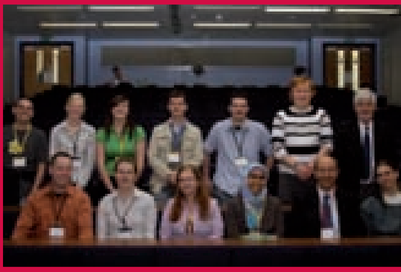
Crystallography News

British Crystallographic Association

Issue No. 109 June 2009
ISSN 1467-2790

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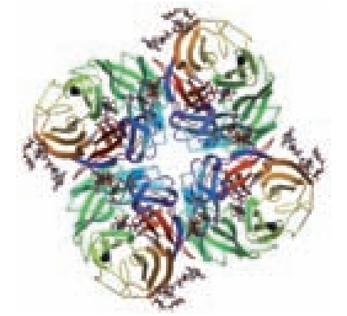

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Crystallography News June 2009

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This month's cover:

President Elspeth Garman, award to Frank Allen, welcoming NN staff, YC's; neuraminidase.

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BCA Administrative Office,
David Massey
Northern Networking Events Ltd.
Glenfinnan Suite, Braeview House
9/11 Braeview Place
East Kilbride G74 3XH
Tel: +44 (0)1355 244 966
Fax: +44 (0)1355 249 959
e-mail: bca@northernnetworking.co.uk

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Carl Schwalbe
School of Life & Health Sciences
Aston University
Aston Triangle
Birmingham B4 7ET
Tel: 0121 204 4009
e-mail: c.h.schwalbe@aston.ac.uk

The British Crystallographic Association is a Registered Charity (#284718)
As required by the DATA PROTECTION ACT, the BCA is notifying members that we store your contact information on a computer database to simplify our administration. These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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From the President

I feel deeply honoured to have been elected at the Loughborough BCA AGM to be the new President of the BCA: the first President of the Association in 1982 was Professor (later Lord) David C. Phillips, who took me on at LMB Oxford as a card carrying experimental nuclear physicist in 1987, with a view to transmuting me into a macromolecular crystallographer! However, I also find it a daunting prospect to succeed **Paul Raithby**. Beneath Paul's unfailingly jovial demeanour there is efficiency and steely determination to do the best for the BCA and the profession of crystallography. Although Paul has made his name as a very creative small molecule crystallographer, he has a sympathetic understanding of other areas of crystallography. Since I started as a physicist and am now in a Biochemistry Department, I hope I can follow his example in this respect. As a recently recruited Co-editor of the Journal of Applied Crystallography and of Acta Crystallographica D, I by necessity am trying to keep abreast of developments in all areas of crystallography.

The Spring meeting in Loughborough attracted over 350 delegates, and at least 80 of them were `Young Crystallographers'. From what I heard and from the part of it in which I was able to partake, it was a diverse and stimulating meeting, with the unifying theme across our subject of `Dynamic Crystallography'. We were glad to have the XRF community sharing the meeting. Many thanks are due to **Simon Parsons**, Chair of the Programme Committee, for masterminding and coordinating the meeting (and the Abstract book) and also to the Session Chairs from the Groups: **John McGeehan**, **Pierre Rizkallah**, **Andrew Bond**, **Amber Thompson**, **Chris Staddon**, **David Taylor**, **David Allan**, **Andrew Goodwin**, **Simon Coles**, **Helen Maynard** and **Owen Johnson**. Northern Networking provided their usual efficient level of organisation for the meeting, backed ably by the local Loughborough staff. We are most grateful to our 24 exhibitors for their support in these `credit crunch' times, and without whom we could quite simply not be able to run the Meeting in its present form. Of particular note was the Symposium held at the end of the meeting in honour of **Frank Allen** on his retirement, and the Tuesday morning YC session themed in special recognition of **Andy Parkin**'s contribution to crystallography. Andy was sadly missed at the meeting, and I especially enjoyed the poster entitled `Andy Parkin's A to Z of Crystallography' with `C is for Crystals' and `P is for φ The Phase Problem'. As a macromolecular crystallographer I can certainly empathise with both of those!

Two crystallographers were made Honorary Members of the BCA at the Meeting: **David Watkin** and **Frank Allen** to acknowledge their significant contribution to the field over many years. Their efforts dovetail beautifully: David's innovative software has helped us to put more structures into the literature, and Frank's guardianship of the Cambridge Structural Database and its analytical tools has enabled us to make sense of this wealth of data.

At the AGM, all three Ordinary Council members (**Bill Clegg**, **Richard Cooper** and myself) came to the end of their three year term, and after many years of service, our Web master, **Jeremy Cockcroft**, stepped down. Council is grateful for their contribution to the Association over the last 3 years, but happily expertise and experience will be retained since **Richard Cooper** is now Web master and **Bill Clegg** has kindly agreed to be a co-opted member of Council for a year. We welcome their replacements: **Alex Griffin**, **Andreas Goeta**, and **David Beveridge**. Following the AGM, Council have agreed to a scheme whereby in future, we will stagger the election of new ordinary members of Council at one a year, instead of a completely new triplet every three years.

My vision for the Association over the next three years involves development of several aspects of our organisation and educational outreach, some of which I know are already ongoing: further development of the new more flexible Website to provide an up-to-date resource for all members, exploring the possibility of linking BCA members in different fields of crystallograhy who are at the same institutions to see if they can offer each other for instance advice or access to facilities, and investigating the reduction of the BCA's paper consumption by offering members (if they so wish) the possibility of receiving their Crystallograhy News electronically in pdf format. I am deeply interested in education in the broadest possible sense, a passion spawned when I was for a year an 18 year old volunteer teacher in a Secondary School in Swaziland, Southern Africa, where I was expected to teach every subject on the curriculum except Zulu (but including Latin and Agriculture). I am lucky to teach on many international summer schools and courses; as a direct result of which there are currently two visiting Mexican graduate students in my group for 6 months, and I revel in the international nature of the field of crystallography.

On the wider front. this summer the ECM25 is being held in Istanbul from 16-21st August, and the programme looks varied and should have something of interest for all crystallographers. At this meeting, the BCA Council will be presenting a bid to hold the 2013 ECM in Warwick. The next issue of the IUCr Newsletter will be Part I of an account of Crystallography in Great Britain and Ireland, tenaciously and skilfully assembled by Bob Gould over the last few years. `Herding cats' is, I think, a more apt description of Bob's achievement on this project, and we are very grateful to him for his hard work on it.

Lastly, for those of you who were at the BCA conference dinner, you will be glad to hear that following my plea for information, the mystery identity of a poster contributor with the name of `Elspeth Garmin', University of Glasgow, is now solved, and I would be happy to share this story with anyone who asks me!

Elspeth Garman

BCA Council 2009

COUNCIL MEMBERS

President (2009)
Prof. Elspeth F. Garman
Department of
Biochemistry
South Parks Road
OXFORD OX1 3QU
elspeth.garman@bioch.ox.ac.uk

Vice President (2010)
Prof. Alexander J. Blake
School of Chemistry,
University of Nottingham
University Park
NOTTINGHAM NG7 2RD
Tel. 0115 9513488
A.J.Blake@nottingham.ac.uk

Secretary (2010)
Dr Georgina Rosair
School of EPS - Chemistry
Perkin Building
Heriot-Watt University
EDINBURGH EH14 4AS
Tel: 0131 451 8036/4241
g.m.rosair@hw.ac.uk

Treasurer (2011)
Dr Harry R. Powell
MRC Laboratory of
Molecular Biology
MRC Centre, Hills Road
CAMBRIDGE CB2 2QH
Tel: (01223) 402423
hrp1000@cam.ac.uk

ORDINARY MEMBERS

Dr David Beveridge
Harman Technology -
ILFORD Photo
Town Lane, Mobberley,
KNUTSFORD WA16 7JL
Tel: 01565 650000
David.Beveridge@
harmantechnology.com

Dr. Andrés E. Goeta
(2012)
Department of Chemistry
Durham University
Science Site, South Road
DURHAM DH1 3LE
Tel.: 0191 334 2102
a.e.goeta@durham.ac.uk

Dr Alexandra Griffin (2012)
oXray Ltd.,
36-37 Pembroke Street
Oxford, OX1 1BP.
Tel: 07525 687 432
alex.griffin@oxray.com

GROUP REPRESENTATIVES

Biological Structures
Dr Darren Thompson
Department of
Biochemistry
University of Sussex
BRIGHTON BN1 9QG
Tel: 01273 876631
D.Thompson@sussex.ac.uk

Chemical Crystallography
Dr Jonathan Charmant
School of Chemistry,
University of Bristol,
BRISTOL BS8 1TS
Tel. (0117) 928 8253
jon.charmant@bris.ac.uk

Industrial
Dr Anne Kavanagh
AstraZeneca
MACCLESFIELD, SK10 2NA
Tel. 01625 517454
Anne.Kavanagh@
astrazeneca.com

Physical Crystallography
Dr Matt Tucker
STFC Rutherford Appleton
Laboratory
DIDCOT OX11 0QX
Tel: 01235 445581
M.G.Tucker@rl.ac.uk

Young Crystallographers
Ms. Susanne Huth
School of Chemistry
University of
Southampton
SOUTHAMPTON SO17 1BJ
Tel: 023 8059 4132
s.huth@soton.ac.uk

CO-OPTED MEMBERS

Prof. William Clegg (2009)
School of Natural Sciences
(Chemistry),
University of Newcastle,
NEWCASTLE UPON TYNE
NE1 7RU
Tel: 0191 222 6649
W.Clegg@newcastle.ac.u

Prof. Paul Fewster
PANalytical Research
Centre
Sussex Innovation Centre
BRIGHTON BN1 9SB
Tel: 01273 704422
paul.fewsterpanalytical.com

EX-OFFICIO MEMBERS

Education Coordinator
Dr Michael R. Probert
Department of Chemistry
Durham University
Science Site, South Road
DURHAM DH1 3LE
Tel: 0191 334 2004
m.r.probert@durham.ac.uk

Editor
"Crystallography News"
Prof Carl H. Schwalbe
School of Life & Health
Sciences
Aston University
BIRMINGHAM B4 7ET
Tel: 0121 204 4009
c.h.schwalbe@aston.ac.uk

Webmaster
Dr Richard Cooper (2009)
oXray Ltd
Oxford Centre for
Innovation
OXFORD OX2 0JX
Tel: 01865 811107
Richard.cooper@ oxray.com

President (2009)
Prof. Paul R. Raithby
Department of Chemistry
University of Bath
Claverton Down
BATH BA2 7AY
Tel: 01225 383183
p.r.raithby@bath.ac.uk

GROUP CHAIRMEN

Biological
Structures Group
Dr Andrea Hadfield
Department of Biochemistry
University of Bristol
BRISTOL BS8 1TD
Tel: 0117 331 2151
a.t.hadfield@bristol.ac.uk

Chemical
Crystallography Group
Dr Andrew D. Bond
Department of Physics and
Chemistry
University of Southern
Denmark, 5230 ODENSE M,
DENMARK
Tel: +45 6550 2545
adb@chem.sdu.dk

Industrial Group
Dr Anne Kavanagh
AstraZeneca
MACCLESFIELD, SK10 2NA
Tel. 01625 517454
Anne.Kavanagh@astrazeneca.com

Physical
Crystallography Group
Prof. David Keen
ISIS Facility, Rutherford
Appleton Laboratory
Harwell Science and
Innovation Campus
DIDCOT Oxfordshire OX11 0QX
Tel: 01235 446556
d.a.keen@rl.ac.uk

Young Crystallographers
Ms. Susanne Huth
School of Chemistry
University of Southampton
SOUTHAMPTON SO17 1BJ
Tel: 023 8059 4132
s.huth@soton.ac.uk

Full committee details on the BCA website **www.crystallography.org.uk**
Spring Meeting Registration and Subscriptions:
www.crystallography-meetings.org.uk

From the Editor

THIS issue will reach a readership that has recently received a fresh charge of energy from the very successful BCA meeting in Loughborough. The title "Dynamic Crystallography" was doubly appropriate: a major part of the meeting was indeed devoted to the crystallographic study of ongoing processes rather than static situations, but more generally it showed how our chosen field is full of vigour and new ideas. A sign of this happy situation is the participation of other scientific societies. Two of our Industrial Group sessions were also under the auspices of the British Association for Crystal Growth, and a strand running throughout the meeting covered the topic of X-ray fluorescence jointly with practitioners of that technique.

This meeting was topped and tailed by two other exciting events. The Young Crystallographers' sessions provided a vibrant start. The enthusiasm was youthful enough, but the polish of the presentations suggested that the speakers had been doing it for years. The lucid and enjoyable summary of the history of crystallography given by **David Watkin** in the Lonsdale Lecture provided the perfect bridge to the main meeting. After the meeting a symposium honoured **Frank Allen** on the occasion of his retirement as Executive Director of the Cambridge Crystallographic Data Centre. The fame of the speakers and the high quality of their presentations mirrored the affection and admiration we feel for Frank. To appreciate his contributions, imagine the following two scenarios: (1) There is no Cambridge Structural Database. Every time we solve and refine a new structure, we have to spend several days in the library lugging bound journals around while we try to find suitable structures for comparison. (2) The CSD exists, but CCDC plc is run by lawyers and bankers, access to the CSD costs £10,000 per year for academic users and £100,000 for industrial/commercial users, and the retiring Executive Director has been awarded a pension pegged to that of Sir **Fred Goodwin**. Now give thanks that we have a CSD efficiently administered by scientists with a CCDC that is staffed by innovators of methodology for the analysis and prediction of crystallographic data, and that generously supports students.

Another person who deserves our gratitude is **Paul Raithby**, whose term as President of the BCA has just finished, leaving the BCA in a healthy state. As Editor I am particularly grateful to Paul. A couple of weeks before each copy deadline, before I could even start to type an e-mail reminding Paul to send me his 'From the President' column", it would arrive, accompanied by the modest request to edit it as I saw fit. Invariably the text was so near-perfect that my only editing might be to add one comma and to change another to a semicolon. I now look forward to working with our new President, **Elspeth Garman**.

Unfortunately, readers will have to wait until September for a detailed account of the sessions at Loughborough. Between the close of the meeting on April 23 and the copy deadline for this issue of April 25, even the most dynamic bursary recipient could not be expected to produce a balanced and well-written report. In this issue we shall have mainly photographs that I hope will bring back good memories. Please pay special attention to the pictures of our sponsors' exhibits. At this time of recession when so many companies are making savage cutbacks it is indeed gratifying that our suppliers are still willing to give their support to the crystallographic community.

The lack of meeting reports leaves space for two other items. One of the Editor's privileges is that I receive newsletters from other crystallographic societies, notable among which is the Swiss Society for Crystallography. Nearly all of their newsletter is written in English. This English is-- dare I say it-- of a higher quality than that of many contributions sent to me from within Britain! I found two articles from their December issue particularly interesting, and I thank **Jürg Schefer**, the Editor, for permission to re-publish them here.

The Swiss are planning the PSI-XFEL, an X-ray Free Electron Laser at the Paul Scherrer Institut in Villigen. As befits a nation that was building fine watches while much of the rest of the world was building grandfather clocks, the PSI-XFEL will be considerably smaller than the world's other XFEL installations thanks to clever design of the electron source. **Bruce Patterson**, the author of the article, specifically welcomes input from interested parties outside of Switzerland.

At recent conferences I have noticed how often the technique of charge-flipping gets mentioned as a means of solving otherwise intractable problems. However, I must admit to a lack of understanding as to how and why it works. The article by Palatinus, Chapuis and Thibault on dual-space iterative phasing methods went a long way to rectifying this situation for me. I thank **Lukas Palatinus** for letting me publish it here, and I hope it will also enhance readers' understanding.

At the time of writing, early May, there is concern about H1N1 swine flu. Fortunately two drugs discovered with the aid of crystal structure analysis, oseltamivir (Tamiflu) and zanamavir (Relenza) can treat it, although resistance is showing up in other variants of influenza. An article in this issue describes how crystallographers are tackling this problem too.

Carl Schwalbe

Puzzle Corner

OUR magnificent DIAMOND synchrotron is now providing valuable data for crystallographers. In 2007 I enjoyed an impressive tour, which I would recommend to any reader. I have just one slight quibble: aside from the name of the synchrotron itself, the names of beamlines (letter-number) and instruments are so prosaic. Only lonely LOLA on I20 adds a splash of colour. Other facilities, beamlines and instruments have more imaginative names, often unrelated to the country where they are sited. What location corresponds to each of the following names, and do they involve neutron or synchrotron radiation?

ALBA

ANKA

BACH

BEAR

GEM

HANARO

MANDI

MUSTANG

NIMROD

OPAL

ORIENT EXPRESS

PEARL

SALSA

SESAME

SNAP

TOMCAT

VESUVIO

VIVALDI

BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
- A 10% discount on exhibition stands on the annual BCA Spring Meeting, OR - A promotional poster at the annual BCA Spring Meeting.
- Free insert in the annual Spring Meeting delegate bag.
- Two free full registrations to the annual Spring Meeting.
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Northern Networking Events Ltd
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Braeview House, 9/11 Braeview Place
East Kilbride G74 3XH
Tel: +44 (0)1355 244 966 Fax: +44 (0)1355 249 959
e-mail **bca@glasconf.demon.co.uk**

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From the Secretary

AS a member of the UK delegation I attended the IUCr General Assembly in Osaka, Japan last August as has been mentioned in the President's report. Whilst we were there, we were all saddened to learn that Andy Parkin had passed away and the Council is looking for an appropriate way to commemorate Andy's contribution to the BCA.

One of the issues raised at the last AGM and at the IUCr meeting in Osaka was the status of the World-wide Directory of Crystallographers. The IUCr are very keen to get this up to date and they have appointed a new General Editor, Professor Torriani. The IUCr will update the interface prior to inviting crystallographers to either join or update their existing entries. I have been asked to be the UK contact. The IUCr plan to generate a printed output of entries for each country and they have asked for this to be reviewed by national associations. However this will take into account data protection issues. The IUCr are open to new ideas for updating so if anyone has any please let me know.

Sandy Blake, the Vice President of the BCA, has been looking at the statutes and by-laws of the BCA with me. There are updates required because of changes accepted at previous AGMs but also as a growing organisation changes and adjustments need to be made so that the statutes of the BCA serve their purpose here and now. One of these is the inclusion of a new group, the Young Crystallographers. We have also been working with the Young Crystallographers to advise them on their constitution, with input from the BCA Council.

I would also like to thank **Paul Raithby** who has both led and served Council very ably and amicably as President and wish him all the best for the future. Thanks also to our Ordinary members **Bill Clegg**, **Richard Cooper** and **Elspeth Garman** for their contributions to Council and whose terms of office as Ordinary members finish at the AGM. Bill is now a co-opted member, Richard is the new webmaster, and Elspeth is the new President. I wish them all the best for the future.

Georgina Rosair, April 2009

Puzzle Corner...
...DECEMBER ANSWER

HERMANN	Author of space group notation
M**A**UGUIN	Author of space group notation
CO**P**PER	Policeman or penny that may become a target
KAP**P**A	Greek axis in Dutch diffractometer
MYOC**Y**TE	Type of cell containing the protein studied by Kendrew
NEUTRON	Beam used in diffraction experiments
P**E**RUTZ	Scientist who shared the Nobel Prize with Kendrew
PO**W**DER	Type of crystalline sample that can be used for identification and, sometimes, structure determination
YTTRIUM	Element used in red phosphors on cathode ray tubes
D**E**BROGLIE	Scientist who postulated wave-particle duality
X-R**A**Y	Beam used in diffraction experiments
FER**R**OUS	Iron (II)

The message was "Happy New Year," and the winning entry came from Jim Trotter.

From the Treasurer

Change of Bank

THE BCA has moved its bank accounts from HSBC to CAF Bank (the Charities Aid Foundation Bank, which is the only bank that the Charity Commission seems to recommend). The principal advantage for the BCA is that CAF treats it as a charity rather than as a commercial organisation.

For most members, this change should make no difference at all to how they interact with the BCA. The people who will be affected are those who choose to pay their annual subscription by standing order. No member who pays by cheque or the online credit card facility will see any change in the ways that things are done.

Standing Orders

ALL standing orders set up currently payable to BCA, for whatever purpose (for most people this means paying their annual subscription), should cease to operate once the HSBC accounts are closed in the middle of this year. In an ideal world, their bank would no longer take the money from their account once the BCA accounts at HSBC cease to exist, but it would be wise to make sure that all standing orders to BCA are cancelled.

While not wishing to labour the point, BCA has no control of any kind over standing orders; if the money is taken from an account to be paid into an account that has ceased to exist, the money essentially disappears into the banking system. It may be recoverable, but that would be a matter for the member and their bank.

Direct Debits

MEMBERSHIP subscriptions to the BCA's CAF accounts will be possible via direct debit, but not by standing order, following discussions by Council. All payments made by the direct debit method are covered by the "direct debit guarantee". The following is taken verbatim from the UK's Financial Ombudsman's web pages:

- If you pay by standing order, it is up to your bank to send the payment. If you pay by direct debit, it is up to the payee's bank to call for the payment, but you will rightly look to your own bank/building society to ensure the smooth running of any direct debits. Mistakes and errors are covered by the direct debit guarantee.

- The direct debit guarantee applies to *all* banks and building societies taking part in the direct debit scheme. It says that:
  - If there is a change in the amount to be paid or the payment date, the person receiving the payment (the originator) must notify the customer in advance.
  - If the originator or the bank/building society makes an error, the customer is guaranteed a full and immediate refund of the amount paid.
  - Customers can cancel a direct debit at any time by writing to their bank or building society.

The main reason for this change is the high proportion of members who pay an incorrect subscription fee to BCA via standing order; this currently runs at just under 50% of standing orders, and thus represents a significant loss in membership subscriptions. In order to encourage take-up of the new direct debit payment, BCA will offer a 10% discount on the applicable subscription rate for those members who wish to take advantage of it.

I understand that there are members who simply do not trust the direct debit system, since it gives a third party some control over what is taken out of their accounts; I can assure all members that any issues arising from incorrect payments will be dealt with in a timely and sensitive manner. Those members who feel that they do not wish to pay their dues by direct debit will be able to pay by cheque or by credit card.

Financial Statement

The British Crystallographic Association

Summary Financial Statements for year ended 31 December 2008

Examining Accountant: R A Young, BSc. FCA
The Young Company, Ground Floor, Unit 2B Vantage Park,
Washingley Road, Huntingdon, Cambridgeshire PE29 6SR

These are consolidated accounts and include the BCA, BSG, IG, CCG and CCG School funds, expressed in pounds sterling (£)

INCOMING RESOURCES:

	2008	2007
Grants and sponsorship	6,700	11,013
Donations	6,341	6,831
Annual conference (5)	93,431	99,195
Meetings of groups	9,406	36,369
Crystallography News	26,945	22,944
Membership Subscriptions	25,503	24,714
Net income from trading	15	16
Investment income	3,090	4,100
Interest received	5,243	4,899
TOTAL INCOME	**176,674**	**210,081**

EXPENSES:

	2008	2007
Direct charitable expenditure (2)	159,029	172,259
Management and administration (3)	31,675	28,884
TOTAL EXPENDITURE	**190,704**	**201,143**

	2008	2007
NET (EXPENDITURE)/INCOME:	(14,030)	8,938
Unrealised (losses) on investment assets	(9,744)	(4,149)
NET MOVEMENT IN FUNDS	**(23,774)**	**4,789**
Balances brought forward at 1 January	222,555	217,766
Balances carried forward at 31 December	198,781	222,555

ASSETS:

Fixed assets	2008	2007
Tangible assets	5	5
Investments	50,848	70,592
Total	50,853	70,597
Current assets		
Stock	493	493
Debtors	1,758	16,928
Cash at Bank	169,491	143,503
Total	171,742	160,924
LIABILITIES: amounts falling due within one year	(22,689)	(7,436)
LIABILITIES: amounts falling due after one year	(1,125)	(1,530)
NET ASSETS	**198,781**	**222,555**

INCOME FUNDS:

	2008	2007
Restricted funds (4)	99,459	95,071
Unrestricted funds (4)	99,322	127,484
Total	**198,781**	**222,555**

NOTES TO THE SUMMARY FINANCIAL STATEMENTS

1. ACCOUNTING POLICIES.

These summary statements are based on financial statements which have been prepared under the historical cost convention, with the exception of investments which are included at market value. The financial statements have been prepared in accordance with the Statement of Recommended Practice, "Accounting and Reporting by Charities" published in March 2005 and applicable accounting standards.

All incoming resources are included in the Statement of Financial Activities when the charity is legally entitled to the income and the amount can be quantified with reasonable accuracy. All expenditure is accounted for on an accruals basis and has been included under expense categories that aggregate all costs for allocation to activities. Investments are stated at market value at the balance sheet date.

Tangible fixed assets are stated at cost less depreciation. Depreciation is provided at rates calculated to write off the cost of fixed assets, less their estimated residual value, over their expected useful lives.

2. DIRECT CHARITABLE EXPENDITURE

	2008	2007
Subscription to International bodies	6,912	6,569
Annual conference (5)	113,405	96,526
Meetings of groups	8,994	8,591
Crystallography News + Newsletters	22,236	24,301
Course fees and accommodation	-	27,000
Grants and sponsorship	2,982	5,440
Awards & bursaries	-	882
Arnold Beevers Bursary Fund	4,500	2,950
Total	**159,029**	**172,259**

3. GOVERNANCE

	2008	2007
Administration fee	18,021	20,781
Administration expenses	8,230	-
Accounting fee	3,967	3,936
Insurance	392	392
Bank and security charges	118	155
Special Interest Group Administration	-	1,958
Council members' expenses	947	1,662
Total	**31,675**	**28,884**

The full BCA accounts for 2008 are available as an e-mail attached file from the BCA administrative office.

The British Crystallographic Association

Summary Financial Statements for year ended 31 December 2008

4. STATEMENT OF FUNDS	Brought Forward	Incoming Resources	Resources Expended	Gains (Losses)	Carried Forward
UNRESTRICTED FUNDS					
General Fund	127,484	155,168	(173,586)	(9,744)	99,322
RESTRICTED FUNDS					
IUCr bursary fund	26,844	3,387	-	-	30,231
Arnold Beevers bursary fund	16,597	926	(4,500)	-	13,023
Dorothy Hodgkin prize fund	8,052	28	-	-	8,080
Chemical group teaching school	11,850	5,800	-	-	17,650
Chemical group fund	3,659	2,492	(3,959)	-	2,192
Industrial group fund	10,022	6,877	(4,416)	-	12,483
Biological Structures group fund	18,047	1,996	(4,243)	-	15,800
Subtotal	**95,071**	**21,506**	**(17,118)**	**-**	**99,459**
Total of Funds	**222,555**	**176,674**	**(190,704)**	**(9,744)**	**198,781**

5. Spring Meeting 2008 University of York	
INCOME	
Sponsorship	961
Registration	70,102
Exhibition	21,268
Bursaries	1,100
Total	**93,431**
EXPENDITURE	
Accommodation & Meals	34,412
Facilities	25,064
Catering	11,786
Social Event	6,875
BCA Speakers Expenses	1,614
Refunds	2,412
Abstract Book	4,870
NNE Fee	15,110
Administration	4,761
Printing & Stationery	2,169
Young Crystallographers	4,332
Total	**113,405**
TOTAL INCOME	**93,431**
TOTAL EXPENDITURE	**113,405**
MEETING DEFICIT	**19,974**

All the transactions for the 2008 Spring Meeting were made through the BCA account, and consequently these detailed meeting accounts are reported as part of the BCA financial report

Treasurer's Report 2008

This was a busy year for the BCA and its constituent groups. Overall we had a deficit of £23,774 during the year ended 31 December 2008; the Association has no material guarantees or commitments which could affect its future solvency.

The general fund had a deficit of £28,162 after a decrease of £9,744 in the value of the investments, but the reserve funds operated by the Groups and the School had an overall surplus of £4,388. The income from our investments brought in £8,333 this year.

The Association moved its main bank accounts to the Charities Aid Foundation Bank in the Autumn. This has the advantage over high street banks in that the Association is treated as a charity rather than as a commercial enterprise; a bonus is that interest rates on capital are substantially higher than we could obtain previously. The major risks to which the Association is exposed are with regard to the cost of the Spring Meeting and its effects on the Association's major reserves. To mitigate those risks the Association has all its investments placed with an independent professional management company. Our investment portfolio was valued at £50,848. The Council's review of the reserves indicates that we should always be striving to generate more income to enable us to plan and encourage even higher levels of educational and scientific activity.

The Young Crystallographers' symposium before the Spring Meeting in York was well attended and appreciated, and sponsors were generous in their support too. Seven bursaries were awarded to the Spring Meeting, of which four were commercially sponsored. We awarded bursaries totalling £3,750 from the Arnold Beevers Bursary Fund to 15 people attending meetings on a wide variety of crystallographic topics, including ten for attendance at the IUCr Congress in Osaka, Japan. The bursary fund for the IUCr was not required by the organisers of the meeting this year, so the monies are accumulating in the reserve fund, and will be offered to the meeting in Madrid 2011 in due course.

Crystallography News has made a small surplus this year on an income of £26,945. The BCA thanks its advertisers and sponsors who generously support our activities. The deficit from the Spring Meeting was an unwelcome reminder of the costs involved in changing location late in the day. The sponsorship was substantially lower than in 2007.

Subscriptions to international bodies were £6,912, covering our membership of the IUCr at the five-vote level; no invoice was received from the European Crystallographic Association, so the subscription will be included in the accounts for 2009. Administration costs, including expenses, are £26,251. The online payment facility for Group meetings has been utilised by both IG and CCG this year. The expertise and hard work of Northern Networking Events Ltd is very much appreciated.

Membership income is up this year by £789. Roughly half the members who pay by standing order have not amended their payment since the increase in dues. Nothing was received from the Inland Revenue in Gift Aid this year due to an oversight on my part; fortunately, claims can be made up to 6 years in arrears so this will be corrected in 2009. The Arnold Beevers Bursary Fund was boosted by a transfer of £901 bank interest income from the BSG, for which the BCA is very grateful.

This is my first report as Treasurer, and I would like to thank everyone, in particular Sheila Gould, my predecessor as Treasurer, Paul Raithby, members of Council, Gill and the team at Northern Networking Events, and our accountant Bob Young for all their help throughout the year.

Harry Powell **Hon Treasurer**

The full BCA accounts for 2008 are available as an e-mail attached file from the BCA administrative office.

News from the groups

Young Crystallographers Group Update

THE BCA Spring Meeting in Loughborough has just passed and I have taken away many inspirations from the excellent contributions focused on "Dynamic Crystallography". As in previous years, the Young Crystallographers Meeting preceded the main meeting; and from the feedback that has reached me, I am proud to say that the talks and posters presented at the YC2009 were again of very high standards. Such a meeting would not be possible without all the input of the contributors and hence a big thank you goes to all speakers and poster presenters! Of course the organisation of this event should not be underestimated and the YCG Committee has put great efforts into making the YC2009 another successful meeting. It has been a true pleasure to be part of this working team and I am looking forward to another term in office!

One of our primary aims for the next year is to raise general awareness amongst potential YCG Members so here is a brief update on YCG business: **Helen Maynard** and **Arefeh Seyedarabi** finished their two year terms as PCG Representative and Ordinary Member, respectively, and they are both thanked for their invaluable contributions to the Committee. New Members were elected onto the Committee at the YCG AGM in Loughborough and we welcome **Samantha Callear** as the new PCG Rep and **Soshichiro Nagano**, **William Lewis** and **Anna Stevenson** as new Ordinary members while Arefeh returns as the new BSG Rep.

Particularly pleasing is that the YCG Constitution met with approval by the YCG Members at the YCG AGM and was subsequently approved by the BCA Council on 23rd April. This is an important step in establishing the YCG as the fifth BCA Special Interest Group and provides the YCG with the necessary foundations for the years to come. As part of the overhaul of the BCA website, the YCG website will move over to the main BCA domain, so if you experience any difficulties please bear with us. In order to make joining the YCG a lot clearer we are working together with Northern Networking on amending the membership form and soon there should be the possibility to join the YCG as part of the on-line form for updating membership details on the BCA webpage.

For the first time there will be a joint IG/YCG autumn meeting taking place on Thursday 5th November this year. More details can be found on the IG and YCG websites and will follow in the next issue of Crystallography News. In Loughborough I also learnt from the ECA President, **John Helliwell**, that a YC Evening Mixer Session will be held at the ECM in Istanbul this August. The organisation is a joint effort of the YCGs in Spain, the Czech Republic and us here in Britain. It is very exciting to see YC movements in the European Countries come together and if successful this might well be the first step for YCs to be recognised as an individual group within the ECA. Keep an eye on the YCG and ECM websites for more details.

So far this is the most important news from the YCG; more information can be found by following the link to our webpage on the BCA website, and announcements are also made on our facebook group and on the x-rayman xforum.

Susanne Huth
YCG chairman

News: CCG Autumn Meeting Announcement

CHEMICAL CRYSTALLOGRAPHY GROUP

The CCG Autumn Meeting will be held at the University of Oxford Chemistry Department on **Wednesday 18th November 2009**
The theme of the meeting is:
"Methods Complementary to Crystallography"

INDUSTRIAL GROUP

Diary Dates and Call For Papers:

British Association of Crystal Growth 40th Anniversary Conference, **6-8 September, 2009**, Bristol.

Call for papers
5th November 2009, new venue to be confirmed. Autumn Meeting - including a Young Crystallographers Session.

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Science Opportunities at the Proposed PSI-XFEL

B.D. Patterson, R. Abela and J.F. van der Veen
Paul Scherrer Institut, CH-5232 Villigen, Switzerland
bruce.patterson@psi.ch

THE Paul Scherrer Institut is planning the construction of an X-ray Free Electron Laser. The PSI-XFEL will produce 60 fs pulses of coherent X-rays in the wavelength range 0.1 - 10 nm, with a peak brightness approximately 10^{10} times that of a third-generation synchrotron. The brightness, coherence and short pulses provide opportunities for performing novel science in the fields of chemistry, biochemistry, solid state physics and materials science. The PSI-XFEL could be operational in the year 2016.

What is an XFEL, and how is the PSI-XFEL special?

The active medium in an X-ray free electron laser consists of a 100 femtosecond pulse of 10^9 relativistic electrons moving in the sinusoidal field of an undulator: a periodic linear array of alternately-poled permanent magnets. As in a synchrotron light source, the transverse acceleration from the Lorentz force causes the electrons to emit X-radiation, but in an XFEL, the undulator is sufficiently long that the growing radiation field influences the trajectory of the electrons. At the "resonance condition", where the radiation overtakes an electron by exactly one wavelength per undulator period, certain of the electrons gain energy and others lose energy, thus splitting the pulse into 10^5 "microbunches". As it moves along the undulator, the microbunched electron pulse then radiates as if it were a single charge of 10^9 e, producing an intense, coherent pulse of "superradiant" X-rays.

Besides the PSI-XFEL there are presently three other projected XFELs worldwide: in Stanford, USA (2009), Hyogo, Japan (2011) and Hamburg, Germany (2014). The maximum electron energy and hence the overall XFEL length (800 m) are significantly lower at PSI than for the other projects. This is made possible by PSI innovations in the high-brightness electron source technology, including nanometer-scale field-emitting tips and initial acceleration in a pulsed field of 1 MV across a 4 mm gap, followed by a novel two-frequency RF-cavity. The individual X-ray pulses will be very similar to those of the larger projects (see Table 1). While the Swiss, US and Japanese XFELs will emit 60-120 pulses per second, the Hamburg machine, due to the use of superconducting accelerator technology, will produce 10 trains of 3000 pulses per second, with a minimum pulse spacing of 200 ns.

With sufficient resources, the PSI-XFEL could have enhanced capabilities which are not presently foreseen at the other projects. These include: rapid tuning of the XFEL wavelength for spectroscopic investigations, the option of circular polarization for magnetic studies, additional beams of pulsed, broadband spontaneous radiation for time-resolved Laue crystallography and wavelength-dispersive spectroscopy, extension of the maximum photon energy to the ultra-narrow Mössbauer resonance of ^{57}Fe at 14.4 keV, and modification of the electron pulses by "seeding" and / or "slicing" to yield substantially narrower spectral widths and / or pulse lengths than those given in the Table. Rapid switching of the electrons will allow the simultaneous operation of three PSI-XFEL branches, covering the photon energies 12.4 - 4.0, 4.4 - 0.4 and 1.2 - 0.13 keV.

Table 1. PSI-XFEL specification

Maximum electron energy	6 GeV
Photon wavelength	0.1 - 10 nm
Photon pulse length (FWHM)	60 fs
Spectral width (FWHM)	0.1 - 0.9 %
Beam size at undulator exit (FWHM)	25 - 35 µm
Peak brilliance	10^{33} - 10^{31} ph/s/mm^2/mrad^2/0.1 % bw
Flux	2 x 10^{11} - 5 x 10^{12} ph/pulse
Pulse repetition rate	100 Hz

Proposed applications

The bright pulses and high degree of coherence of the XFEL radiation will allow time-resolved lensless imaging to be performed on a variety of systems, including ferroelectric and magnetic domains in thin films, biomolecular conformations in solution and molecular diffusion on surfaces. Time-dependent changes can be triggered by a switched electric or magnetic field (see Fig. 1) or by a fs optical laser pulse which is synchronized to the X-ray pulse. On the other hand, *equilibrium* fluctuations on the fs - ns time scale can be studied as a function of wavevector using X-ray Photon Correlation Spectroscopy [3]. All of these techniques require the rapid collection of high-resolution 2D-images and the stepwise variation of a pulse delay. Furthermore, the excited sample must relax to equilibrium before the next pump-probe cycle is initiated. Such processes are compatible with the 100 Hz repetition rate of the PSI-XFEL.

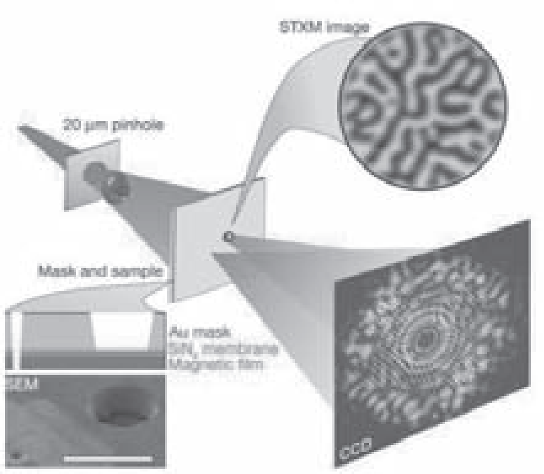

Fig. 1. Static holographic imaging of the sub-µm domain structure in a thin magnetic film, performed at the BESSY synchrotron. Magnetic contrast is provided by using circularly-polarized X-rays at the L3 absorption edge of the magnetic Co ion. At the XFEL, such a pattern can be measured with a single X-ray pulse, allowing sub-ps pump-probe studies of magnetization dynamics. Reprinted by permission from Macmillan Publishers Ltd: [2].

With a tunable XFEL wavelength, X-ray absorption spectroscopy (XAS) can also be used to follow a time-dependent process. For example, it is proposed that a chemical reaction be "gently" initiated on a catalytic surface by using a sub-ps pulse of coherent terahertz radiation [4]. After a variable time delay, the chemical or electronic environment of the reactive species is determined by near-edge (XANES) or far-edge (EXAFS) absorption spectroscopy. It is also foreseen to use time-resolved pump-probe XAS to follow laser-initiated photo-chemical reactions in solution [5]. The time-dependent behavior of solid materials following excitation by a sub-ps laser pulse is a wide field of inquiry, including topics such as non-equilibrium melting, the coherent creation and control of phonons, local structural changes upon the photo-excitation of chromophores, etc. Since the advent of "sliced" synchrotron beams, sub-ps X-ray pulses [6-8] have become available, albeit with very low intensities. At the sliced "FEMTO" beamline of the Swiss Light Source, it has been possible to coherently create and control phonons in a bismuth crystal [8]. Because the PSI-XFEL will deliver vastly more photons per pulse, such pump-probe experiments in solids will become orders of magnitude easier to perform.

The XFEL will also provide several new tools to biochemists. The time-dependent behavior of photosensitive biomolecules in crystalline form can be studied by time-resolved, pump-probe Laue crystallography. Using isolated, 100 ps pulses at a synchrotron, structural changes accompanying the photodetachment of CO from the heme group in myoglobin have been recorded in the ns - µs regime [9] (see Fig. 2). With spontaneous radiation from an incoherent undulator downstream from the XFEL, the same number of broad-bandwidth photons now available in a 100 ps synchrotron pulse will be available in a 100 fs pulse, thus extending time-resolved Laue crystallography into the sub-ps regime.

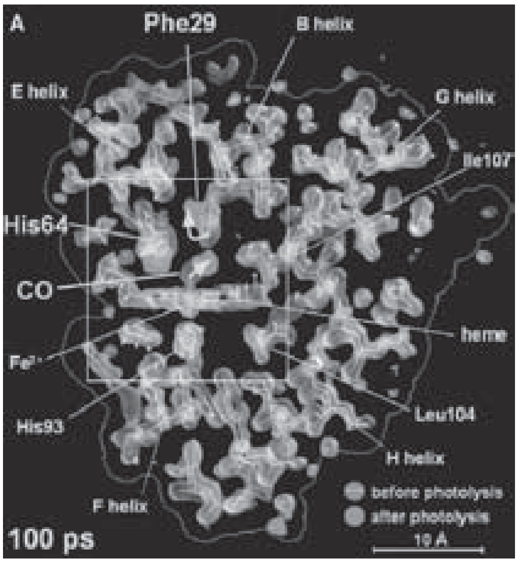

Fig. 2. A comparison of the local structure of a myoglobin molecule before and after the photodetachment of CO from the heme group, produced using 100 ps time-resolved Laue crystallography. The PSI-XFEL, with an additional spontaneous undulator, will extend such investigations to the sub-ps regime. Reprinted by permission of The American Association for the Advancement of Science: [9].

The "holy grail" of XFEL-based structural biology is the structural determination, with atomic resolution, of large, *individual* biomolecules, without the requirement of crystallization. Indeed, the highly-important membrane proteins can generally not be crystallized, and hence their structures remain largely unknown. It is proposed that the hard X-ray XFEL beam be focused down to 100 nm, and that individual protein molecules be synchronously injected, one-by-one, into the XFEL pulses. Of course, the intense X-ray pulse will quickly destroy the molecule (see Fig. 3), but from sliced pulses shorter than several fs, sufficient

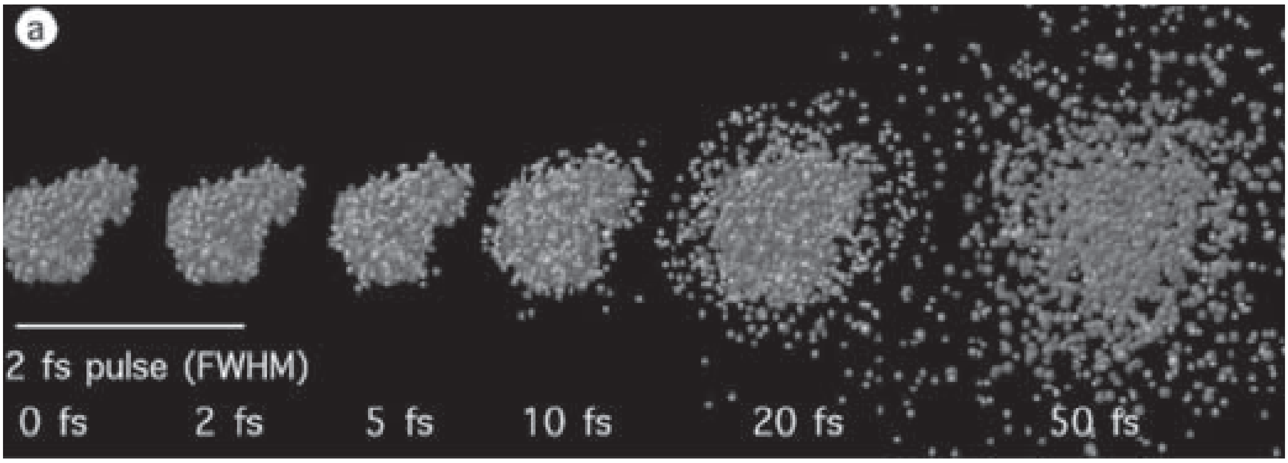

Fig. 3. The simulated "Coulomb explosion" of a protein molecule in a 2-fs XFÈL pulse. Scattered photons yield information on the unperturbed molecule. Reprinted by permission from Macmilllan Publishers Ltd: [10]

scattered photons may possibly be obtained to allow a structural determination. Even with the XFEL in operation, many hurdles must be overcome before this goal can be achieved: pulse shaping and focusing, particle preparation and injection, data collection and, importantly, combining the data from many individual, randomly-oriented molecules.

Conclusion

The qualitative advances in performance by an X-ray free electron laser over all existing X-ray sources make accurate predictions of the relevant photon-matter interactions difficult. Nonetheless, novel science will certainly be made possible by the enormous increases in peak brightness, coherence and time resolution. The Paul Scherrer Institut welcomes input from interested parties inside and outside of Switzerland regarding the conceptual design of the PSI-XFEL facility.

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Fig. 4. The 250 MeV facility

Dual-space Phasing Methods

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Dual-space iterative phasing methods in crystallography

Lukas Palatinus, Gervais Chapuis
Ecole Polytechnique Fédérale de Lausanne, Laboratoire de cristallographie, BSP, 1015 Lausanne, Switzerland; lukas. palatinus@epfl.ch

Pierre Thibault
Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

1. Introduction

THE phase problem in crystallography is almost as ancient as structural crystallography itself. The approaches to this problem have been for a long time driven by the attempts to reduce the computational complexity of the problem because of limited or inexistent access to powerful computers. A lot of efforts have been invested to the development of Patterson and direct methods in order to make them as computationally efficient as possible.

The advent of cheap computer power available on almost everyone's desk has allowed the development of methods that are conceptually simpler than the classical methods, at the expense of stronger requirements in computing power. Among these techniques are direct-space methods (simulated annealing, genetic algorithms...) and extensions of the classical direct methods, like Shake-and-Bake. Recently, a new class of methods not explicitly based on the direct methods or on direct-space approach [1,2,3] have emerged. These methods are based on an iterative modification of an image in both direct and reciprocal (Fourier) space, and therefore can be denoted as dual-space iterative methods. Conceptually similar methods have been used since the seventies in the field of image reconstructions, where, in contrast to crystallography, a non-periodic image occupies a support (a confined area), which is typically considered to be known at least approximately. The most widely used algorithm from this field is probably Fienup's hybrid input-output algorithm (HIO) [4]. Nowadays, these methods find their application also in the field of diffractive imaging (see for instance Ref. 5,6,7,8,9).

The dual-space iterative methods can essentially be described in terms of constraint sets and projections onto them. In this review we outline the basic concepts of this approach with emphasis on the crystallographic applications, and we point out some concepts that go beyond the rigorous "projection-onto-the-constraint set" paradigm.

2. Image, constraint sets, projections, relaxed projections

THE phasing problem in crystallography can be rephrased as: "find a scattering density that is physically meaningful (i.e. that can be interpreted as an assembly of atoms) and that reproduces the experimental data". The experimental data coming from a diffraction experiment are - after appropriate treatment - a set of squared Fourier amplitudes. Let us sample the scattering density on a three-dimensional grid, and represent it by a vector ρ, with each component of the vector being a density value at one grid point. Let the constraint set C_F be the set of all densities ρ such that a Fourier transform of ρ yields Fourier amplitudes in agreement with the experiment. Let the constraint set C_P be a set of all ρ that are physically meaningful (see below for the discussion on what is meant by "physically meaningful"). Then the searched solution ρ_{sol} lies on an intersection of both constraint sets:

$$\rho = C_F \cap C_P$$

Clearly the constraint sets have to be designed in such a way that their intersection defines a unique solution, or a set of closely related solutions.

The problem of finding an element from the intersection of two (or more) constraint sets has been treated by mathematicians many decades ago [10,11]. In the special case of "convex feasibility" or "convex optimisation" problems, where all sets are convex, well-defined iterative procedures exist, with proven convergence properties.[1] For instance, the intersection between two convex constraint sets is always reached simply by alternating projections onto the first and the second set (Fig. 1a). In crystallography, the set associated with the amplitude constraint is unfortunately non-convex. In such case the algorithms developed for

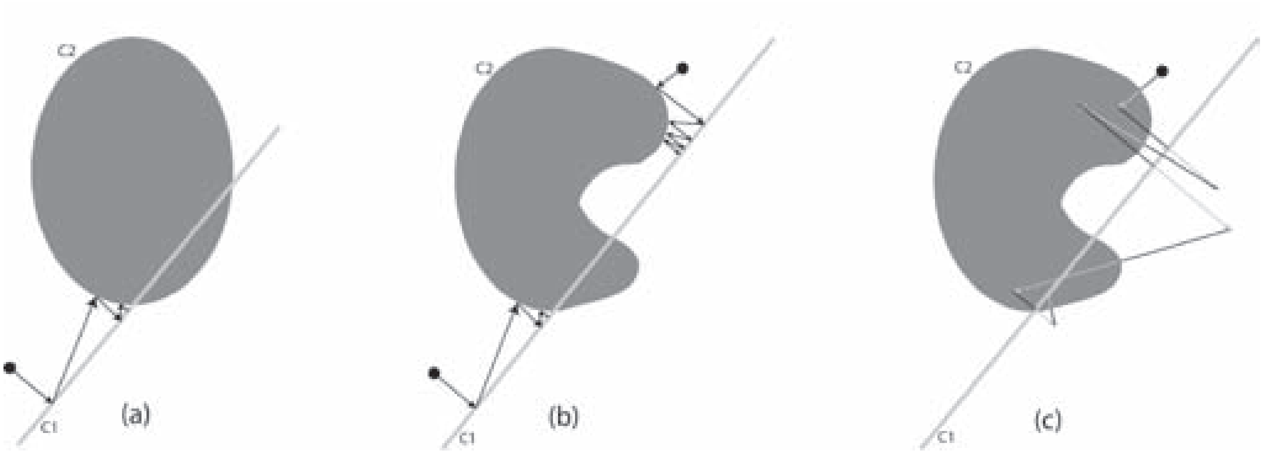

Figure 1: Schematic representation of the search for an intersection of two constraints using iterated projections. C1 (light-grey line) and C2 (dark-grey area) denote two constraints, their intersection represents a set of solutions. Black dots represent a random starting point of the iteration, and arrows indicate the positions after each iteration step. (a) Convex constraints: The solution can be found by repeated application of a simple projection on the two constraint sets. (b) The constraint set C2 is non-convex. For some starting points (upper right) the iteration gets trapped in a local minimum. (c) If relaxed projections are used instead of the true projections, the local minimum is avoided and the true solution can be found. The black part of the arrows indicates a true projection; the grey part indicates the continuation of the displacement along the same direction. The parameter γ of the relaxed projection is in this example equal to 1.

convex sets are not guaranteed to work, because they can get trapped in local minima *(Fig. 1b)*.

It is nevertheless useful to use the terminology and approaches developed for the convex feasibility problem. The three main elements constituting the basis of the algorithms are the image space, the constraint sets and the projections. In the crystallographic context, the image is typically the vector of density values ρ, as it was defined above. The definition of the image is essential, because it defines the space of possible solutions. The constraint sets have also been discussed above: C_F is the set of all densities yielding the experimentally observed Fourier amplitudes, and C_P is the real-space constraint that assures that the solution is physically meaningful. While the definition of C_F is obvious, that of C_P is not. A number of choices have been made in the literature:

a) Positivity constraint: $\forall i : \rho(i) > 0$

b) Band positivity constraint: $\forall i : \rho(i) = 0 \vee \rho(i) > \delta > 0$ [2, 4]

c) Dynamic support constraint: Only a predefined fraction of density values is non-zero [12,13]

d) Constraint on the number of maxima: The number of peaks in the density must be equal to the expected number [3]. This can be understood as a variation of the previous constraint.

Clearly, these constraints alone are not sufficient to assure that the density will represent a chemically and physicaly meaningful crystal structure, but if they are properly combined with C_F, they usually lead to a unique solution.

The third element of the algorithms is the projections. A projection is a mapping from an arbitrary point in the image space onto the nearest point of the constraint set:

$$P : P\rho \in C \text{ and } \|P\rho - \rho\| = \min \tag{1}$$

Applying a projection to an arbitrary density ρ results in a new density that belongs to the constraint set. A projection P_F that projects an arbitrary density ρ on C_F can be written as:

$$P_F = \Phi^{-1} A \Phi \tag{2}$$

where Φ represents a Fourier transform, and A an operation on the Fourier coefficients, where the phases are left intact, and the amplitudes are replaced with the experimentally observed amplitudes.

It was shown in Figure 1 that only "naively" alternating the projections onto the first and second constraint set can be sometimes successful, but it is prone to stagnation at local minima. This drawback can be overcome by replacing simple projections by relaxed projections (overprojections), or combining these relaxed projections in more elaborate schemes. A relaxed projection R is defined as:

$$R^{\gamma} = P + \gamma(P - I) = (1+\gamma)P - \gamma I$$

Thus, a relaxed projection is obtained by "prolongation" of the vector from ρ to $P\rho$ by a factor γ. The special case γ=1 is called a reflection. Fig. 1c illustrates that using relaxed projections may allow the iteration to escape from a local minimum.

Table 1 shows how the dual-space phasing methods used in crystallography can be expressed as combinations of projections and overprojections.

Table 1: Schemes of the most important variants of the dual-space iterative methods used in crystallography. The general iteration scheme is $\rho^{(n+1)}=M\rho^{(n)}$. I denotes an identity mapping.

Low-density elimination [1]	$M = P_1P_2$
Difference map[2] [2]	$M = I + \beta P_1 R_2^{\gamma_2} - \beta P_2 R_1^{\gamma_1}$
Charge flipping [3]	$M = P_1R_2$
Charge flipping “F+ΔF” [11]	$M = R_1R_2$

Although multiple different combinations of projections have been suggested, it must be emphasized that not all possible combinations are useful. A good algorithm is designed in such a way that it searches the image space efficiently, i.e. it does not get trapped in local minima, and explores large parts of the image space. On the other hand, if the iteration approaches the true solution, it must converge close to the solution, and not diverge again. Clearly, the algorithm must be a balance between the perturbing aspect necessary to explore the search space, and the stabilizing aspect needed for stability at the solution. It is therefore not surprising that different types of problems require somewhat different settings and variants of the general scheme.

3. Beyond rigorous projections

A projection has been defined (Eq. 1) as the mapping onto the nearest point on the constraint set. However, in real applications the condition on the minimum distance is not always strictly applied, and sometimes a true projection is replaced by a “projection-like” mapping, that is a mapping that has properties similar to a projection, especially close to the solution, but is not a projection is the strict sense. Such a mapping can be called pseudoprojection. Using pseudoprojections instead of true projections can have two reasons. Either it is computationally more advantageous to calculate the pseudoprojection than the true projection, or the use of a pseudoprojection brings an advantage over the true projection.

An example of the first case is the “peak projection” used in the original formulation of the difference-map algorithm for crystallography [3]. The constraint set used in [3] is the set of all densities that contain a given number N of peaks. Projecting an arbitrary density onto the constraint set requires erasing all but N peaks so that the total amount of erased density is minimal. In the case where the peaks are spatially extended, finding the true minimum requires trying many combinations of erased peaks, and that is a very costly process. Instead, one can keep only the N largest peaks, and obtain a good approximation of the projection. After this operation the density lies in the constraint set, but the minimum distance from the original density is not guaranteed. The tests on real data have shown that the method is very successful in the structure solution despite of this approximation.

While the above example can be understood as a compromise between the theoretical requirements and the computational costs, in other cases the use of a pseudoprojection can be advantageous. This is the case of the so-called “π/2-variant” of the amplitude projection. In this variant the operation A of the standard amplitude projection (the replacement of the amplitudes by the experimental amplitudes, Eq. 2) is replaced by this rule:

$$A\left(\left|F_{cur}\right|\exp(i\varphi)\right)=\begin{cases}\left|F_{obs}\right|\exp(i\varphi) & \text{for large } \left|F_{obs}\right| \\ \left|F_{cur}\right|\exp\left(i\left(\varphi+\frac{\pi}{2}\right)\right) & \text{for small } \left|F_{obs}\right|\end{cases}$$

The current amplitudes (subscript cur) of weak reflections are not replaced by the experimentally observed ones, but kept at their calculated values, but the phases are shifted by π/2. This modification can be intuitively understood as an orthogonal perturbation to the standard amplitude projection. It has been shown [15] that if the standard amplitude projection is replaced by the “π/2-variant, the performance of the classical charge-flipping algorithm is significantly improved.

4. Conclusions

THE principle of function of the dual-space iterative phase retrieval methods can be elucidated using the concept of projections onto constraint sets, and their combinations. This concept provides an intuitive understanding of how and why the methods work. However, the non-convex nature of the constraints, especially of the amplitude constraint, represents a serious complication to an exact mathematical treatment of these methods in the context of crystallography, and in image reconstruction from diffraction data in general. Prediction of the speed of convergence, optimal parameter setting, or even the success/failure of these methods for a given structure has for now eluded formal proof. Nevertheless, the practice shows that these methods are very powerful, and can not only solve most of the structures in the small-molecule field, but can be applied also in macromolecular crystallography [16].

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(Footnotes)

1 A constraint set is convex if: $x \in C \wedge y \in C \Rightarrow \overline{xy} \in C$ where $\overline{xy}$ denotes the set of all points connecting x and y.

2 The name "difference map" comes from the fact that the mapping M is in fact a difference between two mappings, each of them combining one projection and one overprojection. It has nothing to do with Fourier difference maps.

WebCSD: Fast web-based access to the latest crystal structures

http://www.ccdc.cam.ac.uk/products/csd_system/webcsd/

THE CCDC is pleased to announce that internet access to the Cambridge Structural Database (CSD) will soon be available. WebCSD has been developed using CCDC's C++ toolkit and enhances the search, analysis, exploration and validation tools already provided with the CSD System. The software searches on a relational SQL version of the CSD and affords convenient and rapid access to this unique database of approaching one half million crystal structures.

Convenient and rapid access: WebCSD does not require local installation and registration of software; institutions with a site-wide CSD licence need only to provide their IP range(s) and the CSD can immediately be searched or browsed from any computer across their entire site.

Automatic software and database updates: Database updates will be made regularly providing access to the very latest structures. In addition, new features can be made available as soon as they are developed.

Searching and browsing results: WebCSD has been designed with speed, simplicity and convenience of use in mind. In addition to offering a full range of text, numeric and bibliographic search options, WebCSD provides reduced cell, 2D substructure, and similarity search options. Search results are displayed in your browser. This convenient new display offers a choice of embedded 3D visualiser: JMol or AstexViewer. All crystallographic information for a hit structure is presented in a single tabbed pane, including a 2D chemical diagram. Furthermore, selected text fields are hyperlinked allowing immediate retrieval of all other CSD entries containing a particular keyword e.g. *plate, cyclopentadienyl, Allen*.

Use in teaching: With WebCSD teachers obtain a tool that will have great value in the classroom. A range of illustrative teaching exercises that utilise WebCSD are available on the CCDC website: **http://www.ccdc.cam.ac.uk/free_services/teaching/**. WebCSD used in conjunction with these teaching materials help make crystallographic data accessible to the non-specialist. This provides opportunity to showcase the power of crystallography as a technique to a broad audience, and to demonstrate the utility of crystallographic information across the whole of the chemistry curriculum.

For further information, contact **admin@ccdc.cam.ac.uk** or visit **www.ccdc.cam.ac.uk/products/csd_system/webcsd/**

Gary Battle and **Susan Henderson,** CCDC

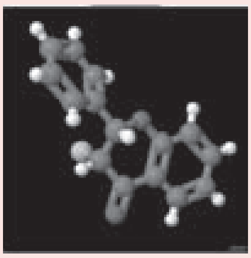

Fig. 1: Search result showing 3-chloroflavanone (CSD refcode KEJBUW); the 3D structure can be manipulated within the embedded visualiser (Jmol).

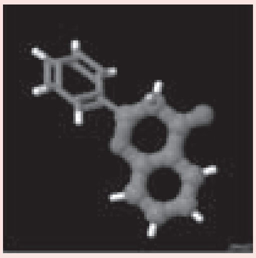

Fig. 2: Additional crystallographic information for hit structures can be viewed alongside the 3D structure.

Crystallography Fights the Flu

AS H1N1 swine flu threatens a pandemic, health services worldwide are relying on their stockpiles of two antiviral drugs, oseltamivir (Tamiflu) and zanamivir (Relenza) to mitigate its effects. The HmNn identification of influenza viruses refers to the nature of their haemagglutinin (H) and neuraminidase (N) macromolecules. Haemagglutinin is involved early in the cycle of viral infection, facilitating entry into the cell. Neuraminidase is involved later on, after the infected cell has manufactured new virus particles. These new virions are stuck to the cell surface and to each other by sialic acid residues. Neuraminidase cleaves these residues, freeing the virions to infect new cells. This enzyme is featured as the beautifully illustrated May 2009 "Molecule of the Month"[1] in the Protein Data Bank (**www.rcsb.org**).

It is important to remember two things: (1) the H and N numbers are general classifications based on their interaction with antibodies, which do not define a single specific sequence and structure, and (2) they do not provide a complete description of a virus. Thus the prevalent strain of 2008-2009 seasonal influenza was a typical, fairly mild, "human flu" virus in class H1N1. The swine flu virus also is H1N1, but its incorporation of genetic material from swine and bird flu viruses has impeded recognition by our immune systems. Another type of influenza virus, H3N2, has caused severe symptoms and significant numbers of deaths in previous outbreaks. The much-feared "bird flu" is H5N1. A comprehensive and approachable account[2] of the composition of influenza viruses, targets for therapy and approaches to drug treatment ranging from fanciful to currently successful was published in 2004.

Our cover shows a subtype N2 neuraminidase, which was the first neuraminidase crystal structure to be determined[3] and which was deposited in its definitive form[4] in the PDB in 1991. Molecular modelling studies based on this structure and another of the complex with sialic acid (Figure 1) led to a proposed mechanism of catalysis and the design of transition-state analogue inhibitors[5]. It was already known that 2-deoxy-2,3-didehydro-N-acetylneuraminic acid (DANA), a dehydrated derivative of sialic acid, was an inhibitor of neuraminidase. Modelling suggested that the C_4 hydroxyl group of DANA approaches a negatively charged region in the neuraminidase active site. Replacement of this hydroxyl group with the protonated form of the strongly basic guanidine moiety enhanced the affinity by providing a salt bridge to a negatively charged glutamate residue. This work resulted in the discovery of zanamivir, which has high affinity for neuraminidase and fairly similar geometrical requirements to the natural substrate. However, with its plethora of highly polar substituent groups zanamivir has insufficient oral bioavailability. Instead it is administered directly to the respiratory tract with an inhaler. This route has the important advantage that the drug is delivered just where it is needed with minimum wastage and minimum potential for side effects elsewhere in the body. However, children, the elderly and patients with impaired respiratory function-precisely those at most risk from influenza infection-may have difficulty using the inhaler, and many other patients find it inconvenient. Another inhibitor, oseltamivir, was designed to have a balance of polar and nonpolar side groups that would allow oral administration. With some local sacrifice of binding power that was restored elsewhere, the large highly polar guanidine was changed to a smaller amino group. The polar side chain with three hydroxyl groups was replaced by a nonpolar pentyloxy substituent. The polarity of the carboxyl group was masked by converting it to an ester; acting as a prodrug, it reverts to the original carboxyl by hydrolysis after being absorbed. The convenience of oral dosing has won a large market share for oseltamivir. However, it differs from the natural substrate in that when the drug is bound, the pentyloxy substituent needs to induce a conformational change in the enzyme to make room for it.

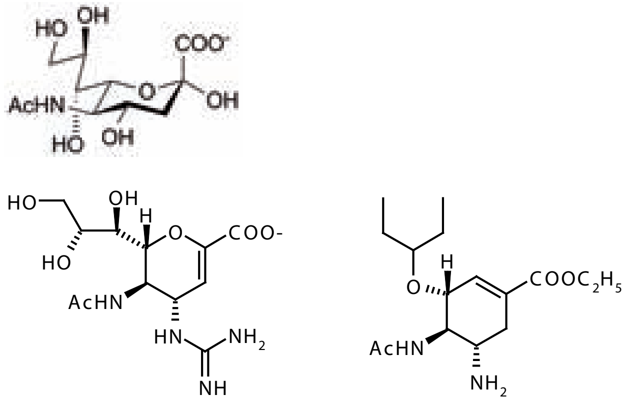

Figure 1. Structures of sialic acid (from Wikimedia Commons) and of zanamivir and oseltamivir

A recent article[6] reported the alarming news that in the 2008-2009 season the circulating H1N1 variety of human flu has become resistant to oseltamivir. Fortunately it remains sensitive to zanamivir, and H1N1 swine flu is sensitive to both. From bitter experience we have learned a lot about the emergence of resistance to anti-infective drugs. For instance, *Staphylococcus aureus* bacteria, which have annoyed most of us by causing spots and boils and which have produced life-threatening infections in some patients, used to be sensitive to penicillin. Our blithe over-use of penicillin facilitated the emergence of penicillin-resistant strains of these bacteria. Development of methicillin, another drug in the penicillin series, provided an effective alternative. Now that selection pressure has also induced the development of resistance to methicillin, we have nearly run out of options to treat MRSA (methicillin resistant *Staphylococcus aureus*). Partly to avoid a similar event with influenza, we have exercised restraint in treating seasonal flu with oseltamivir. We have largely reserved that drug for the "Big One". It therefore has been a shock to learn that, even without widespread use of oseltamivir, a resistant mutant became dominant from one season to the next.

However, the nature of the mutation came as no surprise. The requirement for a change in conformation of neuraminidase to form a pocket for the pentyloxy group was perceived as a weakness. Mutations Arg292Lys, Asn294Ser and His274Tyr were identified as capable of preventing this change. The structural effect of the His274Tyr mutation is clear[1], and this mutation has indeed occurred in the current seasonal H1N1 strain[6]. Eloquent testimony to the diligence and efficiency of macromolecular crystallographers is provided by the fact that a PDB search for “Neuraminidase” produces 16 pages of results. We are witnessing a race where the virus develops new mutants, crystallographers identify the structural changes and drug designers devise new inhibitors.

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Carl Schwalbe

Letter to the Editor

IN the September 2004 edition of Crystallography News, Prof A.C.T. North drew attention to those BCA speakers who, in order to use a laser pen to point to some feature on their PowerPoint presentation, turn their backs to the audience and start talking to themselves. He wondered if anyone could provide a pointer which could be manipulated, with a mouse, on the speaker’s laptop and thus be projected onto the screen.

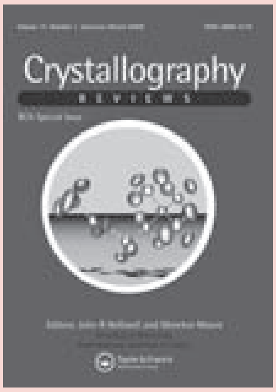
By March 2005, Tony had found such a pointer, a large Golden Arrow, which he made available to readers. For a while the Industrial Group also made it available from their website. The idea was so successful that the organisers of the Florence IUCr Congress installed the Golden Arrow on all the computers used at that meeting.

Sadly, by the BCA in Loughborough this Spring, memory of this simple but effective innovation had faded, and speaker after speaker spent part of their time speaking while turned towards the screen. This might not have been too bad had the speakers been fitted with clip-on microphones, but sadly there was only a static microphone on the lectern. This was itself so ineffective that if “mobile” lecturers moved in and out of its range, the effect heard at the back of the theatre was similar to an old-fashioned shortwave radio broadcast from the far side of the world. The situation was even worse for those lecturers who used a wireless gizmo to change slide while they were almost continuously out of range of the microphone. This was a pity, because there were very many excellent lectures on exciting new work.

There is not a lot the BCA or the speakers can do if the host site provides poor sound systems, but perhaps the BCA can help the more quietly spoken speakers by installing the Golden Arrow on computers, and perhaps also making it available again from the BCA website.

David Watkin

Important Information about Crystallography Reviews for BCA Members



THE Editors of Crystallography Reviews and Taylor & Francis enjoyed meeting so many BCA members at the recent meeting in Loughborough, and we hope that you found your recent special “BCA Issue” of the journal interesting.

Regrettably it will be the last BCA Issue members receive by default; however there is no need to miss out! We are pleased to announce that members will now be entitled to the entire volume (Issues 1-4) of Crystallography Reviews for just £25 by taking up the new special and greatly reduced ‘Members’ Subscription’ rate. Please go to www.tandf.co.uk/journals/gcry and click on News & Offers for more details.

The Editors of Crystallography Reviews would like to commend the BCA for its excellent Annual Conference programs and remain committed to publishing reviews arising from these. We hope that many BCA members take up this new arrangement and we look forward to serving the crystallography community further with our review journal.

John R. Helliwell & **Moreton Moore**
(Editors of Crystallography Reviews)

BCA 2009 Meeting

Impressions of Loughborough

THIS is not-repeat not-a meeting report. That will come in our September issue. Like dabs of paint on canvas that reveal an impression of a scene when you step back, I hope that these glimpses will evoke memories in those of you, numbering over 350, who attended the BCA Spring Meeting. Those of you who didn't, missed a great opportunity! The beautiful flowering tree on the cover, photographed during the meeting, proves the truthfulness of the Loughborough publicity photo featured on our previous cover. It also shows the fine weather we enjoyed.

The four superbly presented Plenary Lectures illuminated four very diverse corners of crystallography. **David Watkin** conveyed important insights via a fascinating history of crystallography. He demonstrated persuasively how purely scientific interest leads to the development of methods that become technology which in turn supports new scientific studies. At present the now well-developed technology of data collection and structure solution facilitates the comparison of intermolecular interactions and crystal packing, but crystal growing remains a Black Art. Addressing one of our most serious concerns, **Nick Marsh** explained the role of X-ray diffraction and X-ray fluorescence in monitoring past episodes of climate change. Planktonic animals and plants create deposits of carbonates and silica in which the ratio of ^{18}O to ^{16}O, measurable by mass spectrometry, is indicative of temperature. However, these deposits may undergo chemical modification or admixture of impurities, and XRD and XRF are valuable in the verification of sample integrity. Giving a masterclass in the use of well-designed illustrations to make a complicated assemblage of biomolecules clear even to a small-molecule crystallographer, **Venki Ramakrishnan** imparted structural insights about the ribosome. Drawing on high-resolution structures of subunits as well as the whole ribosome, he elucidated the dynamic processes at work. Conformational changes creating induced fit are involved at three stages: selection of the correct transfer RNA, peptide bond formation to attach the new amino acid to the nascent chain, and recognition of the stop codon. Finally, **Martin Dove** convinced us that valuable information about dynamics is obtainable from the scattered radiation between the Bragg peaks. Bragg diffraction data give us mean atomic positions suitable for making ball-and-stick diagrams. Additionally, the anisotropic displacement parameters for individual atoms give clues about dynamics. However, total scattering (Bragg diffraction plus diffuse scattering) yields pair distribution functions which enable coordinated motion to be detected.

The "Dynamic Crystallography" theme linked sessions from every Group. The word "Dynamic" appeared in many session titles and in even more abstracts. Many of these studies made use of advanced radiation sources and instrumentation which have recently become available. A very useful additional session was the dSNAP tutorial. Well-designed exercises on the participant's choice of organic or organometallic structures introduced the latest version of dSNAP. This new version with enhanced handling of complex topology and greater user-friendliness can be obtained from http://www.chem.gla.ac.uk/snap.

Two Young Crystallographers gave outstanding Prize Lectures: **Hazel Sparkes** for the CCDC Chemical Crystallography Prize for Younger Scientists 2009 and **Anna Stevenson** for the Industrial Group Prize. The prizes that were awarded at the Conference Dinner reflected a very high standard of scientific content and presentation. Congratulations go to **Eugenio de la Mora** (BSG Special Mention), **Arefeh Seyedarabi** (David Blow Prize), **Samantha Melrose** (CCG Special Mention), **Lynne Thomas** (CCG Prize), **Mark Warren** (IUCr Prize), **Claire Murray** (CrystEngComm Prize), **Jeppe Christensen** (PCG Prize) and **Lynne Thomas** (Durward Cruickshank Prize). The PCG-SCMP PANalytical PCG Thesis Prize awarded to **Aurora Cruz-Cabeza** deserves special mention. One could paraphrase the old adage as "A poster is for Easter; a thesis is for life." Thanks go to PANalytical, the long-time sponsor, and the Committee of the Physical Crystallography Group, whose marathon reading efforts identified the winner from a very strong field of entrants.

Carl Schwalbe

Prize Winners

PSG Thesis Prize

Cruickshank Prize

CCG Special Mention

CCDC Prize

IUCr Prize

IG YC Talk Prize

David Blow Prize

CrystEngComm Prize

CCG Prize

PCG Prize

BSG Special Mention

David Watkin's Award

Exhibitors BCA 2009 Sprin

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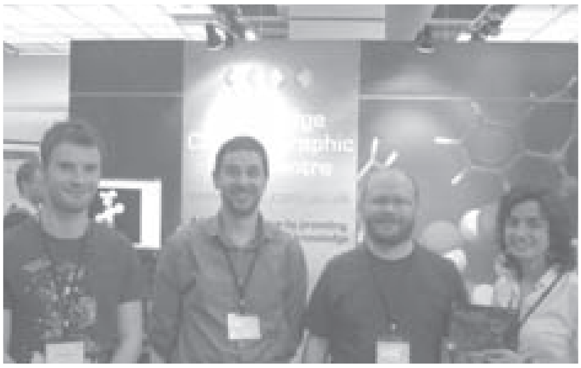

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Bob Carruthers

John Robert (Bob) Carruthers. 15 May 1945 - 17 January 2009

BOB graduated from St Edmund Hall (Oxford) having completed his Part II year doing copper chemistry with Francis Rossotti. He worked for his D. Phil. (still on copper chemistry) with Keith Prout and Francis, and it was during this work that he became interested in crystallography.

For one of the materials he worked on, aquo(maleato) copper(II), he observed “When the diffraction pattern was indexed, it became apparent that the crystals were unlikely to be orthorhombic, as a strange set of absences were found”. The crystals were twinned. “Overlapped reflections were arbitrarily assigned half the measured intensity until a program was written which would include both components in the least squares”. “As there was not sufficient space [memory] it was necessary to rewrite the [AUTOCODE] program in [English Electric Leo Marconi] KDF9 machine language”. AUTOCODE was a symbolic language, rather like a simplified FORTAN. Machine languages are basic to the electronics of the computer, and the programmer has the power and the responsibility of working hands-on with every memory location, even to the extent of synchronising the calculations with the revolutions of the bulk storage devices. So began Bob’s life with computers, and his exceedingly productive partnership with **John Rollett**.

Immediately after writing his DPhil thesis in 1969, Bob was awarded a fellowship from the Accademia Nazionale dei Lincei in collaboration with the Royal Society which enabled him to work in Rome. There, he set about working with Riccardo Spagna re-implementing the Rollett AUTOCODES in FORTRAN. This program included features such as “riding” and rigid-body constraints, and some of the underlying data-structure can still be found in CAOS (Cerrini S. & Spagna R. (1977) Crystallographic software for a mincomputer, IV Eur. Crystallgr.Meet., Oxford, UK, Abstract A-212).

On Bob’s return to Oxford he worked with Rollet and Prout, again re-writing the program from scratch but building upon his experiences in Rome. This new program, called CRYSTALS, could handle up to 9 twin components and had a good range of restraints (including facilities now often called SIMU and DELU). Perhaps the most novel feature was “user-defined restraints”, in which the user could define their own equation of restraint as part of the input data, which was then analytically differentiated by CRYSTALS. The equation parser and differentiating engine were all written in beautiful FORTRAN, and are still working, largely unmodified, in the current version of CRYSTALS. Bob’s attitude to programming combined a meticulous attention to detail with a far reaching ability to plan on an expansive scale.

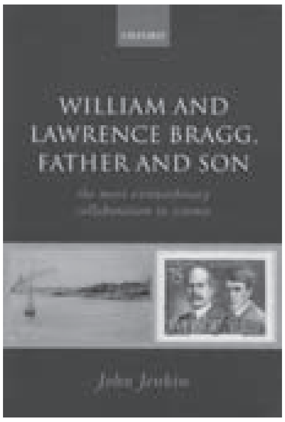
After his Post Doc, Bob started work for Oxford University Computing Service, writing software for data-archiving. However, he continued to work on CRYSTALS whenever he could, and completely re-wrote the underlying data management for a third time when the university upgraded its mainframe to an International Computers Limited (ICL) 2980.

In about 1979 Bob left Oxford to work for Control Data Corporation, implementing meteorology programs on their supercomputers. Apart for a brief period in the 1980’s when he worked with Keith Davies at Chemical Design, Bob has spent most of his career implementing very large FORTRAN program systems, and in recent years modernising massive legacy packages. Weather forecasting may have profited from his work, but there is no doubt that crystallography lost an outstanding programmer when Bob left Oxford.

When not working with computers, Bob was a dependable drinking companion and a formidable Bar Billiards enthusiast. Some of us still remember Bob and **George Sheldrick** working with other young crystallographers to try to drink the bar dry at ECM 4 in Oxford in 1977. His brilliance as a scientist did not spoil his personality - he was always modest, amiable and good fun.

David Watkin

Books



William and Lawrence Bragg, Father and Son: the most extraordinary collaboration in science

JOHN JENKIN

Oxford University Press, 2008
Price £35
ISBN 987-0-19-923520-9, 458 pages

JOHN Jenkin's scholarly and extremely readable biography of William and Lawrence Bragg opens with an extended account of William's early life, from his origins as a farmer's son in Cumberland, through his schooldays on the Isle of Man, to his graduation with high honours in the Cambridge Mathematical Tripos. The story of his subsequent appointment - after only the briefest of interludes - to the Chair of Mathematics and Physics in Adelaide is a most curious one. One morning in 1885, William, then a first-year postgraduate student at the Cavendish, happened to meet his professor and occasional tennis partner J.J. Thomson in King's Parade. Thomson mentioned - apparently in passing - that he had heard the University of Adelaide was seeking a new Professor of Mathematics and Physics, and that, now he came to think about it, Bragg might be a strong candidate for the post if he cared to apply. William, despite his initial astonishment at the idea, made a last-minute telephone application, was shortlisted, arrived at the interview to find Thomson one of his interviewers, and duly got the job! Jenkin's book however makes it clear that the appointment was, in reality, nothing like as haphazard as it sounds - Thomson had identified Bragg as the man for the job as soon as he was approached by Adelaide to advise on suitable candidates.

Jenkin, a retired physicist and now a historian of science at La Trobe University in Melbourne, explores William's 23 years in Adelaide in considerable (some might think relentless) detail. We are provided with copious footnotes, and extensive references to some remarkable source material: *Sport, Class and Community in Colonial South Australia 1836-1890*, and *The Adelaide Gentry, 1880-1905*, are by no means untypical references. A fascinating aside is a description of the young Rutherford calling in to see Professor Bragg in 1895, on his way from New Zealand to Cambridge to become J.J. Thomson's first "B.A. by research" student. The resulting lifelong friendship between Rutherford and Bragg would be crucial in helping William to move successfully into X-ray and atomic research, though only after more than a decade of toil as the University of Adelaide's main teacher and administrator of mathematics and physics. William's marriage in 1889 to Gwendolyn Todd, daughter of the Government Astronomer for South Australia, the birth and education of their children, and their subsequent lives in Australia and England - where William held chairs of physics in Leeds and London, before moving finally to direct the Royal Institution - are all very carefully documented. And of course the climax of the book is the period between 1912 and 1914, covering Laue's discovery of X-ray diffraction, its hugely successful interpretation by William's elder son, Lawrence - then only recently graduated from Cambridge - and their initially collaborative (and rather quickly independent) work on the X-ray analysis of crystal structures.

Jenkin reports the discovery (in the archives of the Royal Institution) of a previously unrecorded letter to William from a Norwegian colleague, Lars Vegard, who had attended a research colloquium by Laue soon after his discovery of X-ray diffraction. Vegard's letter, which arrived in England ahead of Laue's first publication, described the phenomenon in detail and even included a copy of one of Laue's first diffraction photographs. Jenkin contends that William and Lawrence must have discussed the letter during their summer holiday on the Yorkshire coast, and that it was this letter which sparked what Lawrence always referred to as his "Brain Wave" (the discovery of Bragg's Law) on his return to Cambridge in the autumn of 1912. The subsequent "extraordinary collaboration" between Lawrence and his father, which is the pivotal point of the book, was indeed staggeringly productive, and Jenkin makes a strong case that, whatever personal complications and difficulties may have arisen, there was always a close, enduring and affectionate relationship between the two men. Nevertheless, Lawrence must have found William's persistent tendency to refer in his letters to "my boy's work" a little trying!

The present book contains an essentially complete biography of William, but Lawrence's later career is sketched out much more briefly - the last 40 years of his life are covered in only 20 pages. It is perhaps worth recalling what an astonishing career this was. In November 1918, as the guns fell silent in France, Captain W.L. Bragg of the Royal Horse Artillery wrote home to his father, reflecting on his life to date and wondering what sort of job he might hope for back in England. He had survived the War - though his younger brother Bob had died at Gallipoli - and his four years of active service had produced the first effective sound-ranging techniques for locating enemy guns. During the War he had been awarded the Military Cross and the OBE, and was Mentioned in Despatches. He held first-class degrees from Adelaide and Cambridge where, just before the War, he had been elected a Fellow of Trinity College. In 1915, at the age of 25, he had won the Nobel Prize, jointly with his father, for his discovery of the fundamental law governing X-ray diffraction and for applying it to the analysis of crystal structures. In the same year he had published the first book on X-ray crystallography (*X-Rays and Crystal Structure*) and had been awarded the Barnard Gold Medal of Columbia University. By 1918 he had achieved more than most scientists could aspire to in a lifetime, and yet his career had scarcely begun. He would twice succeed Rutherford as Professor of Physics, first in Manchester and then again in Cambridge where, as Sir Lawrence Bragg (he was knighted in 1941), he would direct the research group that determined the first structures of proteins and - almost an aside it must have seemed at the time - the structure of DNA. He would go finally from Cambridge to London, to direct the Royal Institution and rescue it from chaos and political strife after Andrade's brief but autocratic reign. There he would inspire a brilliant new generation of crystallographers to solve the first enzyme structure and establish its mode of action at a molecular level. The Royal Society would admit him as a Fellow in 1921, and later award him the Copley Medal - its highest honour. In 1965, to celebrate the 50th anniversary of his Nobel Prize, BBC television would broadcast a documentary on his life entitled "50 Years a Winner", and in 1967, four years before he died - after a life of unparalled scientific achievement - he would be appointed a Companion of Honour by the Queen, for "services of national importance".

And yet....... the feeling persists among scientists that Lawrence Bragg was badly done to in his lifetime; that his achievements in physics were consistently under-valued because he was the son of a famous father working in the same field. Even the index to the present book contains the slightly startling entry "Bragg, William Lawrence, *lack of recognition*; pp. 340-2, 396-7, 401". It is true that he was regarded by some conservative physicists as a "mere" crystallographer, practically a *chemist* really; and it is said that his colonial background sometimes made life difficult for him in the class-ridden society of England between the Wars. A family legend, quoted by Jenkin, tells that Lawrence (uncharacteristically) let fly with his fist when a rural dean referred to his possible "convict ancestry". However, it seems unlikely that his Australian origins can have ever been a serious issue. The high achievements of Australian and New Zealand scientists are, historically, out of all proportion to their numbers. Jenkin also notes wryly that the concept of Australian nationality is in fact surprisingly recent: until 1949 the residents of Australia were just British subjects who happened to live a little further than usual from London. And the electors to the Fellowship of the Royal Society, to the Manchester Chair of Physics, and finally to the Cavendish Professorship could hardly be accused of ignoring Lawrence's achievements. Objectively, the only real "lack of recognition" in his long career lay in his never becoming President of the Royal Society: as a Nobel laureate and for many years (quoting Max Perutz) "the country's senior scientist", he might reasonably have expected this.

The book ends with an analysis and rebuttal of "the most outrageous accusation" made against Lawrence by a small number of jealous contemporaries and successors who claimed that, despite holding some of the most senior positions in British and international physics, "his work had no great influence on the physics of his time - or after". This is of course complete nonsense. As Jenkin points out, one only has to look at the infrastructure of the modern world: it has been created almost entirely through our understanding, at the atomic and molecular level, of crystalline materials. Lawrence Bragg's work transformed not only solid-state physics, leading directly to the microelectronics revolution, but also mineralogy, metallurgy, materials science, practically the whole of chemistry, most of biology, and no small part of medicine. And crystallographers especially must echo Jenkin's closing thoughts on Lawrence, that "he will be remembered and honoured around the globe, long after his detractors and their words are forgotten".

Howard Colquhoun
University of Reading

Experimental Foundations of Structural Chemistry

STEPAN S. BATSANOV

Moscow University Press
Price USD 80 (GBP 56, EURO 61; exact value depends upon exchange rate) plus postage
ISBN 978-5-211-05468-4

In 550 pages (with 240 tables and 2700 references) the book provides a comprehensive survey of factual data on energy and optical properties, structure and chemical bonding of inorganic, organometallic and organic substances, including:

- ionization potentials of atoms, radicals, molecules, clusters,
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- bond energies in normal and van der Waals molecules,
- heats of phase transitions,
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solids, molecules (including short-lived), liquids, solutions, melts, glasses and crystals of organic, organoelement, binary and complex inorganic compounds.
- Atomic radii for metallic, covalent, ionic and van der Waals radii are systematized.

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The concluding chapter is devoted to experimental studies of the nature of chemical bonding in molecules and solids, including effective atomic charges and effects of high pressure on bond polarity. Mutual influence of atoms in binary and complex compounds is discussed. Relations between various physical properties and the structure of substances are discussed using the concept of electronegativity, capable both to explain and to predict relevant properties and to guide development of new materials.

The book can be useful as supplementary chapters for university courses in crystal chemistry and physical chemistry, materials science and solid state physics, and as a handbook for postgraduate students, teachers and researchers in these fields. The two Russian editions have been published in 1986 and 2000; the present edition has been completely revised and updated and mainly cites the publications of the last 10-15 years.

Requests for the hardbound book in English can be submitted by e-mail to the editor (**editor@mupress.ru**), whereupon the Moscow University Press will send formal quotations. Payment by cheque or bank transfer (in any convertible currency) is required within 28 days after delivery.

Andrei Batsanov
University of Durham

Exceptionally, the reviewer is a relative of the author. Since the review is purely factual, I do not consider that this matters. **Ed.**

CRYSTALS, May 2009

AS CRYSTALS approaches maturity there is less need for frequent updates. The Summer 2009 release mainly removes some annoyances, simplifies day-to-day working and improves CIF generation for Oxford Diffraction instruments. Some specific changes involve:

- Better automatic placement of molecules in the unit cell, numbering of atoms, resolution of name clashes and re-sequencing of hydrogen atom names.
- Better automatic geometric placement of hydrogen atoms, especially near metals and across symmetry operators.
- Improved optimisation of hydrogen atom parameters.
- Unbiased initialisation of the refinement of the Flack parameter (H. D. Flack, G. Bernardinelli, D. A. Clemente, A. Linden and A. L. Spek, *Acta Cryst.* (2006). **B62**, 695–701).
- As part of the Age Concern project, evaluation of the “y” parameter (R. W. W. Hooft, L. H. Straver, A. L. Spek, *J. Appl. Cryst.* (2008), **41**(1), 96-103.) using code based on an original provided by Ton Spek, together with other diagnostics. See A. L. Thompson and D. J. Watkin, *Tetrahedron: Asymmetry*, doi:10.1016/j.tetasy.2009.02.025 for comments on light-atom absolute structure determination using Mo radiation.
- Alert and information displayed based on the value of the p(2) in the SHELXL type weighting scheme.
- Automatic choice of the Chebychev weighting polynomial for either F or F(squared) refinement.
- Better treatment of SHELX-type HKLF5 files, based on code by Simon Parsons.
- Smoother links to SIR97 and SIR2002. Note that these have different characteristics from each other, and with SIR92. One may succeed if another fails to solve a structure.
- Better labelling of symmetry related moieties in CAMERON.
- Drop-down illustrated examples of how to interpret the output from the Analyse and Results menus.
- Automatic handling of deuterium.
- Amber Thompson has drawn on her SHELX experience to write a new Beginners Guide.

We are in discussions about making the code open source. Meanwhile, Windows executables are available from **www.xtl.ox.ac.uk** without charge for not-for-profit organisations or individual users. Some Vista problems remain - contact us for work-rounds. Nothing will be done to the graphics until we have seen Windows 7.

David Watkin

Puzzle Corner...

...MARCH ANSWER

I have received two winning entries which complement each other... scholarly from David Beveridge and lighthearted from Derry Jones. We begin with the contribution from David Beveridge.

As you note, crystallographers do not tend to have their names converted to adjectives by the addition of suffixes such as "-ian". However, there are at least two cases of which I am aware where this has happened. For the first, we have to go back to the prehistory of crystallography, to Johannes Kepler - better known as an astronomer, he did nevertheless publish, in 1611, "Strena, seu de nive sexangula", in which he notes the 6-fold symmetry of snowflakes. Kepler was one of the first - perhaps THE first - to write about crystals. The adjective "Keplerian" is reasonably well-known, to the extent of finding its way into Webster's dictionary. An arch-pedant might, I suppose, argue that Kepler was not a crystallographer after all, because the term "crystallography" (or rather its Latin equivelent, "crystallographia") was not used until 1723. There is another example of which I am aware. I looked in F.C.Phillips' book "An Introduction to Crystallography" and there found "Millerian symbol" and "Millerian notation" - both referring, of course, to Miller indices. These are respectively on pages 42 and 222 of the fourth edition, published in 1971.

It occurs to me that when we refer to Miller indices, or to the Bragg equation, we are using these names, in a sense, as adjectives. They describe the more fundamental noun, and tell us, for instance, what sort of equation we are dealing with. Whether we may consider this to be using these names attributively or adjectivally, they clearly have much in common with adjectives. The modern trend is to use names in this way, rather than appending "-ian" or similar suffixes. Thus, while we would expect to have Newtonian dynamics, we might have either Einstein or Einsteinian dynamics, more probably the former. Thus we have to search the older literature for examples. The very names of some crystallographers militate against the addition of suffixes: consider adding "-ian" to either Haüy or von Laue. Five vowels in a row would produce a result more or less unpronounceable. I have access to few old books on crystallography; one name I would expect to find with a suffix is that of Wollaston, but I have yet to see it. All this early crystallography was, of course, geometrical: this tends to get forgotten nowadays, when crystallography is almost synonymous with the determination of the arrangement of the atoms within a crystal, usually by diffraction methods. I find it worth remembering that Zeitschrift für Kristallographie was founded in 1877, two years before Max von Laue was born.

You ask for examples which do not follow the forms you mention. One well-known case is "Copernican", which follows normal Latin conventions and is rather easier to pronounce than if it ended in "-ian". "Galilean", from another astronomer, again follows Latin convention. I shall leave it to others to attempt to rationalise the suffixes added to names to convert them to adjectives!

Derry Jones decided to remedy the lack of crystallographers-as-adjectives by creating some himself. Here is a selection of his results, assembled from an old World List of Crystallographers.

Surname	Suffix	Meaning	Nationality
Anderson	ic	differently sounding	SWE
Anwar	y	unguarded	GBR
Attard	y	late	USA
Bacon	ic	has neutrons for breakfast	GBR
Benedict	ine	order or drink	DEU
Blaton	ic	just good friends	USA
Bohr	ing	goes on about energy states	DNK
Brock	en	damaged (in Yorkshire)	USA
Crennell	ated	square wave form	GBR
Donn	ish	academic	ZAF
Fu	rious	very cross	CHN
Kar	less	lost an automobile	IND
Lin	ear	straight	CHN
Mackie	avellian	convoluted	USA
Marsh	ian	out of this world	USA
Picken	choose	selective	GBR
Roman	esque	Southern European	ESP
Wooster	ish	Wodehouse-style	GBR

Derry concludes with the serious point that the –ic or –esque form tends to be used for euphony when the root ends in a vowel or in an in/on/eon form that would require a doubling of the consonant.

Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to list please send them to the Editor, c.h.schwalbe@aston.ac.uk. The help of the IUCr listing is gratefully acknowledged.

4-14 June 2009
High Pressure Crystallography: from Novel Experimental Approaches to Applications in Cutting-Edge Technologies. Erice, Italy.
http://crystalerice.org/erice2009/2009.htm

8-12 June 2009
ICDD X-ray Diffraction Clinic. Session I -- Fundamentals of X-ray Powder Diffraction Newtown Square, PA, USA.
http://www.icdd.com/education/xrd.htm

8-12 June 2009
X-ray Techniques for Advanced Materials, Nanostructures and Thin Films: from Laboratory Sources to Synchrotron Radiation. Strasbourg, France.
http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=272

14-19 June 2009
International Conference on the Chemistry of the Organic Solid State, Genoa, Italy.
http://www.iccossxix.mater.unimib.it/

14-19 June 2009
Eleventh International Workshop on Physical Characterization of Pharmaceutical Solids, Stamford, Connecticut, USA.
http://www.assainternational.com/

14-19 June 2009
Liquid Crystals, New London, NH
http://www.grc.org/programs.aspx?year=2009&program=liqucryst

14-20 June 2009
ICC14: XIV International Clay Conference, Castellaneta, Italy.
http://www.14icc.org/

14-22 June 2009
2nd school and workshop on X-ray micro and nanoprobes (XMNP2009), Palinuro (Salerno), Italy.
http://www.ifn.cnr.it/XMNP2009/scientific_motivation.htm

15-19 June 2009
ICDD X-ray Diffraction Clinic. Session II -- Advanced Methods in X-ray Powder Diffraction Newtown Square, PA, USA.
http://www.icdd.com/education/xrd.htm

15-19 June 2009
EMBO / MAX INF2 2009 a Practical Course on Structure Determination in Macromolecular Structure, Grenoble, France.
http://cwp.embo.org/pc09-05/

17-25 June 2009
EMBO Practical Course. High Throughput Methods for Protein Production and Crystallization, Oxford, United Kingdom.
http://cwp.embo.org/pc09-21/

18-20 June 2009
4th TOPAS Users´Meeting, University of Trento, Italy.
http://www.fkf.mpg.de/xray/html/topas.html

21 June 2009
Crystallography online: International School on the use and application of the Bilbao Crystallographic Server, Lekeitio, Spain.
http://www.crystallography.fr/mathcryst/bilbao2009.php

21-26 June 2009
Goldschmidt 2009 'Challenges to our Volatile Planet', Davos, Switzerland.
http://www.goldschmidt2009.org/

22-24 June 2009
Neutrons in Biology. Satellite Meeting of the EBSA Biophysics Congress, Lund, Sweden
http://www.ill.eu/news-events/workshops-events/neutrons-in-biology-2009/

22-24 June 2009
ICNX-2009, International Conference on Neutron and X-Ray Scattering, Kuala Lumpur, Malaysia.
http://icsd.ill.fr/ICNX2009.pdf

22 June - 2 July 2009
ISBMR 9th Course: Biophysics and Structure, Ettore Majorana Foundation and Centre for Scientific Culture, Erice-Sicily Italy.
http://smrl.stanford.edu/erice2009/

25-26 June 2009
Workshop on Diffuse Scattering in Crystalline Materials, Grenoble, France.
http://www.esrf.eu/events/conferences/DiffScatt09/diffuse-scattering-in-crystalline-materials

30 June - 3 July 2009
Practical Workshop on Characterization of Protein Complexes in Structural Biology, EMBL, Hamburg, Germany.
http://www.embl-hamburg.de/protchar2009

1-3 July 2009
Information and Structure in the Nanoworld, St Petersburg, Russia.
http://www.isc.nw.ru/Eng/Conferences.htm

12-15 July 2009
2nd Workshop on Neutron Wavelength Dependent Imaging, Cosener's House, Abingdon, United Kingdom.
http://www.iucr.org/news/notices/meetings/meeting_2009_86

12-17 July 2009
Thin Film & Crystal Growth Mechanisms, New London, NH, USA.
http://www.grc.org/programs.aspx?year=2009&program=thinfilm

14-18 July 2009
EMU School 2009 : Advances in the Characterization of Industrial Minerals, Chania, Greece.
http://www.univie.ac.at/Mineralogie/EMU_School_2009/welcome.htm

19-24 July 2009
Clusters, Nanocrystals & Nanostructures, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2009&program=clusters

23-24 July 2009
MX Frontiers at the One Micron Scale, Brookhaven National Laboratory, NY, USA.
http://www.nsls.bnl.gov/newsroom/events/workshops/2009/mx/

25-30 July 2009
Annual Meeting of the American Crystallographic Association 2009. Toronto, ON, Canada.
http://www.cins.ca/aca2009/

26-31 July 2009
XAFS 14. International Conference, Camerino, Italy.
http://www.xafs14.it/

27-30 July 2009
Energy materials research using neutron and synchrotron radiation, Helmholtz Zentrum Berlin, Germany.
http://www.helmholtz-berlin.de/events/emns2009/

27-31 July 2009
2009 Denver X-ray Conference, Colorado Springs, CO, USA.
http://www.dxcicdd.com/

31 July – 4 August 2009
The SYMMETRY Festival 2009, Budapest, Hungary.
http://conferences.hu/symmetry2009/

2-7 August 2009
X-ray Science, Waterville, ME, USA.
http://www.grc.org/programs.aspx?year=2009&program=xray

2-7 August 2009
SAGAMORE: Charge Spin and Electron Density, Santa Fe, NM, USA.
http://www.sagamoreXVI.org

2-8 August 2009
8th PSI Summer School on Condensed Matter Research on Functional Materials, Zuoz, Switzerland.
http://sls.web.psi.ch/view.php/about/index.html

3-5 August 2009
Polarized Neutrons and Synchrotron X-rays for Magnetism 2009, Bonn, Germany.
http://www.fz-juelich.de/iff/pnsxm2009

8-10 August 2009
Practical Training at the Paul Scherrer Institut - Swiss Synchrotron Light Source, Neutron & Muon Sources, Villigen PSI, Switzerland.
http://school.web.psi.ch/html/index.shtml

14-16 August 2009
Symmetry and Crystallography in Turkish Art and Culture: Satellite Conference of ECM-25, Istanbul, Turkey.
http://www.lcm3b.uhp-nancy.fr/mathcryst/istanbul2009.htm

16-21 August 2009
25th European Crystallographic Meeting, Istanbul, Turkey.
http://www.ecm25.org

30 August – 4 September 2009
GRC Solid State Chemistry Conference: New Frontiers in Materials Synthesis and Characterization, Oxford, UK.
http://www.grc.org/programs.aspx?year=2009&program=sschem

30 August – 12 September 2009
The Zurich School of Crystallography: Bring Your Own Crystal, Zurich, Switzerland.
http://www.oci.uzh.ch/diversa/xtal_school/

31 August – 12 September 2009
11th Oxford School on Neutron Scattering, University of Oxford, UK.
http://www.iucr.org/news/notices/meetings/meeting_2009_30

6-8 September 2009
BACG 40th Anniversary Meeting, 2009, Bristol, United Kingdom.
http://www.bacg.org.uk/BACG.NET/default.aspx?

7-8 September 2009
7th International NCCR Symposium on New Trends In Structural Biology, Swiss Federal Institute of Technology (ETH), Zurich, Switzerland.
http://www.structuralbiology.uzh.ch/symposium2009/

8 September 2009
Annual Meeting of the SGK/SSCr, Fribourg, Switzerland
http://www.sgk-sscr.ch/

8-11 September 2009
Synchrotron Radiation and Polymer Science 4, Rolduc, The Netherlands.
http://srps4.chem.tue.nl/index1.html

13-18 September 2009
Aperiodic09, University of Liverpool, UK.
http://www.aperiodic09.org

13-18 September 2009
XIV International Conference on Small-Angle Scattering (SAS-2009), Oxford, UK.
http://www.sas2009.org/

20-23 September 2009
European Conference on Solid-State Chemistry, University of Münster, Germany.
http://www.gdch.de/vas/tagungen/tg/5585__e.htm

20-23 September 2009
Grazing Incidence Small Angle Scattering (GISAS) Conference DESY, Hamburg Germany
https://indico.desy.de/conferenceDisplay.py?confId=797

20-24 September 2009
XXI Conference on Applied Crystallography, Zakopane, Poland
http://crystallography.us.edu.pl/

21-25 September 2009
Clays, Clay Minerals and Layered Materials – 2009, Moscow, Russia
http://www.cmlm2009.ru/

27 September – 2 October 2009
SRI2009: 10th International Conference on Synchrotron Radiation Instrumentation, Melbourne, Australia.
http://www.sri09.org/

5-7 October 2009
Studying Kinetics with Neutrons by SANS and Reflectometry, SKIN2009, Grenoble, France.
http://www.ill.eu/news-events/workshops-events/skin2009/

5-8 October 2009
JCNS Workshop : Trends and Perspectives in Neutron Scattering on Soft Matter, Tutzing, Germany
http://www.jcns.info/Workshop/

19-23 October 2009
Basic and Advanced Rietveld Refinement & Indexing Workshops, Newtown Square, PA, USA.
http://www.icdd.com/education/rietveld-workshop.htm

28-30 October 2009
International Workshop on the Analysis and Refinement of the Electron Density, Marrakech, Morocco.
http://www.ucam.ac.ma/fssm/adrx/

27-29 January 2010
Flipper 2010: International Workshop on Single-Crystal Diffraction with Polarised Neutrons, Grenoble, France.
http://www.ill.eu/news-events/workshops-events/flipper-2010

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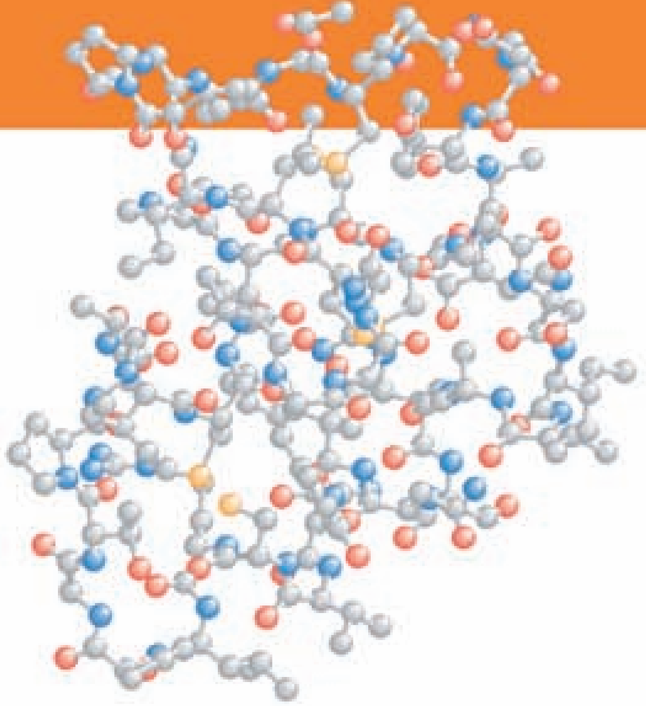

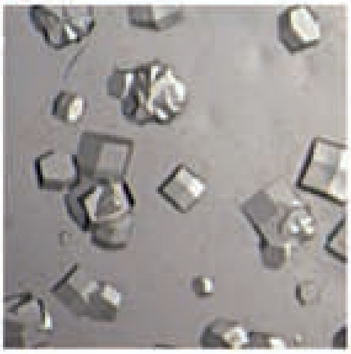

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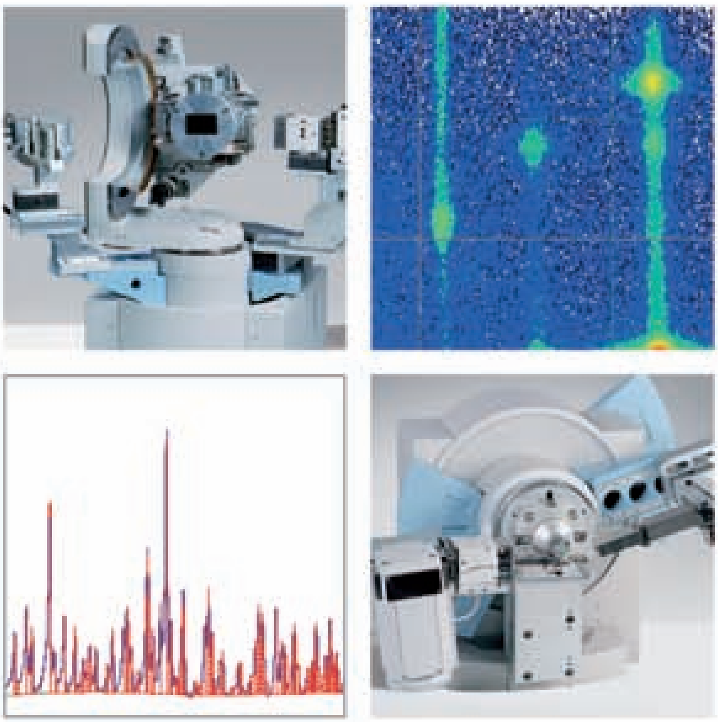

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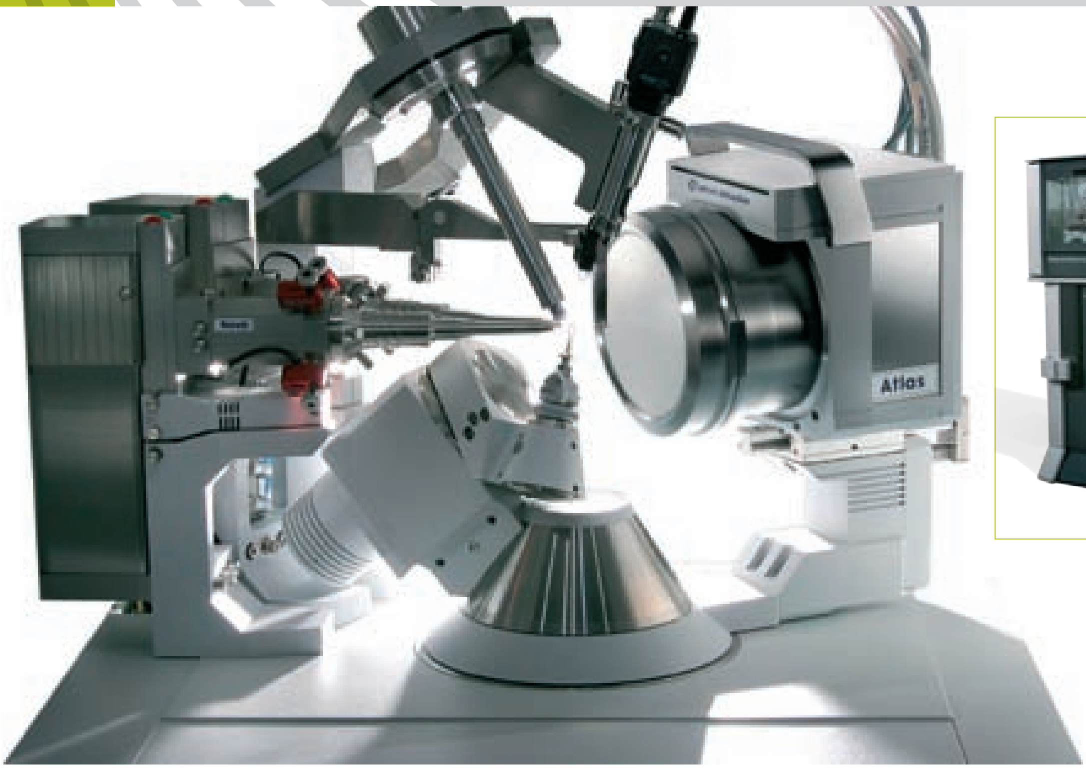

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