxylates and 2–pyridinates (which have 8 different bonding modes) and these have given rise to several different cage morphologies, e.g. M_{12} wheels (Ni, Co) and trigonal prisms (Ni, Co). More complex systems build on these basic shapes, for example the dodecanickel species containing centre penta-capped trigonal prisms.

Changing the carboxylate allows the chemist to modify the metal cage geometry, but the resulting polyhedra are related, and are in fact based on fragments of penta-capped trigonal prisms. Other ligands like Hmpo give rise to larger cages, e.g. $[Ni_{24}(OH)_8(mpo)_{16}(Hmpo)_{10}(O_2CMe)_{24}]$, that was obtained from the reaction with methyl acetate followed by crystallisation from MeCN. There are many hydrogen bonding contacts in the crystal structure.

Crystallographic problems in these species are caused by the state of protonation, and by the occurrence of mixed-metal cages.

Jonathan Steed (King's College, London) discussed "Crystal Frustration - and how to avoid it", concentrating on the causes of and problems encountered with unusual values of Z', the number of formula units in the asymmetric unit. While structures with values of Z' of 0.5, 1 and 2 make up over 95% of all structures in the CSD, those that remain can cause problems. For example, for nucleosides and nucleotides, 20.8% of structures have Z' > 1, and for steroids the figure is 18.8%. Molecular complexity is not a useful guide, e.g. a non-biological structure with an unusual Z' (of 11) is $[MeCl_2(NCMe)(NO)PMe_3)_2]$.

Many of these unusual structures are superspace modulated structures. An example is Me_3SnOH, which has a non-crystallographic helix and Z' = 32. Structures with more than one stacking motif can give rise to polymorphism, resulting in different physical properties. Weak hydrogen bonds can form between CH and X-E groups to give extra local order, grouping molecules together with non-crystallographic symmetry to increase the value of Z'.

Andrei Khlobystov (Nottingham) enlarged on some of the points raised in the first talk of the morning in his discussion of the "Impact of Anion Size on the Structure of Polycationic Chains in Co-ordination Polymers". Using noncovalent self-assembly methodology and employing trans-bipyridyl ligands, chains, helical staricases and perpendicular chains are produced from monomers with the "donor-spacer-donor" ligands linked by metals. The use of quinolyl groups rather than pyridyl always gives rise to chains, which is a big contrast with pyridyl. Essentially, the structure is determined by M-M, M-L and L-L interactions. The bulkier quinolyl groups stack in the solid state, with a large contribution from aromatic interactions, and these ligand-

ligand interactions predominate. Where the stacks interact with metals (e.g. Ag) chains are formed. The mean inter-planar separation is ~ 3.4 – 3.5 Å, but increasing the size of the anion increases the distortion of the stack and the inter-planar separation. This last point gives a clue as to how to control the geometry, e.g. SbF_6^- (large and non-co-ordinating) gives larger voids which can accommodate these anions.

Michaele Hardie (Leeds) began the final session, chaired by CCG Secretary Harry Powell, with "Network structures from the host molecule CTV", cyclotriveratrylene, which has a rigid bowl shape. Unlike calixarenes, it is not a useful host for small guests unless modified by organic chemistry. However, it is a good host for large guest molecules. Three types of complex result, those involving the formation of hydrogen bonding networks, those involving the formation of co-ordination polymers through covalent bonds, and those with both types of interaction.

Group II metals do not chelate to CTV, so hydrogen bond networks can develop. In the presence of $[Co(C_2B_9H_{11})_2]^-$, a large complex is formed with 4 CTV molecules. In the case of the strontium compound with CTV and carborane, the octaaquo structure can be thought of as a cluster at the centre of the complex. The CTV molecules are arranged in a tetrahedron, while $[Sr(H_2O)_8]_6$ groups form an octahedron around this, giving an adamantoid unit. This is a robust structural motif that appears repeatedly with different metals and charges.

Speakers at the CCG Autumn Meeting.

Andrew Bond (Cambridge) concluded the meeting with "Determination and Refinement of the Crystal Structures of Multi-Porphyrin Oligomers" in which he discussed the meaning of the term "mesomolecular crystallography" with reference to a selection of large structures with large unit cells. Andrew began by noting that the average number of non-hydrogen atoms in a CSD entry was 36-40, and that his atypically larger structures would be expected to give problems: a larger unit cell means that the mean intensity of a reflection is reduced. It required 3 days on a Nonius Kappa CCD area detector to obtain adequate intensities for a zinc porphyrin with a P-donor arm. The structure contained large 3_1 helices and hexyl rings which exhibited large displacement parameters.

Another example required data collection on Daresbury's Station 9.8, but this gave a dataset with 72% of data having $I > 2\sigma(I)$ to a resolution of 0.80 Å. Having a Z' of $^1/_2$ kept the size of the asymmetric unit down, and once disorder of hexyl groups had been modelled using occupancy, distance, angle and *U* value restraints there were no outstanding problems with the structure refinement.

His final example had Z = 1 so the unit cell was larger, but it was possible to refine the structure once intermolecular constraints involving the hexyl chain and solvent molecules were taken into account.

Harry Powell

BCA Industrial Group, Autumn Meeting 2001

Pilkington European Technical Centre, Lancashire, 1 November, 2001

Thirty-four people came to this year's meeting. Jack Brettle, Head of Science Support, welcomed us to Pilkington and opened the meeting. He briefly described the scope of the company with manufacturing plants in 25 different countries. Pilkington's major achievement was the development of the process to make float glass in the 1950s. The business is divided into 2 main lines, building and automotive products.

Most of us had an opportunity to view many products in the Exhibition area which is fascinating. It describes how different types of glass are made. Glass can be seen in a wide variety of products from complex curved windows for helicopters and cars, bullet proof glass, thermal control, optical systems and a variety of ascetically pleasing products. We tested it mechanically by using the glass stairs.

Our host and local organiser Mark Farnworth described the sort of X-ray work carried out at Pilkington. Powder diffraction is used to check the quality of raw materials, identify the phases in dusts and corrosion products and do troubleshooting on final products. Many of Pilkington's special products are thin films deposited on glass to improve thermal, optical or mechanical properties. The XRD data can be made surface sensitive by coming in at a glancing angle of 1 or 2 degrees which is useful. Finally these thin films make ideal samples for X-ray reflectometry (or reflectivity). By calculating the data from models and comparing these data with experimental data one can obtain information about the film thickness, density and roughness. Mark showed data from a Round Robin and the agreement was impressive.

The polymorphic form of a drug influences its stability, solubility and hence bioavailability; thus, powder diffraction is an important tool for characterising pharmaceuticals as Anne Kavanagh (Astra Zeneca) described. Current regulations mean that there is a requirement to check samples at all stages in their lifecycle from discovery, through manufacture to trouble shooting. Anne gave a few examples from the literature of polymorphs with different physical properties and emphasised the importance of using complementary techniques such as DSC, TGA and hot stage optical microscopy. High temperature XRPD provides additional information. Mirrors and a position sensitive detector speed up data collection and are beneficial for hot stage work. Astra Zeneca also have a new system with a point source and a 2-dimensional position sensitive detector. This is ideal for very small samples and could be used as a multiple small sample stage or for spatially resolved work.

Matthias Abraham, University of Oxford described how nanocrystalline nickel can be made by electrodeposition. This material is about 5 times harder than conventional large grained nickel and thus has many potential industrial applications. However, during wear, local heating can cause grain growth which reduces the hardness. Thus grain growth and hardness were studied after heat treatments. Line broadening showed that just a few grains grow and the rest remain roughly the same size and the hardness remains high for quite a long time.

Keith Rogers' (Cranfield University) talk covered 3 distinct topics. First he talked about his work on CdTe-CdS solar cells. After describing these systems, Keith showed how diffraction depth profiling had improved the understanding of the structural changes that can occur in the anneal to make a CdTe-CdS heterojunction. It appears that strain is the driving force for recrystallisation. Next he talked about some of his colleagues' work on bone. The challenge is to produce synthetic materials that mimic human bone and can be used to repair breaks and make implants. The effects of ageing and disease are also of great interest. Human bone is poorly crystalline and thus not well defined. We were shown some data from the nose of a whale which was well crystalline and oriented and thus more information could be obtained from it. With thermal treatment new crystalline phases may be observed in bone. Keith showed that with increasing temperature

	Monday 25 March		
Room	C16		
11:00-12:00	BCA Council Meeting (in Room A2)		
12:30-13:00	Registration (in Room A13)		
13:00-14:00	Lunch		
14:00-15:30	Plenary Session: New Methods in Structure Solution and Phasing *Carmello Giacovazzo, Bill David, Kevin Cowtan, Lynne McCusker*		
15:30-16:00	Afternoon Tea		
16:00-17:30	Plenary Session: New Methods in Structure Solution and Phasing (continued)		
17:30-18:15	Education SIG (*Kate Crennell*)		
	Dinner		
20:00-late	Reception Portland Building		
	Tuesday 26 March		
Room	C16	C14	C15
9:00-10:30	DNA Recombination and Repair	Polymorphism and Structural Changes	IG Workshop: Introduction to Thin Films
10:30-11:00	Morning Coffee		
11:00-12:30	DNA Recombination and Repair (continued)	Polymorphism and Structural Changes (continued)	IG Workshop: Powder Diffraction Surgery
12:30-13:00		CCG AGM	
13:00-14:00	Lunch/Exhibition		
14:00-15:30	BSG Oral Poster Presentations	CCG, PCG, & IG Oral Poster Presentations	
15:30-16:00	Afternoon Tea		
16:00-17:30	Detectors	Polymorphism and Structural Changes (continued)	IG Workshop: Introduction to Amorphous Materials
17:30-18:15	Formation of DIAMOND SIG		
	Dinner		
19:30-late	Poster/Exhibition Wine Reception Rooms A13 & A14		

	Wednesday 27 March		
Room	C16	C14	C15
9:00-10:30	New Methods in Structure Solution and Phasing	Protein Crystallography of Drugs and Disease	Thin Films
10:30-11:00	Morning Coffee		
11:30-12:30	New Methods in Structure Solution and Phasing (continued)	Protein Crystallography of Drugs and Disease (continued)	Thin Films (continued)
12:30-13:00	PCG AGM	BSG AGM	
13:00-14:00	Lunch/Exhibition		
14:00-15:30	Prize Lectures: PCG & CCG Awards		CCP4 Workshop in PC Room
15:30-16:00	Afternoon Tea		
16:00-17:00 17:00-18:00	Room C16 BCA AGM BCA Prize Lecture		
19:30-late	Conference Dinner High Stewart Hall		
	Thursday 28 March		
Room	C16	C14	PC
9:00-10:30	Rietveld Refinement	BSG Workshop: Crystallisation	CCG Workshop: CRYSTALS
10:30-11:00	Morning Coffee		
11:00-12:30	Rietveld Refinement (continued)	BSG Workshop: Crystallisation (continued)	CCG Workshop: CRYSTALS (continued)
12:30-13:00	IG AGM		
13:30-16:00	BCA Council Meeting (in Room A2)		

some peaks got sharper and the modulus increased. Continuing the medical theme, the final topic was SAXS on breast tissue with and without cancer. The results show that the collagen in cancerous tissue is less ordered than that in healthy tissue. One hospital is setting up SAXS equipment to investigate the possibility of using this as a diagnostic test on biopsy samples. Current tests usually involve staining and optical microscopy.

Industrial Group Award

Chris Frampton, Chairman of the IG, presented Ian Langford with the Industrial Group Award for his work on profile analysis. Ian started working on powder diffraction in the early days with Arthur Wilson at Cardiff. He has recently retired and now holds an honorary position at Birmingham. He has published extensively and in several of his papers data on zinc oxide were used as an example to describe a particular method of analysis. Thus it was appropriate that Ian chose to have a Beevers model of zinc oxide for his award and then gave a talk on this material.
I had never realised that zinc oxide is used so widely in industry. Uses include: paint, ceramics, catalysts, lubricants, paper, electronic devices, pharmaceuticals and even chemical smoke. Most of these uses relate directly to its crystal structure which has a hexagonal lattice and polar c axis. When pure it is white, but impure it is red and is used as a pigment. The crystallites are often submicron and anisotropic and thus can be characterised by line broadening. Ian mentioned the early work by Scherrer and Debye (1916, 1918) on line broadening, his practical and widely used approach of defining peaks as partly Gaussain and partly Lorenztian, and working with integral breadths and Scardi's approach for analysing size distributions. Looking to the future, Ian said he thought that newer methods of analysis would be based on building physical models and comparing simulated and experimental data. This approach is widely used in many other areas of X-ray scattering.

Most industries are currently in a state of change and Ilford is no exception. David Beveridge's talk started with work relating to silver halide photography and then moved onto the challenges of trying to identify dyes and pigments in new inkjet products. Many of these are poorly crystalline and can occur in several polymorphs. The crystal structure can strongly influence colour. For the silver halides, their standard method of analysis is to remove the gelatine and collect relatively high angle data on the halide particles which have a core shell structure. Changes in the ratio of AgI to AgBr and line broadening can be followed.

Ian Slipper talked about work done at University of Greenwich for Sandberg Testing Laboratories. This involves running samples of Ground Granulated Blast furnace Slag (GGBS) to determine its glass content in accordance with BS6699. GGBS is a by-product of the steel industry, and it is sold on as an additive to cement. It improves various properties of cement such as workability, setting times, permeability and strength, but these improvements require that the material is predominately amorphous. The test method discusses scan speeds, chart paper, separation of crystalline and amorphous peaks, then cutting and weighing the paper to determine the amorphous content. Ian tried to update the procedure using Bruker's software EVA. His experience showed that some things which a person would do automatically require more effort to make a computer program do the job. After some initial difficulties, he was able to obtain comparable results by both approaches.

Many industrial systems are messy and cannot be analysed by classical line profile approaches. The lines are often overlapped, backgrounds non-flat, and for dynamic data there are usually many data sets with poor counting statistics. Thus neither analytical profile fitting nor Rietveld are suitable. Steve Norval (ICI) described a new approach, LOSS, linear optimisation of a simulated set.

This involves simulating data for a given phase, broadening the peaks with a single, or a range of crystallite sizes, microstrain and/or stacking faults and then convoluting this with a parameterised instrumental function. The instrumental function can be checked by using the new NIST lanthanum hexaboride standard. Steve pointed out that although this standard is better than its predecessor it still has a bit of microstrain and it should be stored under nitrogen. Both experimental data and simulated data can be used as input to LOSS. Steve demonstrated this pragmatic approach to analysing real time data with an experimental set for the catalyst support and simulated sets for Ni and NiO. Thus the appearance and disappearance of phases during thermal treatment could be followed.
This meeting was well attended (particularly considering that Lathom is not one of the easiest places for most people to reach). Several well-known faces who are now retired, or no longer still working in diffraction, came and everyone appeared to have enjoyed themselves. Credit for this is due to Judith Shackleton, who put together a meeting which covered a wide range of interesting industrial topics, and to all the speakers. Thanks are also due to Mark Farnworth, the local organiser, for his work and to Pilkington for allowing us to use their excellent facilities.

Mary Vickers, Cambridge University

BCA Physical Crystallography Group, Autumn Meeting 2001

Applications of high pressure in structural studies

Daresbury Laboratory, 5th December 2001

The Physical Crystallography Group organised a one-day meeting to cover the wide-ranging applications of high-pressure techniques in the study of crystal structure. Following registration and coffee, the participants were given a tour of the high-pressure facilities at Daresbury Laboratory, which included both the monochromatic powder and single-crystal diffraction facilities available on stations 9.1 and 9.8 respectively as well as the energy-dispersive diffraction facilities on station 16.4. The high-pressure laboratories of the University of Edinburgh provided the participants with an insight into the apparatus required for the preparation, loading and pressure measurement of diamond-anvil cells - perhaps the most significant investment for the initiation of a new high-pressure research programme. Finally, the high-pressure EXAFS facilities developed for station 9.3 by de Montfort University were demonstrated.

Following lunch, a series of talks were given covering a wide range of high-pressure techniques in structural science. The first speaker was Andy Jephcoat (Department of Earth Science, Oxford University), who discussed the role of Raman spectroscopy in the study of bonding under pressure and the complementarity it offers to x-ray diffraction methods. As well as providing an overview of the Raman technique, he explored the findings of some of his more recent work including studies of diatomic gasses and elemental metals at high-pressure. He rounded off his talk by mentioning the development of SiC anvils for high-pressure Raman spectroscopy. Although they have a lower strength than those made from diamond, SiC anvils have a relatively low absorption across a wider spectral region than diamond, and they are particularly favourable for the study of water in minerals. Just as significantly, however, they are far cheaper.

Moving from Raman spectroscopy to neutron diffraction, Dave Keen (Oxford University and Rutherford Appleton Laboratory) discussed the development of single-crystal techniques at ISIS. He gave a very interesting introduction to the development of high-pressure techniques for neutron diffraction and how, more recently, pressure cells suitable for single-crystal diffraction have been developed from existing powder-diffraction cells or scaled-up versions of diamond-anvil cells. With a more specific reference to ISIS, he outlined the advantages of the fixed-geometry time-of-flight technique for high-pressure

studies and the recent developments of the single-crystal diffractometer, SXD, for high-pressure work. Although the work is in its early stages, a number of extremely promising results were given and the future prospects for high-pressure single-crystal neutron-diffraction were highlighted.

The theme of diffraction at central facilities was continued with a talk by Mohamed Mezouar (ESRF) who discussed high-pressure powder-diffraction using synchrotron radiation. He began with an overview of the range of facilities available at the ESRF and how it was possible to conduct high-pressure powder-diffraction experiments over a large range of P-T space - from temperatures in the range of 20K to 3000K to pressures of 1.5Mbar. He illustrated how these facilities have impacted structural science with a number of interesting examples from the more recent work he has been involved in. For sulfur he demonstrated that the previously established phase diagram was largely incorrectly identified and the work conducted at the ESRF had resulted in a much simpler interpretation. The phase diagram of ZrO_2 was also discussed in the context of the development of a CCD area detector to collect the diffraction data. Finally, the prospects of laser heating techniques were highlighted for in situ chemistry and the recreation of conditions at the Earth's interior.

Returning to single-crystal methods, Simon Parsons (University of Edinburgh), gave a very illuminating talk on the use of CCD detectors in high-pressure crystallography. He shared his practical experience in using the Bruker AXS Smart diffractometer both at his home laboratory and at the SRS Daresbury Laboratory for the collection of high-quality single-crystal data. As well as illustrating a reliable data collection strategy, he emphasised the importance of the data integration procedure for obtaining an optimised data set - perhaps the most crucial stage. Expanding on the general theme of high-pressure, he described the low-temperature *in situ* crystal growth of low melting point small-molecule systems in a capillary held under a cryo-stream device. In his technique, a laser is used to preferentially heat regions of the polycrystalline sample so that a single crystal is obtained. To demonstrate the complementarity between such low-temperature and high-pressure studies, he gave as an example his recent work on formamide.

To conclude the more formal presentations, Sue Bayliss of de Montfort University gave a talk on high-pressure EXAFS with particular reference to the development of the HIPREX facilities on station 9.3 at the SRS Daresbury Laboratory. She gave an overview of what can be achieved with the range of EXAFS techniques currently on offer, and mentioned the activities, focusing particularly on high-pressure, of centres as in France (the ESRF and LURE), the USA, and Japan. Returning to her work at Daresbury, she illustrated what could be achieved from some of her recent studies and for the semiconductor GaSb, she demonstrated the complementarity between X-ray diffraction and EXAFS techniques to determine the nature of the disorder present in its high-pressure phases. She concluded her talk by looking at future prospects for high-pressure EXAFS with particular reference to the proposed GPXS beamline on diamond.

Finally, Malcolm McMahon (University of Edinburgh), and Andrei Sapelkin (de Montfort University), gave short presentations. Malcolm introduced the new Centre for Science at Extreme Conditions which will be based at the University of Edinburgh. It will be housed in a new building which will be open in Autumn 2002. His talk summarised the high-pressure science that would be conducted at the centre and the broad range of facilities and expertise that would be available. Andrei discussed alternative materials to replace the anvils in diamond-anvil cells. Echoing Andy Jephcoat's remarks, he emphasised SiC as a promising alternative as well as polycrystalline diamond, for limited cases. With the possibility of growing single-crystal diamond with vapour deposition techniques, he introduced the concept of so-called smart anvils where electrical leads, for example, could be incorporated within the anvil material. The meeting was then drawn to a close with a general discussion.

The organiser would like to thank all of those who attended for making the meeting both enjoyable and stimulating. It was also extremely heartening to see a number of non high-pressure specialists at the meeting and contributing to the discussions. It is with great appreciation that I thank all those at Daresbury who helped with the organisation, particularly: Steve Collins, who was the local organiser; Alison Mutch, who ensured that everything ran smoothly; and Graham Bushell-Wye for organising the funding from Daresbury Laboratory to allow for free registration, lunch and coffee. I'd also like to thank Ray Jones, Sue Bayliss, Simon Teat and Malcolm McMahon for helping with the tours and allowing their experimental facilities to be open to scrutiny. The meeting was supported by Daresbury Laboratory and the CLRC Centre for Molecular Structure and Dynamics.

Dave Allan

Education News

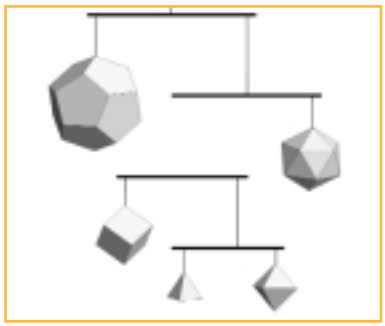
Webpages with instructions for making 3D models

The main education page on the BCA website is http://bca.cryst.bbk.ac.uk/BCA/ed/index.html which now has links to 2 new pages, one for news at .../BCA/ed/news.html the other with instructions for making 3 different kinds of your own 3D card model crystals at .../BCA/ed/Models.html

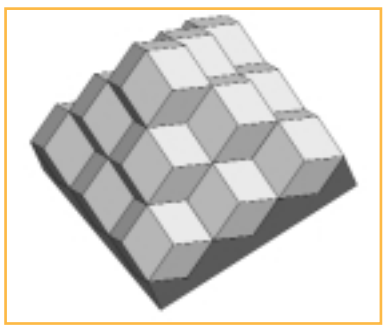
The models are calcite, a mobile showing all the Platonic solids and a set of rhombic dodecahedra and bases to show how these polyhedra fill space.

The calcite is an example of a single A4 page with the planar net of the solid, a 3D shaded view of it, some 'wire' diagrams and some of the symmetry axes illustrated with the standard symbols. Please look at it and let me have your comments, and suggestions as to what other 'crystals' your students would like. The only the Platonic solid which fills space is the cube, others can fill space if you use more than one of them. Many viruses are icosahedral in shape, so making an icosahedron may be a useful exercise for students of biological structure. I hope to make more spacefilling polyhedra soon.

Calcite planar net



Completed mobile



Completed base with rhombic dodecahedra

A new polyhedral model kit from Astro-logix

Astro-logix Design
32 Elmore Road, Horfield, Bristol, BS7 9SD

tel: +44 (0)117 9046768
email: info@astro-logix.net
website: http://www.astro-logix.net

This supplier markets a set of plastic tubes which can be connected together with a variety of 'hubs' to make

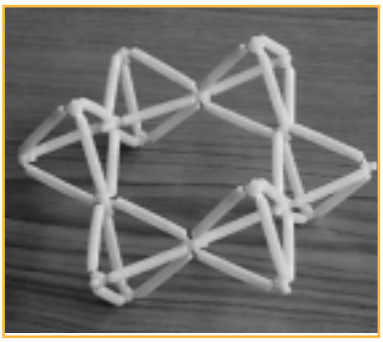


Fig. 2

polyhedra, much like the Cochrane model kits. I tested the 'Solar System' kit (price £7.99) which has 130 parts: 70 40mm long tubes, and 20 each of 3,4 and 5 way connecting hubs. The hubs have a hollow underneath the centre and a small knob on the top, so that polyhedra can be built inside one another or connected at their vertices. These components are all the same colour, a milky white; they will glow in the dark for a short while after they have been in light for some time. The supplier says that tubes in other colours, a cutting tool and 6 way connectors will be available soon. The hubs are not rigid, their arms may be bent which allows flexible model building, but I can see that they may become weak with constant use and then snap off. Triangles are made easily, but polygons with more sides tend to become twisted.

The documentation consists of 2 double sided A4 pages. You should read the one printed in black and white first, it has instructions for assembling the models, including how to connect and disconnect two hubs, with a caution to be gentle when pulling models apart otherwise the hubs may break. Brief instructions are given for making each of the Platonic solids, it is probably a good idea to make those first to find out the problems. My model cube was not rigid and tended to go out of square alignment. The octahedron was better and it can be constructed inside a cube which may help some doubting students to believe that the cube and octahedron have the same symmetries. It is not easy to bend the arms of all the hubs to the correct angle; my rhombic dodecahedron had the right topology but non-planar sides! My attempt to construct quartz is shown in Fig. 2, it is made from tetrahedra linked at their corners; with more pieces and a lot of patience one might be able to model zeolites.

The instructions are only concerned with how to make a particular model, they lack any references to the mathematical theory of polyhedra, which are treated as artistic creations with no indication of where polyhedra occur in the natural world. The coloured A4 page of the documentation shows the possibilities of making larger coloured polyhedra using differing lengths of tube and combining more than one kit. The supplier invites any user who makes a polyhedron not shown on their website to enter it in their competition by sending an image to the website together with instructions on how to make it.

This kit is not recommended for children under 6 because of the smallish parts. However, it is sufficiently cheap that any undergraduate should be able to afford a set and use it to appreciate 3D structures. Teachers who want to make particular polyhedra can ask for a quotation for larger kits suitable for the whole class. Every college bookstore should stock these kits to help undergraduates understand structures better.

New products from the 2002 catalogue from Tarquin Publications

Tarquin Publications
Stradbroke, Diss, Norfolk, IP21 5JP
tel: +44 (0)1379 384 218
email: orders@tarquin-books.demon.co.uk
website http://www.tarquin-books.demon.co.uk

The latest catalogue, Tarquin Mathematics 2002, has new resources. They are now agents for the 'Polydron' kits of fixed sized solid plastic polygons, (triangles, squares, pentagons and hexagons) which can snapped together to make 3D solids. The polygons have the same length of side so that you can make polyhedra with them from more than one type of polygon. A newer product, 'Frameworks', consists of polygons made with just plastic edges; they are compatible with the solid shapes and can be used to make 'see through' polyhedra. The price depends on the size of kit you want; you can order from the website.

They have just started to sell wooden manipulative puzzles, one of which can be used to illustrate the packing of spheres;

20 polished wooden balls are stuck together in 4 pieces, the puzzle is to assemble them into a pyramid on the triangular wooden base. Price £7.50. A set of small polyhedra dice are cheaper; for £1.80 you can buy a set of the 5 Platonic solids and a 10 sided double pyramid.

They have reprinted the 'Altair Designs' colouring pads which can be used to teach symmetry and have other books for teaching tessellations

Personally I liked the set of five A5 sized books by Robert Field (price £2.95 each) 'Geometric Patterns from:', Roman Mosaics, Churches and Cathedrals, Tiles and Brickwork, Islamic Art and Architecture and Patchwork Quilts. They all have photographs and diagrams which could make useful illustrations for student projects to decide on the symmetry of the object shown and help students to realise that symmetrical objects are all around them.

I will try to bring examples of the items described in this article to the Annual meeting in Nottingham for your inspection, come and try out them out for yourselves at my poster.

I hope to make this page a regular item of the newsletter; this news will also accumulate on the BCA Website. Please send educational news items to me, preferably by email to BCA@isise.rl.ac.uk

Kate Crennell

Crystal Growing in Primary Schools

This international project, with which the BCA Council have enthusiastically agreed to be involved, was also featured at the European Crystallographic Meeting in Nancy last year. The following is an account of a project in Edinburgh, sponsored by the Royal Society of Chemistry.

For all those budding Harry Potters and Hermione Graingers out there, the crystal growing competition run by the Royal Society of Chemistry (RSC) Local Section for RSC Chemistry Week in November 2001 was just the ticket! Never mind those magic potions or spells which go awry; growing crystals is a great way of introducing pupils to chemistry with magical results.

Primary school pupils all over Edinburgh, the Lothians, the Borders and Fife were invited to participate in a Crystal Growing competition, Every primary school which elected to participate was sent a crystal growing pack which consisted of samples of aluminium potassium sulphate, and instructions on growing the crystals. In schools all over the region, saturated solutions were prepared and pupils waited in anticipation for the solutions to evaporate and a selection of crystals to form. They selected the best crystal and suspended it in a saturated solution, carefully monitoring the temperature and checking the progress of the growth of the crystal. This was a completely new experience for the children, with jewel-like crystals appearing before their eyes in the initial saturated solution, and their competition crystal growing week by week.

Participating schools were then invited to attend the final of the crystal growing competition which was held at the Science Campus of The University of Edinburgh. Not only had the schools been growing crystals, many pupils who participated in the crystal growing produced wonderful art-work and projects around the theme of crystals. The pupils arrived together with a teacher or classroom helper, and set up their displays of art-work and their crystals.

Some schools had chosen to display their competition crystal in imaginative and exciting ways. We had a crystal in a volcanic setting complete with dinosaurs, crystal in a manger as the guiding star at Christmas, and crystals displayed like fine jewels.

The excitement mounted as the judges (two Members of the Scottish Parliament and our own Dr R. O. Gould) carefully examined the crystals and awarded points for clarity, shape and size. Meanwhile the pupils were kept amused by magical looking potions consisting of dry-ice in water. Copious quantities of juice, biscuits and crisps helped as well. The Department of Chemistry had produced our own display of crystals collected in the department by Arnold

Beevers. One of these specimens, a large reddish-orange group of potassium dichromate crystals bears a stunning resemblance to the Philosopher's Stone in Harry Potter –a fact which was not lost on the children who had read the books or the press who had come to take photographs and cover the event.

The winning schools were Cramond Primary, Abbeyhill and Macmerry who received prizes of cheques totalling £400 to buy equipment for school. The level of enthusiasm shown by the teachers and pupils who participated was an inspiration to all of the staff and students from the Department of Chemistry who participated in the event.

Elizabeth Stevenson

Mary Mulligan MSP, Fiona Hyslop MSP and the Editor with the winning crystal growers from Cramond Primary School, Edinburgh.

CCP4 Study Weekend - High Throughput Structure Determination

The CCP4 study weekend (4-5 January 2002, York), organised by Robert Esnouf (Oxford), David Stuart (Oxford) and Keith Wilson (York), focussed upon the emerging and somewhat controversial topic of "High Throughput Structure Determination". This popular annual event attracted nearly 500 participants from the UK and other European countries as well as the USA, South America and Asia.

Tom Terwillinger (Los Alamos) opened the first session of the meeting with a provocative talk entitled "Structural genomics: foundation for the future of biology?" He is one of the nine members of the NIH supported TB Structural Genomics Consortium. In Mycobacterium tuberculosis (the principal causative agent of TB) there are about 4000 structural genes, of which the consortium has already purified 156 proteins, crystallized 40 and solved the structures of 22. He described methods for improving protein solubility using directed evolution in combination with green fluorescent protein fusions. In addition, he briefly described the recent developments in the SOLVE/RESOLVE software packages used for automated structure solution and density modification based on maximum likelihood techniques. Gerhard Materlik (Chief Executive of Diamond) described the basics of accelerator light source and synchrotron radiation storage ring concepts to be employed during the construction of Diamond in Oxford. The new synchrotron will have a circumference of 560 m and will operate at 3 GeV and 300 mA with a minimum beam lifetime of 10 h. The first 7 stations (3 for protein crystallography) are planned to be ready for users by September 2006. Four new stations are going to be built in each subsequent year up to up a total number of 21.

The second session was geared towards achieving high throughput through the use of bioinformatics and optimal target selection. Malcolm Weir, who recently moved from GSK to Inpharmatica (UK), described the drug design process and his perception of the bottleneck - obtaining integrated and interpreted information. Inpharmatica have developed a bioinformatics platform to address this issue. PharmaCarta is highly focussed on structure and consists of three applications - Biopendium, Chematica, and a chemical structures database. We learned that selection = validation x "druggability." Julian Gough (Cambridge) explained how the SUPERFAMILY web server (http://supfam.org) can assign about half of all new structures to existing superfamilies. SUPERFAMILY relies on profile-based Hidden Markov models of all proteins of known structure, and uses SCOP. Assignment to a structural class might also allow functional implications. Joe Peden provided a strong pitch for the use of Laboratory Information Management Systems (LIMS),

particularly those installed by his Manchester-based company Thermo LabSystems. Traceability is an important concept for any LIMS - untraceable data are worthless. LIMS are more than just streamlining, e.g., the use of information loops, where gained knowledge is used to redesign earlier experiments, is fundamental to a good system. Pedro Alzari from the Pasteur Institute in Paris described the optimisation of 3D structural technologies, following target

CCP4 participants at work

selection in the structural genomics work on TB, as "more of a dream". At this stage, the concern is target selection, for which a number of approaches are under consideration - choosing validated drug targets; genomic analyses (to identify abundant proteins); functional analyses; proteomics; and comparative genomics (comparison to other mycobacteria). This project is part of a collaboration involving the Pasteur Institute, the ESRF, Grenoble, a European initiative X-TB, and the USA TB consortium described by Tom Terwilliger in the first talk of the day. Eric de la Fortelle gave an impressive description of the LIMS that is operational at Structural GenomiX (now 130 employees) in San Diego. The software tracks highly-automated experiments from the cloning stages through protein expression and purification, crystallisation, data collection, structure solution and annotation, and "publishing" in the SGX VirtualJournal. The likelihood of obtaining soluble protein is raised to 80% by varying gene and genome for every target. Membrane-bound targets are being examined using automated detergent screens.

...and at play

Crystallisation robots, including robotics for storage/retrieval (RoboStore) and image capture (Robovision) allow examination of 1000 plates a day. A new beam line on APS (the SGX CAT) is now operational. Eric stressed that the key to automation is understanding the process. Develop the process first, then automate.

The final session of the first day concluded with a number of talks covering techniques which underpin or complement traditional crystallographic approaches. Ian Jones (Reading) opened the session with an overview of the development recombinant protein expression, from the seminal experiments of Cohen and Boyer in the 1970's to currently employed expression systems for utilising bacteria, yeast and eukaryotic hosts. Particular attention was paid to the use of fusion tags (e.g., His, FLAG, GFP, GST) for high throughput expression/purification as well as the advantages and pitfalls of rapid recombination systems. The potential use of the Roche *in vitro* expression system may also prove advantageous in future high throughput efforts. Fergal Hill (Avidis) discussed the optimization of approaches using "evolved" mutant Escherichia coli hosts selected for their ability to overproduce high levels of globular and membrane proteins. The use of such systems is making challenging projects as production of human G-protein coupled receptors tractable, particularly when combined with new refolding technologies such as the chaperone-dependent refolding chromatography developed from Alan Fersht's laboratory in Cambridge. Lajos Nyársik from the Berlin Protein Structure Factory summarised the technical developments associated with one of the 17 subprojects which is specifically devoted to high throughput protein crystallization. The Berlin laboratory has opted for a format using 96-well plates with the vapour diffusion method. Efforts in automation have included a multichannel-pipetting robot for drop preparation and a detection system for identification of crystals. Although it is clear that human intervention is still an important element for success, it is difficult to imagine

undertaking the enormous scale of trials described without modern robotics. Iain Campbell (Oxford) sought to educate the audience about the complementary role that NMR can play in the high-throughput structure determination arena. He opened with a description of the RIKEN facility in Japan which houses the largest expanding collection of high-field NMR machines in the world for structural genomics studies. He then provided an excellent description of the information one can obtain using NMR, including emerging methods such as residual dipolar coupling measurements which can yield improved relative orientation information. He also pointed out that NMR shared the same bottleneck in expression as crystallography but that technical difficulties in construction of high-field NMR machines would still limit the size of proteins that can be solved using this method in the forseeable future. He also described how NMR can be used to increase the coverage of "fold-space" through the determination of identifiable families or domains produced, in some cases from dissection of larger proteins containing multiple folding modules. The day concluded with a very interesting talk from Jan-Pieter Abrahams entitled "Electron crystallography of very small crystals." He provided a convincing case for the use of small ordered crystals in rapid structure determination which he termed "nanocrystallography". However, he also gave a clear account of the technical difficulties associated with developing an integrated system which can cope with everything from dispensing nanovolumes of material, to crystal detection and data collection. Innovation in this area includes the use of electrospray for production of tiny droplets, CCD cameras for detection and microfocus synchrotron beamlines for efficient data collection. He completed his talk with a description of the potential advantages of using electrons rather than X-rays as a method for obtaining diffraction pattern of nanocrystals. His progress in this area may indeed prove fruitful given his obvious determination to make this approach succeed.

Those who could not manage the 9:00 start on Saturday missed an interesting session entitled "Crystallisation / Data Collection". The first speaker was Glen Spraggon from GNF, who addressed the problem of what to do with the hundreds or thousands of crystallisation experiments that a robotic system could produce. He described a system that scans a 96-well plate in 60 seconds, and showed how the system would try to detect crystals. The system then needs to be able to analyse the results. He showed a scoring method that could be fed into a neural net. The database required to manage the data was also discussed. Julie Wilson (York University) followed by showing us how the techniques for automatically detecting crystals work, describing the methods and practice of edge detection with gradients, and how these edges can be classified, grouped and processed into shapes that can be further analysed. Martin Walsh (ESRF-UK) stepped in at the last moment to review advances in data collection automation in the USA. He showed the robotic devices for mounting and de-mounting prefrozen crystals on a goniometer that have been developed at ALS, SSRL, APS, and by MSC/Rigaku. He also described the BLU-ICE integrated software developed at SSRL, and how the APS had integrated data processing software with mounting to automate data collection. In addition, methods for automatic centering of crystals are still being developed. Andy Thompson (EMBL/ESRF) told us about the developments in beamline automation at ESRF, helped by the development of the micro-focus beam-line. He described the automatic beam optimising system and the development of a crystal-mounting robot. The fully automated EH3 was previewed along with the PX–web data collection and processing integration. The use of a Linux farm allowed the handling of the large amounts of data produced. Andrew Leslie (Cambridge) reviewed the needs of an "expert system" to allow the whole process to be reduced (for the user) to pressing a single button. He described the procedures and checks a real expert would perform and how these can be built into a system where the user sets the acceptance parameters. This system could be used (for example) to choose the best crystal from a set and then collect the data and process it. The expert system would be in

overall control, but needs to be interfaced to the various beam line control modules, etc. The session showed that we will soon be taking (or sending) our crystals to the synchrotron in steel blocks in the transport Dewar, probably with bar-codes.

Zbigniew Dauter started the following session on phasing and co-ordinated software developments with a talk entitled "A one-and-a-half wavelength approach to structure determination". The unusual title was derived from the fact that it is often possible to solve a structure from single wavelength anomalous dispersion (SAD) data, and in favourable cases this can be done before data collection of the second wavelength has been completed, leaving the user with one-and-a-half data sets (of which only one is used). Successful examples using the anomalous signal from Se and Br were described, and the basis for the success of the method was explained with Harker diagrams. Martyn Winn then outlined ongoing developments in the CCP4 program package. Some of these, notably the new core libraries, will be mainly invisible to the user but will facilitate maintaining the package as well as simplifying the task of automating the process of structure determination. There is active development of five programs (MOSFLM, ACORN, REFMAC, MOLREP and PHASER) which will improve the individual steps in determining structures. The popular CCP4 GUI is being enhanced to provide further automation of tasks involving several steps, automatic checking, for example of consistent indexing of data sets, and making it easy to install external software packages such as SHELX and Arp/Warp. Data harvesting will become increasingly important in high throughput applications, and is already present in many CCP4 programs. A collaboration with EBI will allow these files to be uploaded automatically when depositing a structure to the PDB. Yao Jia-Xing described the program ACORN, which allows ab-initio structure determination of proteins for which atomic resolution data is available. The program can determine the structure starting with less than 5% of the total scattering, for example a single sulfur or selenium atom, a piece of an a-helix or a small structural motif derived from a homologous structure. Initial phases generated from ACORN-MR are refined using a dynamic density modification procedure. The structure of lysozyme could be determined from the positions of 2 sulfur atoms or even from random starting atoms. ACORN has been successful in several cases where other methods could locate the heavy atoms (sulfur) but were not able to solve the structure. It can also be used to solve a heavy atom substructure at significantly lower resolution (e.g., 2.2 Å) and future developments are aimed at allowing full structure determination using 1.5 to 2.0-Å resolution data. Garib Murshudov talked about recent advances in the REFMAC maximum likelihood refinement program, and highlighted issues that need to be addressed in order to automate the refinement procedure. These include decisions based on the quality of the X-ray data and the stage (early or late) of the refinement. REFMAC could also play a role in automatically validating a molecular replacement solution. The use of both electron density and co-ordinates as part of the model was envisaged, and improved methods of describing the stereochemistry of ligands have already been implemented. Future improvements include automatic weighting of the X-ray terms, faster estimation of non-diagonal terms of the 2nd derivative matrix, a full treatment of models comprising both co-ordinates and electron density and a continuation of the work on the ligand dictionary. Paul Adams concluded the session with a description of the PHENIX software initiative, which is dedicated to providing a crystallographic software package using modern algorithms and taking advantage of the latest computer science techniques. The package will allow automated structure solution while retaining the possibility of user input and control, with the ultimate objective of being able to extend current automatic techniques to medium or low resolution (~3Å). Maximum likelihood algorithms will be used extensively. The collaboration currently involves four groups, Randy Read (molecular replacement), Tom Terwilliger (density modification), Tom Loerger and Jim Sacchettini (automated model building) and Paul Adams

(simulated annealing). A series of strategies will form the "glue" between individual steps, each comprising a network of tasks where the path through the network is determined by the outcome of the previous task. A preliminary version should be available within the next year.

The last session was devoted to molecular graphics and reminded people that however fast you are solving the structures at some point human viewing and thinking about the structure is required. The first presentation was by Dusan Turk who presented improvements to his MAIN (http://www-bmb.ijs.si/doc/) program for automatic building of maps even at moderate resolution. Liz Potterton then presented the plans for the CCP4 viewer and demonstrated it in its current rasmol-like state, which looked nice. The new look CCP4 as an integrated object orientated open source collaborative package is certainly an exciting prospect. Let's hope that Linux hardware stereo on a range of cards is a priority for the viewer. The last formal talk was by Alwyn Jones (http://xray.bmc.uu.se/~alwyn/). The centre piece was the latest bells and whistles on O, to aid the crystallographer in building structures more rapidly rather than automating the process. On the subject of whistles, his EDS server allows anybody to look at the dodgy fits of coordinates to maps where the structure factors are deposited. More worryingly he told us how few structure factors were deposited and that a significant portion of these are wrong. There then followed three short summaries. Gerard Bricogne avoided controversy and instead plugged AutoSHARP (http://www.globalphasing.com). Zbyszek Otwinowski gave an optimistic view of structural genomics (at least this was the opinion of several interventions from the floor). Colin Nave reminded us that there are cultural changes on the way in macromolecular crystallography; you may be worried by this or excited by it but it will happen.

Aside from the aforementioned talks, the meeting dinner on the Friday night was again held at York Racecourse which provided a well received meal, Yorkshire bitter, and a "timeless" disco which proved to be attract a wide range of meeting attendees including numerous members of the BSG committee. In addition, the overall success of the meeting also owes much to the hard work of the CCP4 administrative assistant Maeri Howard Eales along with Pat Broadhurst, Alison Mutch and Sue Waller on the Registration/Help Desk.

In conclusion, the CCP4 Study Weekend 2002 left little doubt that crystallography is central to high-throughput structure determination; however, the volume of the data that such worldwide efforts in this area will yield is daunting and downstream analysis may prove to be the "real bottleneck" in the future.

Biological Structure Group Committee
coordinated by Katy Brown

The Chatt Lecture 2002

The second Chatt lecture was presented by Professor Tom Blundell (Cambridge) on January 25th at the John Innes Centre in Norwich. Professor Ray Dixon (JIC) welcomed the audience of just over 280, and thanked the BCA for sponsoring the event. The lecture is held in honour of Joe Chatt, who was Director of the Nitrogen Fixation Unit from its foundation in 1962 until 1980. Professor Chatt's wife Ethel and their daughter Mrs Elizabeth Simms were present for the occasion.

From left to right: Mrs Elizabeth Simms, Professor Sir Tom Blundell FRS, Professor Ray Dixon and Mrs Ethel Chatt.

In his talk entitled "The post genomic challenge: from sequence, to structure, to function and therapeutic intervention", Tom Blundell presented the thesis that the process of analysis of sequence to structure to function can be automated by using homology modelling to trace evolutionary relationships between protein molecules. However, analysis of published genome data shows that around 30% of protein sequences bear little or no relationship to others.

Within a protein family, there is a strong core similarity, and this

similarity can be used to provide some information about the function of related proteins. As relationships have been shown to exist in small genomes, it is reasonable to infer that many more are likely to exist in large genomes.

While there are difficulties with deriving structures from sequence information, it may be possible to do the reverse, i.e. start with a structure and determine all possible sequences which will fit. The 3D structure can be obtained from prediction or ab initio calculations, or from analytical determination via X-ray or NMR. The search for homologues can be performed by following divergent evolution (by analysis of sequence) or by determining if a protein is from a known family (from its structure).

In Cambridge, the first route can be followed with the program FUGUE (see http://www-cryst.bioc.cam.ac.uk) using environment-specific substitution matrices to search for homologues and similarities in sequences; FUGUE does this with the use of database searching and alignment.

In general, homology recognition performance by automated methods is not very reliable, but very occasionally, these methods do give useful information with regard to the protein's function. A combination of methods allows relationships to be determined between different families.

The second method involves the automation of all the processes involved in X-ray or NMR methods of structure solution in a production line. It can be targetted towards interesting problems e.g. metabolic signalling or regulatory pathways. So far, this approach has been used to good effect, e.g. to determine the structures of all four enzymes involved in the pantothenate synthetase pathway. Another use of this approach is to focus on particular gene products, e.g. determining the functional organization of the S. Cerivisiae genome by systematic analysis of protein complexes.

Large complexes give high signal:noise in their function. Their formation is controlled initially by weak binary interactions, which give rise to multi-component complexes with large interaction surfaces. For example, fibroblast growth factor (FGF) receptors form a dimer of dimers, while simultaneously binding to heparin sulfate. Single mutations in this protein are found in human bladder and cervix carcinomas, and another single mutation gives rise to craniosynostosis (a facial deformity) and is implicated in the formation of webbed fingers and toes.

Pre-clinical discovery for pharmaceutical and agrochemical currently uses a random "hit - lead compound - screening" approach, but X-ray structures can be used for "virtual screening", for example by using the CCDC program GOLD. This has two main advantages; in the first place, potential drugs found by virtual screening could be used to form a cocktail solution for soaking protein crystals, and the resulting complexes analysed by X-ray diffraction; any compound bound preferentially could then be investigated further. The computational approach can pick up low affinity leads which can then be developed rapidly. Secondly, the other chief advantage is to screen out compounds which are readily metabolized before they can act on the target. At present, about 50% of drugs are metabolised by cytochrome P450, so pre-screening for P450 activity could be useful for eliminating potential drugs with this problem.

Harry Powell

Meetings of Interest

Puzzle Corner

The following is offered in an attempt to revive a small entertainment item for this magazine. Suggestions will be most welcome of almost anything with a crystallographic flavour. Word squares, crosswords, cryptograms, spot-the-difference or more literary things like finish-the-limerick are all possibilities. A Book Token for £10 will be offered for any offering used.

Many of you will have received a Christmas Card from what I had better call 'a leading firm of instrument manufacturers' with the attractive design shown above. It looks crystalline but has the apparent amazing point group 8mm (C_{8v} for Schoenflies enthusiasts). The background indicates that this crystalline aggregate might be a type of snowflake. A book token of £10 is offered for the best explanation of this illustration received by 19 April 2002. And, as Algernon requests in The Importance of Being Earnest, "Pray make it improbable".

The Editor

Meetings of Interest

These announcements are necessarily brief, but 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. A much more comprehensive list is maintained by Simon Parsons (s.parsons@ed.ac.uk) on the IUCR website – http//www.iucr.ac.uk – click on "Meetings" under "News Online" on the service bar. Simon would welcome comments on and contributions to this list.

March 18-22, 2002
Ice Focus Sessions at the 2002 March American Physical Society Meeting, Indianapolis, IN, USA
[http://www.chem.northwestern.edu/~geigerf/index.html]

March 23-28, 2002
9th International Conference on the Crystallization of Biological Macromolecules, Jena, Germany,
[http://www.conventus.de/iccbm9/]

March 25 - 28, 2002
BCA Annual Meeting, Nottingham University (Final details in this issue – see December 2001 issue as well)

April 2 - 4, 2002
Spring Meeting of the Materials Research Society, San Francisco, CA, USA
[http://www.mrs.org/meetings/spring2002/]

April 3 - 5, 2002
Biomolecular Interactions, Molecular Graphics and Modelling Society Annual International Conference in conjunction with the British Biophysical Society, Bristol.
[http://www.chm.bris.ac.uk/enzyme/mgms/outline.html]

April 7 – 11, 2002
The 19th General Conference of the Condensed Matter Division of the European Physical Society and CMMP 2002 : Condensed Matter and Materials Physics Conference of the Institute of Physics, Brighton.
[http://physics.iop.org/IOP/Confs/CMD19/]

May 15 - 17, 2002
European Synchrotron Source European Conference, Bundeshaus, Bonn, Germany
[http://www.ess-europe.de]

May 23 - June 2, 2002
From Genes to Drugs via Crystallography, Erice, Italy
[http://www.geomin.unibo.it/orgv/erice/drugdesi.htm]

May 23 - 26, 2002.
EPDIC-8 - 8th European Powder Diffraction Conference, Uppsala, Sweden
[http://www.mkem.uu.se/epdic8]

May 25 - 30, 2002
ACA American Crystallographic Association Meeting, San Antonio, TX, USA
[http://www.nexus.hwi.buffalo.edu/ACA/ACA-Annual/futuremeetings.html]

June 19 –21, 2002
11th Annual Fibre Diffraction and Non Crystalline Diffraction Meeting, Keele University, Staffordshire.
[http//www.ccp13.ac.uk]

June 23-27, 2002
American Conference on Neutron Scattering, Knoxville, TN, USA , sponsored by the Neutron Scattering Society of America (NSSA) and the Spallation Neutron Source High Flux Isotope Reactor User Group (SHUG). Deadline for abstract submission: March 25, 2002 [http://www.sns.gov/acns]

June 24 - 26, 2002
Time-Resolved Chemistry: From Structure to Function, Manchester.
[http://www.rsc.org/pdf/confs/faradisc/fara122/pdf]

July 14 - 19, 2002.
International Conference on the Physics and Chemistry of Ice , Newfoundland, Canada
[http://www.housing.mun.ca/conf/pci/]

July 29 - August 2, 2002.
Denver X-ray Conference, Denver, USA
[http://www.dxicdd.com/02/]

July 31 – August 2, 2002
Exploring Modern Computational

Chemistry , University of Nottingham. Organised in association with the Royal Society of Chemistry Theoretical Chemistry Group. [http://www.nottingham.ac.uk/chemistry/emc2]

August 4 - 6, 2002
Neutron and Synchrotron X-Ray Scattering in Condensed-Matter Research, Villingen, Switzerland [http://www.psi.ch/sls/NSCmr2002]

August 6 - 15, 2002
IUCr XIX - XIX Congress and General Assembly of the International of Crystallography, Geneva, Switzerland [http://www.kenes.com/iucr/ also at http://www.unige.ch/crystal/ahdf/geneva02.html]

August 25 - 29, 2002
SAS 2002, XII International Conference on Small Angle Scattering, VENICE, Italy with some satellite meetings at ELETTRA in Trieste. [Contact: A.Benedetti, Dipartimento di Chimica Fisica, Calle Larga S.Marta D.D. 2137, 30123 Venezia -ITALY [fax +39 041 257 8594, E-mail: sas2002@unive.it, http://www.isf.unian.it/isf/SAS/Home-SAS.htm]

September 1 – 6, 2002
International Mineralogical Association (IMA2002), Edinburgh [http://www.minersoc.org/IMA2002]

September 4 – 6, 2002
Synchrotron Radiation in Polymer Science II, European Physical Society Conference on Macromolecular Physics, Sheffield. [http://www.polymercentre.org.uk/srps/]

September 8 – 10, 2002
British Association of Crystal Growth Annual Conference, Liverpool [http://www.bacg.newi.ac.uk/index.htm]

September 15 – 18, 2002
15th International Symposium on Industrial Crystallisation, Sorrento, Italy [http://www.aidic.it/ISIC15/index.html]

April 14 - 17, 2003
BCA Annual Meeting, York University. Last day is Maundy Thursday

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

Corporate Members

Anachem Ltd

Astex Technology

Bede Scientific Instruments Ltd

Bruker/Nonius

Cambridge Crystallographic Data Centre

Hampton Research

International Centre for Diffraction Data

Oxford Cryosystems

Oxford Diffraction

Philips Analytical

Rigaku MSC

BCA Corporate Membership

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

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

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

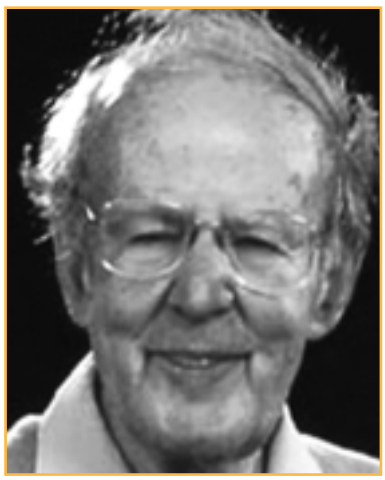
The cost of this membership is £600.00 per annum

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

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

Phone 01355 244966
Fax 01355 249959
e-mail bca@glasconf.demon.co.uk

Max Perutz 1914 - 2002



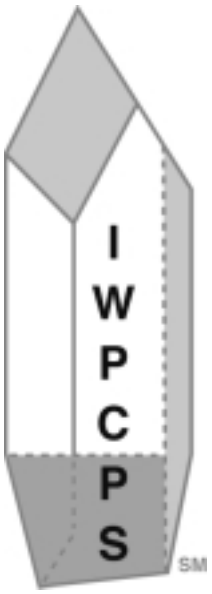
The following note is based on that written by Richard Henderson on the day Max died. A full obituary will be published in the June issue of Crystallography News.

Max Perutz died early in the morning of February 6th from cancer which developed during the last few months.

Max was the Chairman of the MRC Laboratory at Cambridge from its opening in 1962 in the present building until 1979 when he continued as a "retired worker", publishing over 100 papers and articles during his retirement. Until the Friday before Christmas he was active in the lab almost every day, submitting his last paper just a few days before then. This paper, on the structure of the glutamine repeats in Huntington's Disease, is now in press in PNAS.

Max will be remembered for his pioneering work in protein crystallography using X-ray diffraction, which led to the determination of the atomic structures of oxy and deoxy haemoglobin and the growth of the flourishing field of macromolecular crystallography. He was a gifted writer and lecturer who wrote many essays, books and book reviews. He had a special talent for attracting and supporting other outstanding scientists whose work laid the foundations of Molecular Biology, first in the MRC Unit for Molecular Biology in the Cavendish and, later, on the Hills Road site in the MRC Laboratory of Molecular Biology. He took particular pleasure in talking with students and other young scientists about their work.

We shall miss him and long remember the splendid example he has set for us all.



Third International Workshop on Physical Characterization of Pharmaceutical Solids[SM]

IWPCPS[SM]-3 www.**assa***international*.com June 9 - 14, 2002

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

The Preliminary Workshop Topics* include:

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

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

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

Find more information about the workshop, scheduled speakers and abstract submission as well as online registration at **www.assa*international*.com** or contact us at **workshops@assa*international*.com**.

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

International Centre for Diffraction Data

1941—Sixty Years—2001
Serving the Scientific Community

Release 2001
of the
Powder Diffraction File™

Featuring

- ❖ Over 87,500 experimental patterns
- ❖ 2,500 new experimental patterns added for Release 2001
- ❖ Over 49,000 patterns calculated from the ICSD database
- ❖ 2,821 new calculated patterns added for Release 2001
- ❖ Chemical formula, compound name, mineral name, structural formula, crystal system, physical data, experimental parameters, and references when available
- ❖ Interplanar (d) spacings, relative intensities (Int), and Miller indices
- ❖ Quality mark for each experimental pattern for estimate of reliability
- ❖ Entries indexed for subfile searches
- ❖ Dedication to detail and scientific purpose
- ❖ Four-tiered editorial process
- ❖ Highest standards for accuracy and quality

Visit us at www.icdd.com

Ask about our special Anniversary pricing!

Phone: 610.325.9814 ❖ Sales: 610.325.9810 ❖ Fax: 610.325.9823 ❖ info@icdd.com