



FROM THE CHAIRMAN

The second issue of the Group Newsletter, which once again sees the light thanks to Ivana Evans' initiative, provides me with the opportunity for a quick review of this year's activities and of the plans for the year ahead.

PCG presence at the BCA 2007 Spring Meeting at the University of Kent was weighty in both quantity and quality, with three sessions on "Computational Methods in Crystallography", "New Science from Big Facilities" and "Disordered, Amorphous and Liquids", aptly introduced by an excellent plenary lecture on "Modelling and Predicting Structures of complex Solids and Nanoclusters" delivered by Richard Catlow. Picking from the rich scientific menu offered to the BCA attendees in Canterbury, I would also like to mention two lectures from distinguished past members of the PCG-SCMP Committee: Bill David (former Chair) delivered the Lonsdale Lecture, on "Combinatorial Studies of Hydrogen Storage Materials – playing the odds", and Chick Wilson (former Secretary) provided education and entertainment by lecturing on "Beans, Sausages and Pancakes: a Recipe for Understanding Thermal Motion in Crystals".

The AGM in Canterbury was, as usual, an opportunity for thanking retiring Committee members (Jon Wright, Mina Golshan) and welcoming new members (Andrew Goodwin and Andrew Wills, who was re-elected as an Ordinary Member). Professor Peter Hatton from Durham University was subsequently co-opted to the Committee and Helen Maynard from the University of Edinburgh has agreed to act as a liaison between the PCG-SCMP Committee and the Young Crystallographers Group.

This year's PCG prize winners were Lynne Thomas (PANalytical PhD Thesis Prize) and Alistar Davidson (PCG Poster Prize).

Winter is traditionally the busiest time for the year for PCG-SCMP. This year, we are proposing a new edition of the ever popular Magnetic Rietveld Workshop, which, exceptionally, will be combined with the PCG Winter Meeting, in the form of a day workshop on "New Techniques and Instrumentation for Magnetic Structure Solution".

This will provide a foretaste of the BCA 2008 Spring Meeting on "Structure, Property and Function", packed with PCG sessions, thanks to our very own Ivana Evans and John Evans who played a major role in setting the programme.

Finally, I would like to join the other Committee members in thanking John Finney for his distinguished service as the vice-chair of the BCA.

Paolo G. Radaelli
PGG-SCMP Chairman
p.g.radaelli@rl.ac.uk

ANNOUNCEMENTS

Physical Crystallography Prize 2008

Call for Nominations

The Physical Crystallography Prize is awarded for the best recently published work by a person in the early stages of their career, working in the field of Physical Crystallography, whose research is expected to make a significant impact in the field. The award is traditionally presented at the BCA Spring Meeting and the winner gives a Prize Lecture at that meeting. The Physical Crystallography Prize currently consists of a cash award of £1000 plus expenses for attending the Spring Meeting to deliver the Prize Lecture.

Nominations for the prize must be submitted to the Chair of the Physical Crystallography Group, Prof. Paolo Radaelli (p.g.radaelli@rl.ac.uk), by

1st April 2008 and the Prize will be awarded at the 2008 BCA Spring Meeting in York, 8-10th April 2008.

Thesis Prize 2008

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 1st September 2006 to 31st December 2007. 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 to progress their nomination further (current rate £10 per annum or £27.50 for 3 years of the PhD degree).

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 defined on the website www.pcg-scmp.org 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.

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.

Nominations for the prize must be submitted to the Chair of the Physical Crystallography Group, Prof. Paolo Radaelli (p.g.radaelli@rl.ac.uk), by 1st April 2008 and the Prize will be awarded at the 2008 BCA Spring Meeting in York, 8-10th April 2008.

Vacancies on the PCG-SCMP Committee

Call for Nominations

There are vacancies arising on the PCG-SCMP Committee for the positions of Chairman and Vice-Chairman. Nominations for these positions are invited and should be sent to the Honorary Secretary (m.g.tucker@rl.ac.uk).

Nominations should include the name of the proposer, the name of the seconder and the nomination acceptance by the nominee, confirming his/her willingness to contribute to the Committee efforts by actively participating in BCA and PCG-SCMP meetings, meeting organisation and our educational activities. Informal enquiries about the Officers' roles should be directed to the current Chairman (p.g.radaelli@rl.ac.uk).

Elections for these positions will be held at the Annual General Meeting of the PCG-SCMP, which will be held during the BCA Spring Meeting in York, on Wednesday, 9th April 2008.

NEWS

Prizes and Awards

The 2007 Lewy-Bertaut Prize of the European Crystallographic Association and the European Neutron Scattering Association was awarded to Henrik Rønnow of the Ecole Polytechnique Fédérale de Lausanne, Switzerland. Dr. Rønnow's research is focused on experimental and theoretical aspects of quantum magnetism (including spin dynamics in the two-dimensional magnet copper deuterioformate tetradeuterate (CFTD), manganites, germanates as well as the high T_c cuprates). The award was presented at the European Conference on Neutron Scattering in Lund, Sweden.

The PANalytical Thesis Prize in Physical Crystallography 2007 was awarded to Lynne Thomas (Cambridge) for her thesis entitled "Disorder in Substituted Benzenes by Combined Diffraction and Computational Studies". Reg Nicolls of PANalytical presented Lynn the award at the BCA Spring Meeting in Canterbury.

Software News – SARAh Update

For those interested in magnetic structures, there is a new version of the program SARAh.

SARAh is a suite of two programs that use the calculations of representational analysis to determine the different symmetry types of magnetic structure, and facilitate refinement of

the neutron diffraction data (with GSAS and FullProf) in terms of the results. As well as calculating the irreducible representations, SARAh contains those of the tabulated work of Kovalev.

Specific improvements include:

- Automatic updates (please allow SARAh to check for them through your firewall/virus checker)
- A rewritten routine that determines the type of k-vector in Kovalev's notation.
- Better translation of Kovalev's monoclinic space groups to those used today in the International Tables
- Output from both GSAS exp file and FullProf pcr file of a file for FullProf Studio, to allow simple visualisation of the magnetic structure
- Restructured help system with example pdf files
- Change of installer

Other features of SARAh are:

- Choice of source of irreducible representations- Kovalev or calculated
- Simple choice of International Tables convention space group
- Automatic identification of Kovalev's k-vector from the centred International Tables setting
- Detailed output of space groups, irreducible representations, basis function calculations in plain text and LaTeX format files
- A clip on front-end that allows reverse monte carlo refinement of magnetic structures in GSAS without need of the Shubnikov space groups
- Generation of example phases for a FullProf pcr
- Automatic editing of pcr file to facilitate exploration of trial structures with FullProf
- Output of FullProf Studio fst file from both GSAS exp file and FullProf pcr file
- Nice and simple Windows menu system

The new version is available from: www.ccp14.ac.uk

Please note:

Previous versions should be uninstalled before installation of the new version.

Other News

Prof. John Finney (UCL) has finished his term as the vice-president of the BCA. This has left the PCG-SCMP group without representation among the BCA officers and with only two representatives on the 17-member Council (Dr. Matt Tucker, ordinary member and Prof. Paul Fewster, co-opted member).

Prof. Peter Hatton (Durham) has been co-opted as a new PCG-SCMP committee member. Peter's interests are in the development of X-ray scattering techniques and scattering studies of strongly correlated electron systems such as transition metal oxides.

FUTURE EVENTS

Meeting Calendar

- Magnetic Rietveld workshop, 14-17th January 2008
- PCG Winter Meeting, 17th January 2008
- Powder Diffraction and Rietveld Refinement School, 30th March-3rd April 2008
- BCA 2008 Satellite: PDF Workshop, 7-8th April 2008, York
- BCA Spring Meeting, 8-10th April 2008, York

Magnetic Rietveld Workshop, 14-17th January 2008

This highly interactive workshop is aimed at providing the essential theoretical foundations and some working experience on solving and refining magnetic structures from neutron powder diffraction data.

The essential formalism of propagation vectors, Shubnikov groups and representation analysis will be covered in a series of lectures, and applied in tutorials sessions, with the help of computer programmes such as SARAh. Neutron instrumentation for magnetic powder diffraction studies will be presented, and refinement techniques using popular packages such as GSAS and FULLPROF will be discussed. The participants will have the opportunity to apply these methods on example data sets, and are highly encouraged to bring their own data, which will be analysed with the help of the tutors.

The team of lecturers and tutors will include Dr. Aziz Daoud-Aladine, Dr. Laurent Chapon, Prof. Paolo Radaelli, Dr. Juan Rodriguez-Carvajal and Dr. Andrew Wills.

The workshop will be held at the Cosener's House in Abingdon.

More information about the workshop, including the online registration page, is available at: <http://www.isis.rl.ac.uk/conferences/magneticdiffraction/2008/index.htm>.

You can also contact the local organiser Laurent Chapon (L.C.Chapon@rl.ac.uk) with any inquiries.

PCG Winter Meeting, 17th January 2008

The PCG Winter Meeting will take place at the Cosener's House in Abingdon, in conjunction with the Magnetic Rietveld workshop and will be entitled "Novel Instrumentation and Methods for Magnetic Structure Determination".

The programme will be advertised nearer the time on the PCG-SCMP wiki at: www.pcg-scmp.org

Powder Diffraction and Rietveld Refinement School, 30th March-3rd April 2008

The biennial Powder Diffraction and Rietveld Refinement School will take place in Durham, from 30th March until 3rd April 2008. The course will offer a combination of lectures covering the theoretical aspects of powder diffraction and Rietveld refinement, supported by extensive hands-on practical sessions using a variety of modern software packages.

Topics to be covered will include:

- Data collection strategies for X-ray and neutron diffraction
- Constant wavelength and time of flight diffraction
- Modelling peak shapes
- Indexing powder patterns
- Rietveld, Le Bail and Pawley fitting methods
- X-ray and neutron combined Rietveld refinement
- Restrained refinements
- Rigid body refinements

Examples and tutorials will cover both extended and molecular systems. Lectures will be given by Prof. John Evans, Dr. Ivana Evans, Dr. Jeremy Cockroft and Prof. Andy Fitch.

Online applications will be accepted from late 2007 at the School website: http://www.dur.ac.uk/john.evans/webpages/pcg_rietveld_school_2008.htm.

BCA Spring Meeting, 8-10th April 2008, York

The BCA Spring Meeting will take place from 8-10th April 2008 in York. The meeting is themed "Structure, Property and Function". Over three days, it will feature a number of scientific sessions of interest to a wide condensed matter community, solid state chemists, physicists and materials scientists alike.

The PCG plenary lecture, entitled *Charge Order in Oxides - Putting the Fun into Functional Materials*, will be given by Professor Paul Attfield (University of Edinburgh).

Symposia titles include:

- Local structure and disorder in crystalline materials
- Strongly correlated electron systems
- Crystal chemistry of functional molecular materials
- Crystal chemistry of functional extended solids
- Design of solid state functional materials
- Deriving property from structure
- Applications of powder diffraction to pharmaceutical materials

Call for abstracts for oral presentations has been issued. There are slots reserved in each of the symposia listed above for contributed talks. Please submit abstracts for consideration using the word template (available from the conference website at: <http://www.crystallography-meetings.org.uk/abstracts.htm>) by Friday, 28th September. Applicants will be informed by 25th October whether their talk has been accepted.

The full scientific programme, further details about the conference and the form for online abstract submission can be found at: www.crystallography-meetings.org.uk

BCA 2008 Satellite: PDF Workshop, 7-8th April 2008, York

Matt Tucker (ISIS) and Thomas Proffen (LANSCE) will run a full day hands-on PDF workshop.

The importance of local structure and disorder in crystalline materials is increasingly being recognised as a key property of many functional materials. From negative thermal expansion to solid state amorphisation and the 'nanoscale' problem to improved fuel cell technology, a clear picture of the local atomic structure is essential to understanding these phenomena and solving the associated problems.

A powerful technique for exploring the local structure of materials is total scattering, also known as the PDF method. Synchrotron X-ray and/or neutron powder diffraction data can be used to obtain information on the local, medium and long range atomic structure simultaneously. To gain the maximum information from the data, specialised refinement methods are required. Two of the most powerful methods currently available for refining this type of data are RMCPProfile and PDFFIT.

The aim of this workshop is to provide an overview of the methods and the opportunity to gain some hands-on experience of applying them to total scattering data. No previous experience is required.

For more information about the workshop please email Matt Tucker (m.g.tucker@rl.ac.uk) or Ivana Evans (ivana.radosavljevic@durham.ac.uk).

YOUNG CRYSTALLOGRAPHERS

YC Meeting, 7th April 2008, York

I'd like to take this chance to recommend to all young crystallographers (Ph.D. students and those in their first two post-doc positions) to attend the YC satellite meeting just before the BCA spring meeting in York, 2008. The idea of the meeting is to provide an opportunity for you to present your work in a friendly and un-hostile setting, in front of people who are in the same boat as you. It's also a great opportunity to meet new people (starting your own network connections) and to see what sort of work is going on out there.

The format will be the same as last year (http://bca.cryst.bbk.ac.uk/BCA/YC/homepage_files/Page563.htm) and is free to register for, so what'll be stopping you?

Science Policy Internships

Are you interested in science policy? Does the prospect of pitching your science to the great and the good appeal to you? In that case, you may be interested in applying for an internship with the parliamentary office of science and technology (POST), based in Westminster.

EPSRC funded PhD students can apply through this research council until 5th October 2007. SCMP members can apply through the Institute of Physics, with the closing date on 26th October 2007.

Further details of the scheme and links to application forms can be found at:

http://www.parliament.uk/parliamentary_offices/post/about6.cfm.

YC Contact

As the representative for the PCG-SCMP on the Young Crystallographers committee (and the representative for young crystallographers on the PCG-SCMP committee), if there is anything that you would like brought up, or indeed any more information that you would like please let me know.

Helen Maynard, Edinburgh University
(h.e.maynard@sms.ed.ac.uk.)

RECENT EVENTS

BCA Spring Meeting, 17-19th April 2007, Canterbury

The week started very early on Monday morning to arrive in time for the start of the Young Crystallographer's (YC) satellite meeting. The newly-formed 5th special interest group of the BCA is still in its infancy, but the number of high-quality oral and poster presentations clearly demonstrates that the younger BCA members are helping to take the association forward. This session provides an opportunity for postgraduates and first term postdocs to present and discuss their work in a relaxed environment surrounded by people in a similar position.

The YC keynote talks by Roy Copley and Andres Goeta were of particular interest. Roy showed how varied and complementary techniques were used within the pharmaceutical industry to solve both compound structures and problems as they are discovered within production, particularly with respect to crystallisation and polymorphism. Andres gave us a useful teaching session on the use of low temperature crystallography, with particular reference to in-situ powder and single crystal techniques used to study spin crossover compounds.

As the main meeting commenced, we attended the "New Science from Big Facilities" session. Richard Ibberson outlined some of the recent work undertaken at HRPD, OSIRIS and GEM and also gave us insights into future possibilities. The improved facilities at HRPD following the current super-mirror guide upgrade should greatly improve the flux available at the station, particularly at short d-spacings; this will be greatly beneficial to research where very small changes in structure result in small changes to the diffraction patterns, changes that may remain unresolved on lower resolution instruments.

Our research also makes use of solid state NMR. Some of the relevant sessions were on glasses (we have some delightful amorphous samples!) and also some talks on computational methods. We are interested in combining both X-ray and NMR data in order to solve complex inorganic structures.

We especially enjoyed the Bragg Lecture, given this year by Professor Sir Roger Penrose. The fields of quasi-crystals and disorder within crystal systems are expanding rapidly, and Professor Penrose's lecture gave us much to think about by combining symmetry and crystal growth with quantum theory.

The campus at Kent was scenic and with the cultural centre of Canterbury being near by, it made for a wonderful location. The conference was organised very well, making the 4 day meeting very enjoyable. Thankfully, the weather was very warm throughout the conference, and we hope that next year's conference in York will be as successful.

Anne Soleilhouvop and Sarah Lister
Durham University

Developments and Directions of Powder Diffraction on Proteins, 22nd-23rd June 2007, Grenoble, France

45 participants from 14 different countries came together in Grenoble this summer to discuss the use of powder diffraction with proteins. The meeting was opened by Sine Larson, director of research at the ESRF, France, who highlighted the importance of synchrotron radiation for diffraction studies and welcomed the participants to Grenoble.

Our first scientific presentation was fittingly given by Bob Von Dreele (APS, USA), who has done so much of the pioneering work on powder diffraction with proteins. Bob gave an excellent explanation of how he came to be working on protein structures from powder data. Trials began with "in-silico" based tests on simulated data, then progressed to real experimental data, and with the addition of a series stereo-chemical restraints, it is now routinely possible to refine protein structures using GSAS.

Celine Besnard (EPFL, Switzerland) showed some exciting progress in using isomorphous replacement techniques with powder data. By using data from several heavy atom derivatives electron density maps can be obtained which show clear secondary structural features.

Despite the beautiful powder profiles which can be obtained at a synchrotron, many scientists

still find it more convenient to collect data in the home laboratory. Detlef Beckers (Panalytical, The Netherlands) showed that a useful profile can be obtained in around 10 minutes using a focussing geometry, which of course improves with longer counting times. Screening of plates containing ~1 mg samples is already possible. Automatic peak searches and indexing algorithms were able to find the correct unit cells for several examples of small proteins, and the data can also be used for Rietveld refinements of the protein structure.

John Helliwell (Manchester, UK) described progress towards the application of MAD techniques with powder data. When using a single crystal and anomalous diffraction one can measure the Friedel differences $F(h,k,l)$ and $F(-h,-k,-l)$, however, with a powder these reflections are completely overlapped! Nevertheless, by exploiting the dispersive differences in f' , phasing might still be possible.

Keiko Miura (Spring8, Japan) reported on the progress with the "Large Guinier Camera", which is a 1 meter radius image plate instrument that is optimised for large unit cells. Excellent quality powder profiles have been collected with sharp peaks and superb counting statistics. The data have been used for indexing and structure refinements and also for a "2D" crystal structure of a purple membrane protein.

The extra challenge in powder diffraction comes from the overlap of the peaks when 3D reciprocal space is collapsed into the single dimension of a powder pattern. Jon Wright (ESRF, France) talked about this overlap problem and the ways in which we can use anisotropic unit cell changes or preferred orientation to untangle the overlapped peaks. Problems which arise from peak overlaps in twinned crystals are very similar to the powder case and so this leads to hope that software packages for single crystal and powder diffraction may find more common ground in the future.

Irene Margiolaki (ESRF, France) talked about experimental phasing using multiple isomorphous replacement with dispersive differences and powder data. By using data collected near the absorption edges of a series of derivatives with different concentrations of heavy atoms, the phasing power can be significantly improved in comparison to a single derivative. A robotic sample changer combined the high resolution data available at the powder diffraction beamline (ID31) at the ESRF helped to make these studies possible.

In recent years, one of the major players in structure solution methods for small molecules

with powder diffraction data has been the EXPO software package. Carmelo Giacobozzo (Bari, Italy) described the progress which has been made in adapting this suite to be applied to proteins. Already it is possible to carry out automatic indexing and also space group determination successfully in a number of test cases. Molecular replacement also works using the Remo software, which accounts for peak overlaps.

Bernd Hinrichsen (Bruker, Germany) described the charge flipping algorithm and how it can be applied to powder data. By using the tangent formula within the charge flipping algorithm the performance can be improved. Impressive results have already been obtained for several small molecule and inorganic examples.

Thomas Degen (Panalytical, The Netherlands) tackled the problem of high throughput data analysis. By using Cluster analysis it is possible to rapidly and automatically classify powder profiles coming from screening experiments. These classification methods can also be integrated with automatic indexing and Le Bail fits to perform phase identification.

Lanthanide complexes can generate enormous Bijvoet ratios at low resolution and Richard Kahn (IBS, France) described a series of different organometallic compounds which have been used for phasing protein structures. With single crystal data these derivatives lead to superb maps even from laboratory diffractometer based data.

Micheal Kokkinidis (IMBB-Forth, Greece) showed how a host of different structural tools have been applied to the structure of the Bacterial type III secretion system. Different length scales are covered, from electron microscopy studies of the needle like structures used to inject pathogens into cells, down atomic detail in the crystal structures of the individual proteins. The use of solution scattering (SAXS) and molecular dynamics are also critical to understanding the function of flexible proteins.

Nikos Pinotsis (EMBL, Germany) described how the structure of the second SH3 domain of Ponsin has been solved using powder diffraction data. This protein spontaneously formed microcrystals during purification. A set of intensities extracted from powder data were sufficient for molecular replacement and model building from a starting model with 40% sequence homology. The 544 atom structure contains 67 amino acids and 36 water molecules and was later found to agree with a single crystal analysis.

Mathias Norrman (Novo Nordisk, Denmark) explained that medical formulations of insulin often contain micro-crystals and that insulin is stored in micro-crystalline form in the pancreas. Powder methods are particularly applicable in this case, as the native state is also the crystalline state. Principal Component Analysis has been used for phase identification and also to identify new crystalline forms.

Likelihood methods applied to powder data were described by Anders Markvardsen (ISIS, UK). These approaches allow errors in a model to be described mathematically, together with the errors on the data coming from both counting statistics and peak overlaps. Applications included the computation of rotation functions for molecular replacement and also the extraction of integrated intensities from powder profiles.

Bill David (ISIS, UK) explained how the powder overlap problem is equivalent to a "hyper"-phase problem. For small molecule structures this problem has largely been overcome using multi-dimensional searches, in software like DASH, where a likelihood based figure of merit has already been tested. Bill also showed the dramatic improvements in Fourier maps which can be obtained using maximum entropy algorithms.

Ralf Grosse-Kunstleve (LBL, USA) described the many components which go together to make up the computation crystallographic initiative and the phenix.refine software. There are already many features present; for example simulated annealing, handling of twinning and joint x-ray and neutron refinement. With the current active development of this package it might be possible in the future to include powder data also.

Jordi Rius (CSIC, Spain) showed how an FFT algorithm can be used for phase refinement together with the origin free modulus sum function. This approach has been successfully applied with powder data for several framework materials and can also be used for substructures.

One of the difficulties with powder data and molecular replacement is that there is no unique Patterson function, due to peak overlaps. Nicholas Glykos (Thrace, Greece) showed how this problem might be avoided in the Queen of Spades program which carries out simulated annealing by comparing the data to the model in reciprocal space.

Garib Murshudov (York, UK) showed how twinning can be handled with single crystal data. The developments lead to the possibility to handle unmerged data, split crystals and also twinned crystals. It seems that accounting for

twinning improve crystallographic R-factors more than the electron density maps.

Marc Schiltz (EPFL, Switzerland) gave excellent summary of progress in powder diffraction with proteins so far. Applications to materials science, structure refinements, molecular replacement and ligand binding have already been well demonstrated. There is a window of opportunity for powder methods to access crystallite sizes smaller than those allowed by radiation damage effects at micro-crystal diffraction beamlines (eg about 20 microns).

Throughout the workshop we enjoyed many lively discussions and these continued during a dinner at “La Panse” in downtown Grenoble. There were many interchanges of ideas and we look forwards to seeing even more progress in this exciting area in the next few years.

Irene Margiolaki and Jon Wright,
ESRF

ACKNOWLEDGEMENT

Many thanks to everyone who contributed to this issue of the PCG-SCMP Newsletter.

Ivana Evans
Durham

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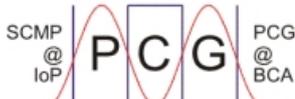
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Third Workshop on



Magnetic Structure Determination from Neutron Diffraction Data

14th -17th January 2008

The Cosener's House Abingdon (UK)

Theory of Magnetic Scattering
Magnetic Shubnikov Groups
Representation Analysis
Rietveld Refinement
Refinement of Single Crystal Data

Confirmed Speakers:
Dr A. Daoud-Aladine
Dr. L.C. Chapon
Prof. P.G. Radaelli
Dr. J. Rodriguez-Carvajal
Dr. A.S. Wills

www.isis.rl.ac.uk/conferences/magneticdiffraction/2008