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Text should preferably be sent electronically
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Diagrams and figures are most welcome,
but please send them separately from text
as .jpg, .gif, .tif, or .bmp files.

Items may include technical articles, news
about people (e.g. awards, honours,
retirements etc.), reports on past meetings
of interest to crystallographers, notices of
future meetings, historical reminiscences,
letters to the editor, book, hardware or
software reviews.

Please ensure that items for inclusion in
the **December 2005** issue are sent to the
Editor to arrive before **25th October 2005**.

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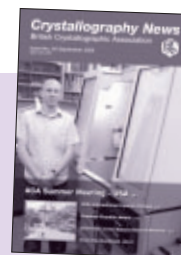
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**This month's
cover:** Dominic
Fortes (shown
with his
diffractometer)
was the winner

of this year's PCG Thesis Prize at
Loughborough (see page 17). The
inset is a view of Lancaster, venue
for next year's Spring Meeting.



From the President



AS I write this column, my summer vacation is over, IUCr in Florence is a few weeks away and my own preparations for attending that meeting are in full swing. Of course, by the time you read this IUCr will be over, but nonetheless I will outline my activities there to indicate how the

BCA is represented on this international stage.

It will be a busy time, primarily because of the wide range of science we will get the chance to listen to and discuss. However, there is also much other business undertaken at an international crystallography congress. I am honoured to be leading the UK delegation to the General Assembly of the International Union of Crystallography, and to be accompanied on that delegation by colleagues **Sheila Gould, Elspeth Garman, John Evans** and **Bob Gould**. We will do our best to represent the UK in that forum and be fully involved in what look like being some lively discussions. We are of course optimistic that our nominee for the IUCr Executive, **Chris Gilmore**, will be elected.

When it is not IUCr business in Florence, part of my time will be spent on European Crystallographic Association matters. Among other issues, ECA Council will decide on a location for ECMs 25 and 26, in 2009 and 2010; as you will know we have made a bid to host one of those European Meetings in Edinburgh, at the Edinburgh International Conference Centre. The bid has benefited enormously from input and assistance from Northern Networking, in the person of **Gill Moore**, and from our colleagues at the EICC. The competition to host these meetings is keen as ever, with Darmstadt and Istanbul both submitting strong bids. We shall do our best to bring ECM to the UK.



That is what is timetabled, but in the nature of these things, the BCA president is always "on duty" at crystallographic conferences and I anticipate many interesting discussions and debates. (Note to potential candidates for BCA President next year - this is a GOOD THING).

On issues which will not be resolved by the time this issue of Crystallography News arrives at you, it is my pleasure to issue a Call for Nominations for Honorary Members of the BCA. This, our highest membership accolade, is awarded to a small and select band of colleagues who have contributed significantly to crystallographic science and to the work of the BCA. Last year we elected **Paul Barnes, Mike Glazer** and **George Sheldrick**, and we anticipate electing around the same number of new Honorary Members in 2005. Your nominations are welcome, with a short supporting case, to me at president@crystallography.org.uk, by the end of October please.

In this issue of Crystallography News you will find the outline programme for the 2006 Spring Meeting in Lancaster, with its emphasis on crystallisation - fittingly in collaboration with the British Association of Crystal Growth. Programme Chair **Paul Raithby** is pulling it all together, with **Kevin Roberts** leading for the BACG; I hope you agree the evolving programme once again looks exciting and compelling - we look forward to attracting once again a large number of delegates. The BCA Young Crystallographers, who will once again be organising sessions at the Lancaster meeting, are being organised along the lines of a special interest group, in order to ensure continuity of their involvement within the BCA. This input from the Young Crystallographers, as well as being scientifically relevant, is also important with respect to the educational remit of our Association. On that issue, the draft BCA Education web-site should be available in early September at its temporary home www.chem.gla.ac.uk/BCAEducation, initially for comment before migrating to the main Web-site.

Chick Wilson

BCA Council: Front Row Christine Cardin, John Finney, Chick Wilson and Sheila Gould. Back row: Bob Gould, John Helliwell, Sandy Blake, Jeremy Cockcroft, Sheila Gover, Elspeth Garman, Georgina Rosair, John Evans and Peter Moody.

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2004-05

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www.crystallography.org.uk

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From the Editor



ONCE again, the IUCr is about to take place as we go to press, and, as the President points out, you will not be reading this until after it is over. From the point of view of crystallography news, with or without capital letters, it is a quiet time of year. Those of you who are on the verge of sending in something

but didn't do it have missed a good chance - but be of good cheer, even for the December issue, we have a high acceptance rate!

There are a number of small general "News Items" in this issue, serious, and not-so-serious. Many thanks to Kate Crennell who is the spotter of most of these. However, anything you spot in the newspapers or on the net which interests or amuses you may well amuse or interest others too, so please do E-mail any such discoveries to me!

In years of international meetings, there are no European meetings, but the American Crystallographic Association meets early, and, traditionally, in the southern part of the USA. This year's meeting was in Orlando FL, within Walt Disney World, and was, as always, an impressive affair, despite the somewhat bizarre setting. I have written an account of a small part of the meeting. I'm also indebted to Lachlan Cranswick for sending a copy of the report of one of the Special Interest Groups which airs matters which will be relevant to both the BCA and the ECA.

An unusual feature in this issue is **David Watkin's** advertisement for a post-doctoral research assistant. We are always glad to print these on behalf of members, but are rarely sent them. The main problem, of course, is the fact that we only appear four times a year. If, however, you have a post which you would like to advertise early in March, June, September or December, let us know about it. Printed in this issue are application forms for membership of the BCA and for attendance at the CCG meeting at Daresbury. I need hardly say what bargains they both are! Naturally, we hope that you will photocopy rather than rip these out. Not having extra paper to stuff in saves both money and time in getting Crystallography News to you.

A cheerful face appearing for the first time in this issue is that of Elaine Fulton, who is now, as Assistant to Gill Moore, the main "voice on the phone" at the BCA Office. Unusually for this day-and-age, you will have to learn her surname, as there are two Elaines at Northern Networking Events. Our one does, however, respond to the Welsh-style "Elaine-the-BCA"!

I receive some house journals from our related organizations on the Continent. I have included a couple of brief extracts from the Swiss and German journals, SGK/SSCR Newsletter and Mitteilung der DGK e.V. and hope you will like them.

Plans are going ahead well for next year's spring meeting in Lancaster, both with planning the scientific meeting and looking over the site and its facilities. There will be much more about it in the December issue, but meantime, mark the dates of April 4-6 2006 in that part of your diary that gets transferred to next year's!

Bob Gould



Puzzle Corner

SUDOKU seems to have swept the country, but I've not been able to think of a puzzle with a crystallographic bias.

So for this issue, here is something that looks like a Sudoku diagram but isn't! Each of the nine blocks contains a nine-letter word after the style of Wordsearch in the Radio Times. Starting anywhere, proceed in any direction to build a nine-letter word, using each letter only once. All of the words here are connected with structural science, taken in a broad sense! To get you started, the word in the upper left hand corner is "GALACTOSE". When you have finished, the first letters of the resulting words may be arranged into a tenth nine-letter word, which is the solution to the puzzle. Happy unscrambling!

O	T	C	S	U	O	M	Y	R
S	A	G	A	R	H	O	E	D
E	A	L	O	M	P	R	H	E
N	G	A	I	O	N	C	I	H
O	A	X	X	L	E	M	I	P
L	E	H	E	R	F	D	O	R
E	N	S	O	P	H	E	T	A
I	L	O	L	O	P	A	T	S
B	U	L	M	Y	R	R	P	A

Last month's £10 book token was won by Tim Weakley who enquired why the font was specified. The only reason for this was that Arial/Helvetica does not have extra serifs which might confuse the symmetry relating the letters b, d, p and q. Here is one solution, with a 2-fold rotation point at each vertex and glide lines bisecting each rectangle in both directions. It is an interesting exercise to use arrangements of these four letters to represent all of the oblique and rectangular plane groups.

b	p	b	p	b	p	b
d	q	d	q	d	q	d
b	p	b	p	b	p	b
d	q	d	q	d	q	d
b	p	b	p	b	p	b



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 December 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.
- Ten complimentary copies of the quarterly BCA Newsletter.
- Corporate Members will be listed in every BCA Newsletter and on the BCA Web Site with links to your corporate site.

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

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

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ACA Summer Meeting



ACA at Walt Disney World

WELL, the Magic Kingdom was an odd place to choose to have a scientific meeting. After we had wound our way through the endless maze of lanes encountering no comforting signs saying “ACA this way”, we eventually arrived at the Swan Hotel. We then learnt that guiding notices outside the hotel weren’t allowed, as they weren’t deemed appropriately magic! It is opposite the Dolphin Hotel, and the symbols of the two looked disconcertingly related by pseudo-symmetry, albeit one had its face at the small end and the other at the large one.



Happily, once inside, we found the hustle and bustle of crystallographers just as good as ever, and quite magical enough! As usual, there was a lively British contingent represented in all sections of the meeting. A highlight was the presentation of the Patterson Prize to **Alwyn Jones** (Uppsala). His following lecture was the usual mixture of fascinating science and hilarious clowning - he, at least, seemed to bridge the gap into the Magic Kingdom. It was a description of the development of his famous program “O”, and, as usual, he refused, Lohengrin-like, to reveal the origin of its name!

My favourite session, which covered a very wide range of topics I will attempt to summarise, was entitled *Advances and Insights in Small Molecule Crystallisation and Handling* was opened by **Douglas Ho**, appropriately, if unconvincingly, clad as a Jedi lord in a dressing gown and towels. The speakers, however, preferred a standard laser pointer to the sabre that he offered. (But see letter from **David Watkin** in this issue about pointers of any sort!)

The first talk, by **Bart Kahr** (Washington State), was called *Dyeing Crystals*, but featured much more. He pointed out that the nineteenth century educator, Froebel, was a crystallographer, who was offered the chair of Mineralogy in Stockholm, but decided instead to invent the kindergarten, and produce some very sophisticated teaching materials emphasising symmetry concepts. He pointed out the similarities between some paintings by Klee and Mondrian and some by well educated kindergarteners. The actual crystal dyeing demonstrated different habits (and hues) of K_2HPO_4 crystals grown in the presence of dyes, whose adsorption on different faces affected crystal growth, as well as giving colour to the crystals. **Marilyn Olmsted**'s (Davis, CA) talk *Application of CO_2 to Crystallisation of highly fluorinated compounds*, showed that the use of sub- and supercritical CO_2 in mixed solvents could greatly increase the chance of crystallising some difficult to crystallise materials, including perfluorinated hydrocarbons and peracetylated sugars.

Kenneth Poppelmeier (Evanston IL) in *Crystal Growth that targets Non-centrosymmetric Structures* illustrated some solid state reactions carried out in sealed Teflon pouches producing, among other things $Ag_4V_2O_6F_{12}$, a battery material suitable for medical implants, and lasting 7-10 years. The technique was described as “lending itself to serendipity”. **Andy Parkin** (Glasgow) examined *In situ Crystallography; the effect of an Applied Electric Potential on Crystal Structures and their Formation*. He described the construction of a cell, complete with a three electrode system, suitable for mounting in an X-ray beam, in order to study both material as it was deposited and the possible change in an electrolysed crystal. **Vic Young** (Minneapolis MN) with *Handling Difficult Small-molecule Specimens*, said that he had “never seen a farmer who hadn’t invented something to revolutionise farming - look in any barn, and you’ll find it under a tarpaulin somewhere. Crystallographers are rather like that!” He then gave some of his ideas for keeping solvent in and keeping air out, including the use of sTp oil - something well known to any American farmer (American for WD-40). **Victor Rosso** and **John DiMarco**, (Bristol-Myers-Squibb) *High Throughput of Small Molecule Crystallisation and Problematic Crystal Forms discovered therefrom*, looked at adopting protein techniques for small molecule crystallisation. The standard plastic equipment could not be used, since it was incompatible with many solvents used and interferes with optical investigations; also, a greater range of temperature is required. Vials intended for HPLC were often suitable. An example was given with 35 hits from a total sample of 40mg. Another experiment using only 1 mg of the same sample gave 34 hits, of which only 28 were common to the two! A drug “X” had given 23 crystal structures including 21 solvates; there were 11 unique crystal forms. **Robert Bau** (Southern California) Presented work on

$\text{OsH}_3\text{Cl}(\text{PPh}_3)_3$ in which an H_2 -ligand connected η -2 has a “stretched” H-H bond length of 1.47Å. The session was concluded by **Colin Seaton** (Bradford) on the structure of a glucose-sulfathiazole adduct which gave only very small crystals. Application of powder diffraction, solid-state NMR and structure prediction is particularly difficult for molecular adducts. In this case, success found that the “adduct” was actually a compound!

It was, as usual, a big meeting, and while mainly macromolecular, had plenty else too. Next year's meeting is scheduled to be in Hawaii, which is well off the centre of gravity of crystallographers. Since, however, the ACA is, like the ECA, the recognised regional body for the whole of the Americas, presumably it will have to have some meetings in Latin America soon? Anyone for Tierra del Fuego?

Bob Gould

Materials Special Interest Group of the American Crystallographic Association (ACA) : Chairman's Report - 2005

(This report was sent to us by the author, and seems to touch several issues relevant to planning our meetings. Ed.)

THE Materials SIG has recently been in a rather moribund state such that the Powder and Neutron SIGs deserve the credit for this year's MATSIG oriented sessions in ACA 2005 at Disney World, Orlando.

To try and reverse this sorry state in the ACA Materials SIG, rather than continuing to propose sessions in near isolation, a significant number of materials topics were proposed with other SIGs (Neutron, Powder, Small Molecule, Service Crystallography, Industrial and Small Angle Scattering). Coordination with these SIG chairs was arranged prior to the 2006 planning meeting to afford minimum chance of session conflicts, and thus attempt maximum interest to potential attendees. Within the constraints of a large number of SIGs divvying up 4 parallel sessions, this has resulted in a good set of proposals for 2006 meeting agenda for single crystal oriented materials crystallographers, and a fair agenda for powder materials crystallographers. The constraints of a 4 parallel sessions limit for a diverse area such as crystallography are very apparent. Especially when compared to an equivalent yearly crystallographic conference in field and numbers of attendees, the (usually) 6 parallel session European Crystallographic Association (ECA) meeting. As was stated in a verbal report to the ACA Council, this is not a chicken and egg issue. If lacking a consistent and continuous

stream of relevant sessions, crystallographers will make the logical and appropriate decision of not bothering to attend. The comment of two “invited” materials speakers at this year's meeting are quite similar: they each attended an ACA meeting around 10 years ago but were alienated by an unbalanced program with perhaps two to three sessions of interest during the entire 5 days. They never intended to come again, and only some strong-arming to attend as invited lecturers changed their minds; for this year. On chatting to some other SIG chairs, this does not sound a problem unique to the Materials SIG.

The other relevant issue relates to a possible lack of consideration in keeping the ACA meetings affordable by i) choice of location and ii) ensuring there is a wide variety of economy accommodation available. According to some other SIG chairs, this is not just affecting materials crystallographers and their students. It is profoundly futile to plan a good stream of sessions if the intended audience cannot afford the “total cost” to attend in reasonable numbers. The Hawaii 2006 meeting is a first class example. It has apparently become routine for the ACA to only recommend high-end accommodation and herd all participants into it. For a North American academic, a “cheap” room in a 5 star hotel, single or shared, can be a bitter financial pill to swallow. To a majority of Latin or South American crystallographers the ACA claims to encompass, it is completely impractical. This year's planning meeting in Orlando for Hawaii 2006 gave the impression that the criteria for a successful ACA meeting, is that of how many rooms are filled in a 5 star conference hotel. This definition of “success” (if accurate) is not financially compatible with the research funding and budgets of academics involved in American materials crystallography. Various attendees at the materials SIG and related SIG meetings made it very plain they will not be able to attend the ACA 2006 due to the total cost of attendance being too high. There are indications that unless cheaper accommodation is also promoted, the default total attendance cost of ACA 2006 in Hawaii will have a significant negative effect on the ability for academic materials crystallographers and students to participate. Contrary to statements made at the Orlando planning session for Hawaii 2006, there is multiple student-and-academic-affordable hostel style accommodation in or near Waikiki, Honolulu; this includes the Banana Bungalow Waikiki Beach and Polynesian Hostel Beach Club. It is hoped, in so much as it is possible to achieve, the ACA can make its annual meetings as available to students and academics as possible by providing practical pathways for participants to minimize total attendance cost.

Lachlan Cranswick

British Crystallographic Association/ British Association for Crystal Growth

Spring Meeting 2006

to be held at the University of Lancaster on 4th - 6th April

Keynote Lecturers include:

- **Professor Mike Glazer** (Oxford)
- **Professor Mark Spackman** (Western Australia)
- **Professor Ulrich Griesser** (Innsbruck)

Provisional Session Titles include:

High Pressure, Liquids & Surfaces
Powder Diffraction in Industry
Customised Crystallisation
Charge Density Studies
Crystal Engineering
Exhibitors Forum

Hot Topics in Crystallisation Methods
Topology
Pharmaceutical Crystallography
Nanocrystallography
Getting the most out of your crystal?

In addition there will be a workshop on powder diffraction and a short workshop on TOPAS.

Satellite Sessions will include:

The Young Crystallographers Meeting
SRS Users Meeting
ISIS Users Meeting
Symposium in Honour of Prof Mike Hursthouse

For further details please contact the Programme Chair, **Professor Paul Raithby**, Department of Chemistry, University of Bath, e-mail: p.r.raithby@bath.ac.uk further details will appear in the December Issue of *Crystallography News*.





Membership Form 2006

British Crystallographic Association Charity Registration Number 284718

WEB SITE: <http://www.crystallography.org.uk/>

Return this form to: **British Crystallographic Association, Administrative Office, 1 Tennant Avenue, College Milton South, East Kilbride, Glasgow G74 5NA UK.** Tel +44 01355 244966, Fax +44 01355 249959, E-mail: BCA@glasconf.demon.co.uk.

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

Title _____ Initials _____ Name _____

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- A current BCA Member
 - A lapsed BCA Member
 - Not previously a BCA Member
 - Unemployed*
 - Retired*
 - A full time student*

Main	Group	Special
<input type="checkbox"/>	Industrial	<input type="checkbox"/>
<input type="checkbox"/>	Chemical Crystallography	<input type="checkbox"/>
<input type="checkbox"/>	Physical Crystallography	<input type="checkbox"/>
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For Students only - Signature of Supervisor: _____

Course completion date: _____

- FEES:** Full *Reduced *ONLY Students, Retired and Unemployed
- £15 £7.50* in Pounds Sterling by cheque (UK Bank) or credit card (Mastercard, Visa, Delta ONLY)
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I wish to add a donation to my fees as specified below:

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£.....:.....p to the **Arnold Beevers Bursary Fund** of the British Crystallographic Association.

£.....:.....p to the **Dorothy Hodgkin Prize (DHP)** fund.

£.....:.....p **TOTAL PAYABLE to British Crystallographic Association in pounds sterling.**

Tick here if you are a UK taxpayer and would like Gift Aid to be paid on your contribution.

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- Banker's Order - please complete section (B) below. Credit card - please complete the following:

(eg Visa, Mastercard, Delta **NOT** Switch)

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Signed Date.....

Thank you for supporting the British Crystallographic Association

38th International Course at Erice: 9-18 June 2006 Structure and function of Large Molecular Assemblies: Crystallographic Targeting of Pathogenic Viruses to Recognize and Neutralize potential Terrorism Agents.



Purpose of the course

Crystallography and electron microscopy are pre-eminent techniques for obtaining the structure of biological macromolecules at atomic resolution. These structures, components of living organisms and viruses, are central to the understanding of the detailed mechanisms of biological processes, and to discover novel therapeutics using a structure-based

approach. Almost weekly, international journals such as *Nature*, *Science*, and *Cell* show striking drawings of large biological molecular assemblies, and the articles therein explain the role and function in their biological environments. To counter the myriad modern threats of disease and terrorism, there is an urgent need to interpret the significance of the hundreds macromolecular structures published nowadays. This meeting will train upcoming generations of scientists to undertake this important task.

The present scientific programme will focus on the most recent achievements in structural studies of large molecular assemblies.

Formal lectures in the main hall will be integrated with practical hands-on sessions, by exploiting the most recent advances in Information Technology, in several smaller and well equipped rooms available at the Ettore Majorana Centre.

The present Course is designed also to provoke the birth of centres for macromolecular crystallography in several eastern European countries where this field has only recently started to develop.

Applications

Interested candidates should register by 30 November 2005 using the format available at <http://www.chimica.unipd.it/erice> or writing to the Executive Secretary of the International School of Crystallography:

Professor Paola SPADON - Executive Secretary
International School of Crystallography

Dipartimento di Scienze
Chimiche Via Marzolo

1- 35131 PADOVA, Italy

Tel ++39.049.8275275 Fax ++39.049.8275239

e-mail: paola.spadon@unipd.it

Specifying:

- i) full name(s), age, sex, citizenship;
- ii) postal address, phone, fax, electronic mail;
- iii) present academic position and scientific interests;
- iv) the title or abstract of a scientific contribution to the poster session(s) which might be included in the programme.

Young researchers should add a list of no more than five scientific publications and a letter of recommendation from the group leader or a senior scientist, where the amount of support, if needed, is justified. In order to reflect the multi-disciplinary nature of the course, attendance will be encouraged on the basis of the scientific discipline, publication record and the correspondence between the current research of the applying scientists and the listed topics.

Control and Prediction of the Organic Solid State

THIS Basic Technology project will be holding its Open Day on Tuesday 13th September 2005 in the Old Refectory at University College London.

The Open Day provides an opportunity for anyone interested in the organic solid state to see what we have learnt about polymorphism and the development of computational predictions as we approach the half-way point of our project. All are welcome, but please register with **Dr Louise Price** by 5th September, either by phone (020 7679 7583), email (l.s.price@ucl.ac.uk) or on the website (<http://www.cposs.org.uk>). The full programme for the day is now available on the website, along with directions for how to get to UCL.

Louise S. Price

Revision of .cif Dictionaries

(The following is an announcement from the IUCr office in Chester - Ed.)

IN association with the publication of "International Tables for Crystallography Volume G: Definition and Exchange of Crystallographic Data" (expected mid-August 2005), revised versions of all current CIF dictionaries have been released on the IUCr web site:

core CIF dictionary

version 2.3.1 dated 2005-06-27

powder CIF dictionary

version 1.0.1 dated 2005-06-14

modulated structures CIF dictionary

version 1.0.1 dated 2005-06-16

electron density CIF dictionary

version 1.0.1 dated 2005-06-14

macromolecular CIF dictionary

version 2.0.09 dated 2005-06-27

image CIF dictionary

version 1.3.2 dated 2005-06-25

symmetry CIF dictionary

version 1.0.1 dated 2005-06-17

DDL1 dictionary

version 1.4.1 dated 2005-06-29

DDL2 dictionary

version 2.1.3 dated 2000-10-16

DDL2 dictionary

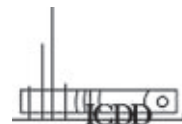
version 2.1.6 dated 2004-04-15

(Note that DDL2 dictionary version 2.1.3 has had some typos corrected, and is released in this form, but with an unaltered release date, because it is discussed in detail in International Tables G. The current version of DDL2 is 2.1.6.)

All these dictionaries may be accessed from the IUCr CIF home page <http://www.iucr.org/iucr-top/cif/index.html>. The IUCr web site now contains HTML versions of all these dictionaries, and the utility to search for a CIF data name (<http://www.iucr.org/iucr-top/cif/cifsearch.html>) has been extended to include all the dictionaries.

These are all minor version upgrades (although one new data name has been added to the core dictionary) and reflect editorial changes and minor corrections arising from the work on Volume G. Complete details of changes may be found in the revision history section of each dictionary.

Ludo Frevel Crystallography Scholarship Awards Sponsored by the International Centre for Diffraction Data Application



Deadline: 31 October 2005

TO encourage promising graduate students to pursue crystallography oriented research, the International Centre for Diffraction Data (ICDD) has established the Ludo Frevel Crystallography Scholarship Fund.

Multiple recipients are selected on a competitive basis, each receiving an award of \$2,250. Applications must be received by the ICDD by 31 October 2005.

Qualifications for the applicant:

The applicant should be enrolled in a graduate degree program during the 2006 calendar year with major interest in crystallography, e.g. crystal structure analysis, crystal morphology, modulated structures, correlation of atomic structure with physical properties, systematic classification of crystal structures, phase identification and materials characterization. There are no restrictions on country, race, age or sex. The term of the scholarship is one year.

Submit:

- Curriculum vitae, listing degree(s) held and degree(s) sought.
- A one page summary by the graduate student describing the type of crystallographic research being pursued in satisfying the requirements of an advanced degree and the applicant's expected date of graduation.
- A supportive letter from the sponsoring professor of an accredited university or an institute of technology on institution letterhead.

Scholarship awards are made possible by donations from both private and industrial sectors. Donations can be directed to the Ludo Frevel Crystallography Scholarship at the address below.

Visit our web site at: <http://www.icdd.com/resources/awards/frevel.htm>

Please mail to:

Scholarship Committee
c/o Corporate Secretary
International Centre for Diffraction Data
12 Campus Boulevard
Newtown Square, PA 19073-3273 U.S.A.

UKRC Return Campaign

THE United Kingdom Research Councils' Return Campaign to encourage women to return to careers in Science, Engineering and Technology was officially launched on 11 May 2005.

See <http://news.bbc.co.uk/1/hi/sci/tech/4534177.stm> for BBC coverage.

The Return Campaign encompasses:

- Information, referral and follow-up support from the UKRC
- On-line course run by the Open University - T160
- Mentoring and networking support
- Links with employers (under development)
- Services offered by regional hubs in the JIVE project and other partners.

For further information please contact **Jane Butcher**, Women Returners Manager

email: j.butcher@bradfordcollege.ac.uk

Rosalind Franklin Award



Rosalind Franklin



Christine Davies

PROFESSOR Christine Davies of Glasgow University, whose research interests are mainly in the phenomenology of the strong interaction described by a theory called Quantum Chromodynamics, and who is an active member of the Women In Physics Group of the IoP, has won the Royal Society Rosalind Franklin Award this year.

The Award, made annually to an individual for an outstanding contribution to any area of natural science, engineering or technology (SET) consists of a medal and about £30,000 and the recipient is called upon to deliver a lecture as part of the Society's public lecture series.

SET for Women Unit Resources

AS a result of the reorganisation of the DTI the UKRC have received the valuable collection of resources, including books, reports and papers, which have been built up over the 10 years since the Promoting SET for Women Unit was established.

These will be catalogued and incorporated into the UKRC Library. All the resources held at the UKRC are available to anyone wishing to reference them for research purposes. And we hold copies of many publications which can be mailed out. Our online Publications Catalogue is an ever growing bibliography signposting to many other available resources on Women in SET. Please visit the Resource Bank on the website and your feedback and comments would be most welcomed. For further information please contact **Erica Williams** at the UKRC (e.williams@bradfordcollege.ac.uk).

Synchrotron Radiation Users Meeting 2005

13th-14th September 2005 | Palace Hotel, Manchester

The meeting this year will celebrate 40 years of the SRS. There is a vibrant and active programme of plenary lectures and satellite meetings. Further details of the meeting and registration may be found on the SRS website www.srs.ac.uk/srum05/intro.html.



A satellite meeting of particular interest to crystallographers is:

Structures and Change: dynamic EXAFS and XRD

Abstract

Time resolved studies have long been the prerogative of spectroscopists, but recent advances in technology mean that diffraction methods can now be used to study fast reactions and identify transient species. Recently, there have been cutting edge time resolved single crystal studies on macromolecular and molecular systems where lasers have been used to induce photoexcited states with lifetimes in the nanosecond to microsecond range. EXAFS spectroscopy has also been used successfully to probe structural changes in short lifetime photoexcited species. In this symposium the complementarity of time resolved spectroscopic and diffraction will be illustrated by a series of keynote lectures from experts in the area.

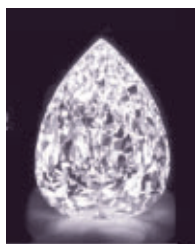
Refugee Academics

THE council for assisting refugee academics is pleased to announce a call for applications for its September 2005 funding round. We would be grateful if you could post and/or distribute the attached notice to your clients and networks as appropriate.

We provide grants to academic refugees who are now living in the UK, and seeking to further their educational or vocational goals. Grants may cover expenses such as course, exam, or bench fees; associated research, travel and equipment costs; conference costs; childcare expenses; and in limited cases maintenance.

For further information please contact **Marieke Stroink**, Programme Officer Council for assisting refugee academics phone: +44 (0) 207 021 0880; email: schreiber.cara@lsbu.ac.uk; web: www.academic-refugees.org

Diamonds at the Natural History Museum



THE Natural History Museum in London has an exhibition on diamonds which started 8 July 2005 and ends 25 February 2006.

Admission to the museum is free but a charge is made to see the exhibition; it is by timed ticket. The

cost depends on your age; there are concessions for children and pensioners. The organisers suggest advance booking to avoid disappointment if you just turn up on the day. You can also buy a glossy 'Book of the Exhibition'.

The website has several sections: VIP large, History, Discovery, Technology and Design. I did not look through them all closely but I failed to find anything on structure. Plenty of details of making artificial diamonds and pretty pictures of famous diamonds some of which are on show in the exhibition, including some of the 'De Beers' millennium jewels which were on display in the Millennium Dome during 2000. (See the front cover of 'Crystallography News' no 71 December 1999, inside on page 9 and the puzzle pages 62 and 63, which I plan to store on the BCA website with the other puzzles, (see <http://bca.cryst.bbk.ac.uk/BCA/Cnews/Comp/index.html>)

Further details are on the web site at: <http://www.nhm.ac.uk/diamonds/exhibition.html>

This site is a useful set of pages on the diamond, but the Museum states that the pages will only be kept for a short time. I should like the BCA to urge the pages be kept indefinitely, if not on the Museum website perhaps on ours.

Kate Crennell

Applied Crystallographic Programming

(The following course, advertised by the Abingdon and Witney College, was sent in by Kevin Knight who thought it might interest some of our readers. Ed.)

Equine Studies: Introduction to Crystal Therapy for Horses - NEW

Course code: ECCB203P

Location: Witney Stud Farm.

Length of Course: 1 day - Part-time

Times: 10.00am - 4.00pm, Saturday.

Fees: £45

Course begins on 08 October 2005

Course Description

This is an introduction to the Crystal Healing for equines. You will learn the basics of working with auric fields, chakras and dowers to enhance your horse's well-being. You will learn about choosing, cleansing, dedicating, resting and programming crystals and different types of methods that can be used when healing horses.

Contact

Pam Willsher T: 01993 208025

E: inquiry@abingdon-witney.ac.uk



Russian website on the drawing of minerals

DEAR colleagues!

We invite everyone who is interested in minerals, mineralogy and the fine arts to visit a new unique Site of the Project "Drawing Minerals": <http://mindraw.narod.ru/>

You can also see some pictures on <http://www.mineralogist.ru/> in "Science"

Yours faithfully

Victor Slyotov and **Vladimir Makarenko** (the authors)

(Some interesting material here, but be warned - the website downloads very slowly! Ed.)

Letters to Ed.

From Dr David Watkin

Dear Bob,

In the March 2005 issue of the British Crystallographic Association 'Crystallography News', Prof Tony North wrote about the advantages of using the mouse pointer in PowerPoint presentations (rather than using a laser pointer). He explained that main advantage is that if the speaker has the monitor and mouse between herself and the audience, she does not have to turn her back on the audience to use the pointer. If the speaker does use the mouse pointer, it is also an advantage to use a large brightly coloured (e.g. gold) one.

Since reading that, I have watched speakers at the BCA intensive course, and the BCA Spring Meeting, and must agree that Prof North is correct. If you could check this out for yourself, I'm sure you will also agree, and perhaps then be able to encourage the BCA to make a gold cursor downloadable from a website - perhaps CCP14.

The cursor file should be put in WINDOWS\CURSORS, and then be selected via

START > SETTINGS > CONTROL PANEL > MOUSE > POINTERS > BROWSE.

Note that pressing CTRL/A during a PPT presentation keeps the cursor on the screen even if it is inactive.

Best wishes,

David Watkin
Past Chair
IUCr Computing Commission.

Ed. (David enclosed two attractive pointers with his letter - sadly, they don't print very helpfully in monochrome, but we will try to see that something is done about his suggestion for making them generally available! Ed.)

From Dr Mike Webster

Dear Dr Gould,

I was recently reading through the June Crystallography News and noticed that a number of photos did not give the names of the people photographed. In large group photos it is probably not appropriate and in others of a single person it follows from the context. Your photo on page 4, for example, in the 'From the Editor' needs no caption! However the photos on page 7,8,10, 12,13 and 15 for example have no information and whilst I may recognise some faces there are many who are unfamiliar. Some photos do have a caption, for example on page 20, and in your editorial role you may feel some general views may not warrant one.

However, I think it might help to give a friendlier feel to the pictures with the names particularly if less formal settings were used. The IUCr Newsletter usually manages to give the names. This is a minor point in an otherwise excellent newsletter.

Best wishes,

Mike Webster, University of Southampton

Ed. Dear Mike,

Thanks very much for your comments. I completely agree about names - the problem is that I sometimes don't get them at the time; you'd be surprised how disinterested people are in their photographs at the time of their being taken. At least one photograph in the June issue has the wrong name! Less formal settings would also be a good idea - but not every set of lecturers readily relaxes into such less formal arrangements as that of the tutors at the CCG School on page 4! Generally, I have trouble getting people into any sort of array in which they can actually be seen and recognized. I've also occasionally ended up with such dreadful expressions that I've had to cut people out.

Anyway - I'll try harder, and really do appreciate comments! - Editor.

From Dr Ron Stenkamp

Hi.

While I enjoy receiving your newsletter, I feel I should let you know that I'm no longer one of the co-editors for the ACA Newsletter. Accordingly, if you're feeling like trimming your distribution list (and saving some postage), I should probably be removed from it.

Yours is a very good looking newsletter, and I like the humor shown in it.

Thanks,

Ron

Ed. Dear Ron,

After receiving flattery like that, how could I possibly disconnect you! There will certainly be more humour/humor in the next issue!

All the best,

Bob

University of Oxford Department of Chemistry

Chemical Crystallography Laboratory

POSTDOCTORAL RESEARCH ASSISTANT IN CRYSTALLOGRAPHIC COMPUTING

Applications are invited for a Postdoctoral Research Assistant to work on a crystallographic software project. This PDRA position is a joint collaboration between the Universities of Oxford and Durham and in the first instance is funded by the EPSRC for one year. The work aims to implement a new set of algorithms in object oriented, open source code that will preserve the immense knowledge-base that exists in the field of crystallography, and to provide a platform for future developments.

The post holder must have experience in designing and writing computer programs to good modern standards, and knowledge and proven practical skills in the areas of crystal structure analysis using X-rays or neutrons. Experience with powders and extended lattice (inorganic) materials would be an advantage.

Brief job description

The post holder must be able to make a significant contribution to the following tasks in adding modules to the software system:

- Preparing clear plain-text descriptions of the crystallographic function and use of each module.
- Prepare clear and complete descriptions of the mathematics involved in the module, including issues of precision, latent singularities, and limits of applicability.
- Prepare a clear specification of how the module will interface to other modules and the underlying database.
- Prepare a clear description of how the user will interact with the module.
- Prepare suitable test data and results and if possible validate them with existing programs.
- Write code complying to both ANSI standards and the style adopted for the whole project.
- Validate the new code.
- Prepare end-user documentation.

It is planned to appoint on the Research Grade 2 II scale for University Research staff, salary (£27,116 - £29,128), depending upon age and experience. However we would be prepared to consider applicants who are not yet seasoned specialists, who would like some mentored time to develop in the post in which case the appointment would be made on the RS1A Grade scale.

Further details are available from the Administrator, Inorganic Chemistry Laboratory, South Parks Road, Oxford OX1 3QR (quoting ref DH05009/DJW), or by email from rita.higgs@chem.ox.ac.uk and these must be obtained before application is made. Informal enquiries may be made to Dr David Watkin (e-mail: david.watkin@chem.ox.ac.uk). Applications by e-mail are not acceptable. The closing date is 30 September 2005.

Groups



PCG News

THE PCG/SCMP annual general meeting was held during the Loughborough BCA spring meeting.

Pam Thomas reviewed another active year for the PCG/SCMP including a successful winter meeting on neutrons in biology (thanks to **Paolo Radaelli** as local organiser and **John Helliwell**); a white beam satellite workshop to the BCA spring meeting (thanks to **Mina Golshan**); a teaching and research session on phase transitions at the BCA spring meeting (thanks to **Mike Glazer**); a two day Rietveld workshop (thanks to **Jeremy Cockcroft, Ivana Evans, Kevin Knight** and **John Evans**). Other important events included the inaugural PCG/SCMP/PANalytical thesis prize which was awarded to **Dominic Fortes** of UCL (thanks to PANalytical for £500 sponsorship). **Jacqui Cole** (Cambridge) was congratulated on receiving the poster prize for PP7 on "Rare Earth Phosphate Glasses", and **Matt Hampson** (Durham) who was awarded "Highly Commended" for his poster on ^{17}O NMR studies of oxide mobility in ZrW_2O_8 .

Pam thanked retiring members of the committee and ran elections for their replacements. **Paolo Radaelli** was elected as Chair, and gave a short speech on his plans which include maintaining the PCG's focus on education. **Dave Allan** was elected as Vice Chair and **Dave Laundry** and **Jacqui Cole** as Ordinary Members. **John Evans** was co-opted to serve for a further 12 months as Honorary Secretary/Treasurer to provide continuity amongst the officers.



The AGM closed with Pam thanking all those who served with her during her 13 (!) years on the PCG committee. The current committee presented her with a "long service certificate", a small but

suitably alcoholic gift, and expressed their gratitude for her services to the PCG/SCMP. As secretary during Pam's years as president I would like to add my personal thanks for all she's done for the PCG/SCMP over many years - her many contributions will be greatly missed.

Future planned activities include a second workshop on Magnetic Rietveld refinement to be co-organised by Paolo Radaelli and Andrew Wills, and a winter meeting on physical crystallography to be organised by John Loveday. More details on these events appear opposite.

Finally, a reminder that the PCG will be organising a prize for the best young(ish) physical crystallographer

to be awarded at the BCA spring meeting in 2006 - the successor to the PANalytical prize (PANalytical now sponsor our new thesis prize). Start thinking now about worthy recipients and expect a deadline for nominations in mid January 2006.

John Evans

Current Committee:

Name	Grade	Since
Paolo Radaelli	Chairman	2005
Dave Allan	Vice Chairman	2005
John Evans	Honorary Secretary/Treasurer	2002
John Loveday	Ordinary Member	2003
Mina Golshan	Ordinary Member	2004
Andrew Wills	Ordinary Member	2004
Jonathan Wright	Ordinary Member	2004
Jacqui Cole	Ordinary Member	2005
Dave Laundry	Ordinary Member	2005

PCG Winter Meeting

The Physical Crystallography group is planning a one day winter meeting in Edinburgh on 14 December entitled "Physical Crystallography in the U.K." It will be at the Centre for Science at Extreme Conditions, Kings Buildings Edinburgh, Organiser **John Loveday** (j.Loveday@ed.ac.uk) from whom more information can be obtained.

BSG Poster Prize - Spring Meeting, 2005



SINCERE apologies from the Editor for wrongly identifying the winner of the Biological Poster Prize!

The correct identity, supplied by **Sheila Gover**, was **Michael Hough** of Daresbury Laboratory, who received the prize as first author on

BP-14 "Catalysis and Electron Transfer in Copper Nitrite Reductase from *Alcaligenes xylosoxidans*."

PANalytical Thesis Prize for Physical Crystallography - Call for Nominations

THE Physical Crystallography Group is pleased to invite entries for the PANalytical Thesis Prize in Physical Crystallography.

The prize will be awarded for the best use of techniques or methods of Physical Crystallography in a **successfully-examined thesis submitted in the period from September 1st 2004 to December 31st 2005**. The amount of the prize, which will be sponsored by PANalytical Ltd, will be £500. To be eligible for the prize, candidates must be a member of the Structural Condensed Matter Group of the IOP and/or the British Crystallographic Association (BCA). Non-members may enter the competition but will be required to join the BCA at the student rate (currently £7.00) to progress their nomination further.

To enter the competition, candidates must submit:

- (a) a copy of the Thesis on CD-ROM.
- (b) a personal statement of not more than 500 words explaining why the Thesis should be considered for the prize and including a clear description of the role of Physical Crystallography (as interpreted below or otherwise) in the research.
- (c) The names and contact details of two academic referees, one of whom may be the Thesis supervisor, who will be able to comment on the Thesis research of the candidate.

Nominations for the prize must be submitted to the Chair of the Physical Crystallography Group, **Professor Paolo Radaelli**, by **February 28th 2006** and the prize will be awarded at the 2006 BCA Spring Meeting in Lancaster, April 2006.

Remit of Physical Crystallography in connection with the PANalytical Thesis Prize

Methods and techniques of Physical Crystallography will be interpreted in a broad fashion, for example, to include x-ray and neutron diffraction or scattering, Rietveld analysis and structure refinement, structure-property relationships, development of structure-solution techniques, crystallography under non-ambient conditions, use of complementary techniques to diffraction (e.g. optical studies, NMR), computational crystallography and modelling, electron diffraction, diffuse scattering, applications of physical crystallography in biology. In order for a thesis to be eligible for the award, the Physical Crystallography element must be central to the work of the thesis, which must also demonstrate a context over and above structural work for its own sake.

Professor Paolo Radaelli,

Chair of the Physical Crystallography Group,
Isis Facility Rutherford Appleton Laboratory,
Chilton, DIDCOT OX11 0QX
tel: 01235 445685 p.g.radaelli@rl.ac.uk



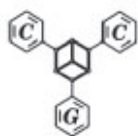
PANalytical Physical Crystallography Award 2005

AS part of its support of the British Crystallography Association, PANalytical sponsors the Physical Crystallography Group Award for the best physical crystallography PhD thesis of the year.

At the Spring BCA meeting, the adjudicators under the leadership of **Dr. Pam Thomas** (Chair of the PCG), judged the thesis of **Dr Dominic Fortes** of UCL as being the best amongst the nominees. The award was announced by the Chair of the BCA Council, **Prof. Chick Wilson**, at the Conference Dinner. The title of Dr Fortes' winning thesis is "Experimental and computational studies of solids in the ammonia-water system".



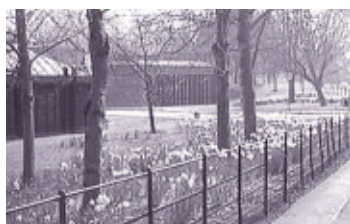
Dr. Fortes performs his research in the Department of Earth Sciences at University College London. His work involves the study of phases and compounds which are believed to exist on some of the large icy moons of the Solar System's Gas Giant planets. The Department at UCL has recently taken delivery of a PANalytical X'Pert MPD Pro diffractometer which is being used by Dr. Fortes in his investigations into these "alien" phases. The resolution achieved by the Alpha-1 system will aid the identification and indexing of the unusual phases derived from ammonia and salt hydrates, so allowing a better understanding of the processes acting in these large planets.



BCA / CCGroup : Eleventh Intensive Course in X-ray Structural Analysis

THE next Intensive Course will take place in Trevelyan College at the University of Durham, England, between 24 March and 2 April 2007.

It is intended primarily for younger scientists with some experience of structure analysis as well as other scientists who wish to improve their understanding of the underlying principles and practice of chemical crystallography.



Further details will appear in *Crystallography News* in due course, and on the Web at <http://crystallography.org.uk/CCG/ccg.html>.

Biological Structures Group Winter Meeting and A.G.M.

THIS meeting will take place in Bristol on Monday 19th December.

Organisers: **Andrea Hadfield** (A.T.Hadfield@bristol.ac.uk) and **Jim Spencer** (Jim.Spencer@bristol.ac.uk). The theme will be: "Structural Enzymology" and we aim to include both contributions from invited speakers and shorter presentations from selected abstracts. We intend to combine lunch with a poster session and to include the Biological Structures Group Annual General Meeting.

Further details will be posted on the Biological Structures Group web page <http://bca.cryst.bbk.ac.uk/bca/bsg/welcome.htm> as they become available.

Bristol is easily accessible by train and air. Direct flights from UK airports include:

Aberdeen	(Eastern Airways)
Inverness	(Easyjet)
Edinburgh	(Easyjet / BA)
Glasgow	(Easyjet / BA)
Newcastle	(Easyjet)
Manchester	(Airsouthwest)
Leeds-Bradford	(Airsouthwest)
Plymouth	(Airsouthwest)

More details on <http://www.bristolairport.co.uk/information/flightinfo/findaflight.aspx>

CCG Autumn Meeting - Computational Methods applied to Crystallography



oxford diffraction



ANGELO Gavezzotti (Milan) and **Graeme Day** (Cambridge) will be among the speakers at the CCG Autumn meeting on 16 November at Daresbury Laboratories. The planned topics include:

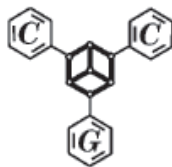
Density Functional Theory (DFT)
Methods in CRYSTAL98
Intermolecular perturbation theory (IMPT)
Modelling diffuse scattering
Lattice energy from structure

The programme at the time of going to press is:

- 10.15 Registration
- 10.50 Welcome (SP) - also safety procedures if necessary (JEW)
- 11.00 A. Gavezzotti - Milan
- 11.45 G. Day -CCDC & Pfizer Institute, Cambridge University
- 12.30 Lunch & possible tour of facilities (I)
- 14.00 Stewart Clark - Durham
- 14.30 N. Harrison -Daresbury
- 15.00 Student presentation
- 15.20 Coffee
- 15.50 TBA
- 16.20 Another student presentation
- 16.40 Close, tour of facilities (II).

Further information should appear on the Group Website, and an application form is included with this issue. We greatly appreciate the sponsorship of the meeting by Oxford Diffraction, and of student attendance by Pfizer.





British Crystallographic Association
Chemical Crystallography Group
Autumn Meeting 2005



Application of Computational Methods to Crystallography

Daresbury Laboratories
Wednesday 16th November 2005

Sponsored by  **oxford diffraction**

Title _____ Initials _____ Surname _____

Address _____

Tel: _____ Fax: _____

e-mail: _____

Name and affiliation for badge _____

Meeting fees (including morning and afternoon refreshments and lunch):

BCA Member	Standard	£15	<input type="checkbox"/>	Non-member	Standard	£27	<input type="checkbox"/>
	Student	<i>nil</i> *			Student	£16	<input type="checkbox"/>
	Retired/etc	<i>nil</i>			Retired/etc	£16	<input type="checkbox"/>

* we would like to thank Pfizer Ltd for supporting student attendance at the meeting

If you are a *non-member* and wish to convert your meeting fee into BCA membership for 2006 at the appropriate rate, mark the box on the right and complete & return a membership form to the registration desk

Please note that there is no parking available on site and the use of public transport is strongly encouraged; if you cannot use public transport, please contact the organizers directly.

Please indicate any special requirements, *e.g.* wheelchair access or dietary needs:

Cheques should be made payable to “**Chemical Crystallography Group**” and sent with the completed registration form to the CCG Secretary/Treasurer, Georgina Rosair (e-mail: G.M.Rosair@hw.ac.uk):

Dr Georgina Rosair, William Perkin Building, School of Engineering & Physical Sciences,
Heriot Watt University, Edinburgh EH14 4AS

Please note: registrations will be acknowledged by e-mail

From the Continent



From the July Mitteilungen der Deutsche Gesellschaft für Kristallographie

Statistics from the Köln Meeting

(I found the following both interesting and amusing. I'm not sure whether we shouldn't do the same thing - but do we want to know ourselves so well? Apologies to the authors for any errors in translation - Ed.)

AS usual, it falls to the organizers of the Spring Meeting in Köln to give a summary of the statistics and the events of the meeting.

The meeting was well attended, with 510 participants from 13 countries. 64 of these came from abroad: 29 from Austria, 17 from Switzerland, 4 from the USA, 3 from Spain, 2 from each of Great Britain, the Netherlands and the Czech Republic, and 1 from each of Canada, France, Ireland, Russia and Sweden. Women were definitely under-represented at 20% of those attending.

The scientific program had 145 lectures (8 plenaries, 1 prize lecture, 95 in thematic microsymbiosia, 18 from the special interest groups and 23 from the German Association for Crystal Growth (DGKK).) In

addition, there were 259 posters (80 associated with the microsymbiosia, 167 from the special interest groups and 12 from the DGKK). More than 20 of the scientific contributions were presented in both oral and poster form. The group presenting the most contributions was, as it has been for many years, the Chemical Crystallography Group, with 83 posters.

To the joy of the organizers, the number of abstracts received before the deadline was a splendid 75%.

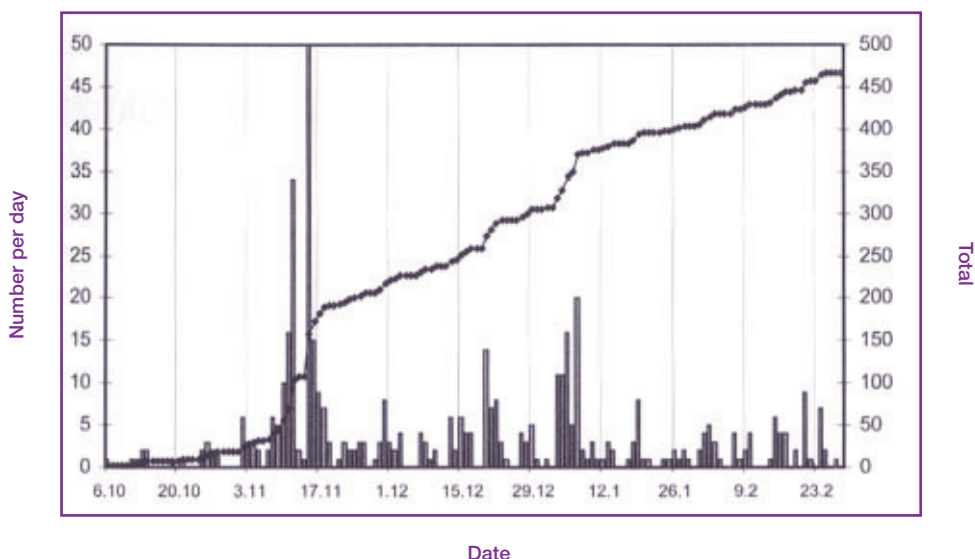
Nearly 80% of the 395 abstracts were almost error-free, at least if one ignores idiosyncratic ways of giving references. About 12% of the "difficult" abstracts were sorted by a short E-mail. The remainder did require a more or less intensive going-over. We are very grateful for the authors' good collaboration!

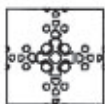
A glance at the registration statistics, however, shows that our members are rather lackadaisical over getting themselves registered! We hope that for future meetings they will give a little thought to the unhappy organizers, who do have to know the approximate numbers very early for such things as getting the right number of abstract books printed.

And a final observation: This year, during the meeting, Köln had the untypical average temperature of -2° !

The Organising Team DGK-, DGKK- & NK-ÖAW-Meeting Köln 2005

Progress of Registration of Participants





From SGK/SSCr Newsletter

Swiss Society for Crystallography:
Section for Crystal Growth and Crystal Technology
Annual Meeting 2005: Lausanne: Thursday, October 13
Auditoire 410, Collège propédeutique 2,
Université de Lausanne, Dorigny

General Theme Crystallography and Physics Programme

- 09.25 - 09.30 Welcome by the President Radovan Cerny, and the local organisers Gervais Chapuis and Marc Schiltz
- 09h30 - 10.20 Edgar Weckert, DESY, Hamburg: "The new radiation sources, PETRA III and the European XFEL at DESY"
- 10.20 - 11.10 Andras Sütö, Hungarian Academy of Science, Budapest: "Ab Initio structure determination by charge flipping"
- 11.10 - 11.50 Coffee break I Poster session.
- 11.50 - 12.10 Contribution from the University of Geneva
- 12.10 - 12.30 Contribution from the EPFL
- 12.30 - 14.00 Lunch I Coffee I Poster session

- 14.00 - 14.50 Jean-Louis Hodeau: CNRS Grenoble: "Resonant diffraction"
- 14.50 - 15.40 Franz Pfeifer (PSI, Würenlingen): "Coherent x-ray diffraction"
- 15.40 - 16.00 Selected poster presentation
- 16.00 - 16.40 Coffee break I Poster session
- 16.40 - 17.00 Contribution from the ETHZ
- 17.00 - 18.00 General Assembly of the Swiss Society for Crystallography
- 18.00 - 18.20 Information from the Swiss Steering Committee of the SNBL
- From 18.30 Aperó followed by Dinner at the Restaurant de Dorigny



Meetings of interest

Further information may be obtained from the website given. If you have news of any meetings to add to list please send them to the BCA Web Master cockcroft@img.cryst.bbk.ac.uk or to the Editor. The help of Dr Simon Parsons and the IUCr listing is gratefully acknowledged.

1-2 September 2005

Magnetism, Neutrons and High-Pressure.
Edinburgh
www.csec.ed.ac.uk/NSG_main.html

2-8 September 2005

Electron Crystallography School 2005 - ELCRYST 2005.
Brussels, Belgium
www.elcryst2005.de

4-6 September 2005

Annual Conference, British Association for Crystal Growth.
Sheffield
www.bacg.org.uk

4-7 September 2005

Neutrons in Biology - A Satellite Meeting of the IUPAB/EBSA Biophysics Congress.
Grenoble, France
www.ill.fr/neutbio2005/

5-15 September, 2005

9th Oxford School on Neutron Scattering - An ideal introduction to the theory, techniques and applications of neutron scattering to the study of condensed matter.
University of Oxford
www.isis.rl.ac.uk/conferences/osns2005/

7-9 September 2005

12th CCP4 Protein Structure Workshop.
Galashiels
www.ccp4.ac.uk/

8-10 September 2005

Neutron Spin-Echo Workshop 2005.
Institut Laue-Langevin,
Grenoble, France
www.ill.fr/YellowBook/IN11/NSE2005

9 September 2005

Neutron Research at NIST - A one-day symposium honouring Mike Rowe and Jack Rush.
Rockville, MD, USA
www.ncnr.nist.gov/nran/

13 September 2005

Control and Prediction of the Organic Solid State.
University College London
Information from:
l.s.price@ucl.ac.uk

15-17 September, 2005

Murnau Conference - Structural Biology of Molecular Recognition,
Murnau, Germany
www.murnauconference.de

22-23 September 2005

The 13th BENS Users' Meeting HMI.
Germany
www.hmi.de/bensc

22-24 September 2005

7th International Meeting on Single Nucleotide Polymorphism and Complex Genome Analysis.
Hinckley, Leics
snp2005.nci.nih.gov/

25-30 September 2005

ICXOM 2005 - 18th International Conference on X-ray Optics and Microanalysis.
Frascati Rome, Italy
www.lnf.infn.it/conference/2005/icxom/

29-30 September

Molsoft LLC ICM workshop: Protein Structure and Drug Design.
La Jolla, CA, USA
www.molsoft.com/training.html

3-7 October 2005

4th NCCR Practical Course - Synchrotron Data Acquisition Techniques in Macromolecular Crystallography.
Swiss Light Source, Villigen, Switzerland
www.structuralbiology.unizh.ch/course05.asp

6-7 October 2005

Watching the Action: Powder Diffraction at non-ambient conditions.
Max-Planck-Institute for Solid State Research,
Stuttgart, Germany
www.fkf.mpg.de/xray/

10-14 October 2005

Autumn School - Application of Neutron and Synchrotron Radiation in Engineering Materials Science.
Hamburg, Germany
www.tu-berlin.de/%7Eepnam/

13 October 2005

Swiss Society for Crystallography
Annual Meeting, Lausanne CH
www.sgk-sscr.ch

17-19 October 2005

3rd MECA SENS Conference on
Stress Evaluation by Neutron and
Synchrotron X-Ray Radiation.
Bishop's Lodge Resort,
Santa Fe, NM USA
[www.lansce.lanl.gov/
mecasens2005/](http://www.lansce.lanl.gov/mecasens2005/)

24-27 October 2005

ROG2005 - International
Workshop on Reflectometry,
Off-specular Scattering and
GISANS.
PSI, Villigen, Switzerland
[www.ill.fr/YellowBook/D16/
ROG2005/](http://www.ill.fr/YellowBook/D16/ROG2005/)

30 October 2005

International Workshop - Recent
Advances in Phasing Methods for
High-Throughput Protein Structure
Determination.
Peking University, Beijing, China.
www.ccs.pku.edu.cn/wp2005/

16 November 2005

CCG Autumn Meeting, Daresbury
Laboratory
www.crystallography.org.uk/ccg

19 November 2005

Canadian Light Source 8th Annual
Users' Meeting.
University of Saskatchewan,
Canada
[www.cls.usask.ca/enews/
upcomingevents.php](http://www.cls.usask.ca/enews/upcomingevents.php)

**27 November -
2 December 2005**

International Conference on
Neutron Scattering 2005.
Sydney, Australia
sct.gu.edu.au/icns2005

14 December 2005

PCG Winter Meeting, Centre for
Science at Extreme Conditions,
Edinburgh
www.csec.ed.ac.uk/pcg.htm

4-6 April 2006

BCA/BACG Spring Meeting.
University of Lancaster
www.crystallography.org.uk

10 May 2006

X-Ray Fluorescence meeting of
general interest, British Geological
Survey.
Keyworth, Nottingham
www.crystallography.org.uk/ig

9-18 June 2006

The Structure Biology of Large
Molecular Assemblies: The 38th
crystallographic course at the
Ettore Majorana Centre, Erice, Italy
crystalerice.org/futuremeet.htm

9-13 July 2006

SAS2006 - The XIII-th International
Conference on Small-Angle
Scattering. Kyoto, Japan
[www2.scphys.kyoto-u.ac.jp/
sas2006/index.html](http://www2.scphys.kyoto-u.ac.jp/sas2006/index.html)

22-27 July 2006

ACA 2006 - The American
Crystallographic Association
Annual Meeting (2006).
Honolulu, HI, USA
www.hwi.buffalo.edu/aca/

4-6 August 2006

ECM-23 Satellite Meeting on
Mathematical and Theoretical
Crystallography.
Leuven Belgium
[www.lcm3b.uhp-nancy.fr/
mathcryst/leuven2006.htm](http://www.lcm3b.uhp-nancy.fr/mathcryst/leuven2006.htm)

6-8 August 2006

23rd European Crystallographic
Meeting, Leuven BE
www.ecm23.be

13-18 August 2006

Sagamore XV: The fifteenth
international conference on
Electron Charge Spin and
Momentum Densities.
Bosworth Hall Hotel, Warwickshire
www.sagamore2006.com

28 August - 2 September 2006

Summer School - Ecole
thematique: Analyse structurale
par diffraction des rayons X,
cristallographie sous perturbation.
Nancy, France
[www.lcm3b.uhp-nancy.fr/
nancy2006/](http://www.lcm3b.uhp-nancy.fr/nancy2006/)

1-4 September 2006

EPDIC 10, European Powder
Diffraction Conference.
Geneva
[www.sgk-sscr.ch/EPDIC10/
EPDIC10.html](http://www.sgk-sscr.ch/EPDIC10/EPDIC10.html)

13-15 September 2006

ECRS 7 - The 7th European
Conference on Residual Stresses.
Berlin, Germany
www.ECRS7.de/

25-28 September 2006

PNCMI 2006 - The sixth
International Workshop on
Polarised Neutrons in Condensed
Matter Investigations.
Berlin, Germany
www.hmi.de/bensc/pncmi2006/

7-17 June 2007

Engineering of Crystalline
Materials Properties: the 39th
crystallographic course at the
Ettore Majorana Centre.
Erice, Italy
crystalerice.org/futuremeet.htm

22-27 August 2007

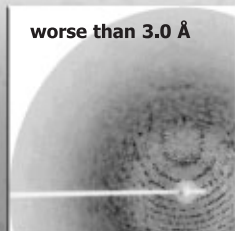
24th European Crystallographic
Meeting, Marrakech, MA
www.ucam.ac.ma/fssm/ecm24

Don't throw away that crystal

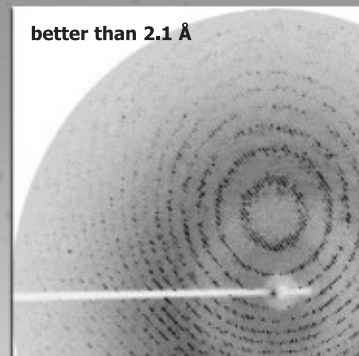
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Diffraction pattern of CODH crystal in native state (left) compared to FMS-processed and optimized pattern (bottom).



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