



SCMP @ IoP PCG @ BCA

Newsletter

Spring 2008

FROM THE CHAIRMAN

The Spring 08 issue of the PCG-SCMP group Newsletter is also the last to which I will contribute as Chair of the Group (my term of office ends in April). This Editorial is therefore a good opportunity for me to draw a balance of our work and achievements over the last three years, and to illustrate some of the lessons we learned, hopefully to the benefit of the new Officers.

The past winter has again been a period of intense activity for the PCG-SCMP group. For the first time, we were able to organise three major training events – the 3rd edition of the Magnetic Structure Workshop, which took place at the Cosener's House on 14-17th January 2008, the Powder Diffraction and Rietveld Refinement School, which is about to kick off on March 30th to April 3rd 2008 and the BCA 2008 Satellite: PDF Workshop, which will take place on 7-8th April 2008 in York. In conjunction with the Magnetic Structure Workshop, we also held the PCG-SCMP Winter Meeting, which was focussed on magnetic neutron and X-ray magnetic diffraction, giving the Workshop attendees the opportunity to hear about state-of-the-art applications of the techniques they have been learning over the previous days (for more details see articles in this Newsletters).

Looking back at these workshops and also to their previous editions over the period of my tenure as Chair of the group, I can say with confidence and with a considerable amount of collective pride, on behalf of the Committee, that our decision to invest in education has paid handsomely. By organising these activities, which always require a very significant investment of personal time, the Group Officers and the teachers/instructors they manage to attract to the Schools have provided an extremely valuable service to the Structural Condensed Matter community as a whole. The young UK and overseas students who attended

and will attend these events will form the backbone of the next generation of Facilities users, and will provide the key human component required to deliver returns on the considerable infrastructure investments in this field.

The upcoming BCA 2008 Spring Meeting on "Structure, Property & Function" will also be a major showcase for the PCG science, with one Plenary and five Parallel Sessions in addition to the Satellite PDF workshop (see related articles in this issue). I am extremely pleased with the quality of the speakers we were able attract to York this year and I have no doubt that these sessions would not be out of place in a major international topical conference. Here again, looking back at my tenure as a Chair of the group, I am convinced that the quality of our activities in the field of structural science dissemination have always been excellent. However, I must also take stock of the fact that neither the BCA conference nor the CMMP conference, to which we actively and enthusiastically contributed over the years, have quite managed to become the national focal points we were hoping to create for our constituencies. The ambition of PCG-SCMP is to represent the UK community employing physical structural science as a principal tool. This community is large and diverse, spanning aspects of physics, chemistry and materials science, and has an internationally recognized track record of excellence, yet is still does not have a UK "home". Completing this home will be one of the main tasks of the next Committee. And on this note I conclude, inviting you to participate in this process by electing the new Chair and Vice Chair at the next AGM (at the BCA Spring Meeting in York, on Wednesday, 9th April at 11:45).

Paolo G. Radaelli
PCG-SCMP Chairman

ANNOUNCEMENTS

There are still a few days left to nominate someone or get yourself nominated for one of the two PCG-SCMP Prizes. The deadline for nominations for both Prizes is Friday, 14th March 2008.

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 14th March 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 14th March 2008 and the Prize will be awarded at the 2008 BCA Spring Meeting in York, 8-10th April 2008.

FUTURE EVENTS

Meeting Calendar

- Neutron & Muon User Meeting, 18-19th March 2008, Nottingham
- Powder Diffraction and Rietveld Refinement School, 30th March-3rd April 2008, Durham
- BCA 2008 Satellite: PDF Workshop, 7-8th April 2008, York
- BCA Spring Meeting, 8-10th April 2008, York
- XXI IUCr Congress and General Assembly, 23rd-31st August 2008, Osaka, Japan
- 11th European Powder Diffraction Conference (EPDIC), 18-22nd September 2008, Warsaw, Poland

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 & 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) on **Wednesday, 9th April, 9:00-9:45**.

PCG parallel sessions include:

Local Structure and Disorder in Crystalline Materials (Tuesday 8th April, 13:30-15:00)

This session will focus on total scattering methods which aim to obtain information on both long and short range order. For many functional materials structural knowledge on a range of length scales is vital for understanding their properties.

13:30-14:00: Thomas Proffen (Los Alamos Neutron Science Center): *Total Scattering: the Key to Understanding the Local- and Medium-Range Structure of Materials*

14:00-14:30: Sharon Ashbrook (St Andrews): *Investigating Local Structure and Disorder by MAS NMR*

14:30-14:45: Simon Hibble (Reading): *Not So Simple: The Structures and Dynamics of Simple Transition-Metal Cyanides from Total Diffraction*

14:45-15:00: Alex Hannon (ISIS): *Polyhedral Distortion in Glasses and Crystals*

Crystal Chemistry of Functional Extended Solids (Wednesday 9th April, 10:15-11:45)

Properties of solid state materials and their functionalities are inherently related to their crystal structures. This session will highlight examples of structure-property relationship studies in extended solids, such as inorganic oxides and chalcogenides.

10:15-10:45: Peter Slater (Surrey): *Relationship between Structure and Conductivity in New Ionic Conductors*

10:45-11:15: Edmund Cussen (Strathclyde): *Switching on Fast Lithium Ion Conductivity: Structure and Transport Properties of the Garnet Structure*

11:15-11:45: Ian Reaney (Sheffield): *Crystal Chemistry of Dielectric Ceramics*

Functional Molecular Materials II (Wednesday 9th April, 15:30-17:00)

The field of molecule-based materials has seen a very rapid progress since the discovery of compounds with a variety of technologically important properties such as conductivity, superconductivity and ferromagnetism. One of the major opportunities offered by this area is the possibility of designing building blocks which combine properties allowing the preparation of multifunctional materials. This session will focus on the new discoveries and achievements in the field.

15:30-16:00: Kosmas Prassides (Durham): *Fullerene Superconductivity: Are There Any Surprises Left?*

16:00-16:30: Darren Bradshaw (Liverpool): *Pressure-Dependent Hysteretic Sorption Behaviour in a Flexible Metal-Organic Framework*

16:30-17:00: Alessandro Prescimone (Edinburgh): *High Pressure And Magneto-Structural Correlations in Single Molecule Magnets*

Strongly Correlated Electron Systems I (Thursday 10th April, 10:15-11:45)

Strongly correlated systems where changes in structural properties are intimately linked with changes in electronic/magnetic properties remain an extremely topical area in condensed matter physics. These sessions will cover various aspects of this field such as multiferroics, materials displaying charge ordering, materials with electronic and or magnetic phase transitions and GMR materials.

10:15-10:45: Des McMorrow (UCL): *XRS Study of the Electric Control of Chiral Magnetic Domains in Multiferroic TbMnO₃*

10:45-11:15: Claudio Mazzoli (ESRF): *New Magnetic Spin State Evidenced by XRS in a Frustrated Spin System*

11:15-11:45: Martin Lees (Warwick): *Magnetic Order in Ca₃Co₂O₆*

Strongly Correlated Electron Systems II (Thursday 10th April, 12:00-13:30)

12:00-12:30: Radu Coldea (Bristol): *Charge Order to Remove Orbital Degeneracy in Triangular Antiferromagnet AgNiO₂*

12:30-13:00: Neil Mathur (Cambridge): *Limited Local Electron-Lattice Coupling in Manganites*

13:00-13:30: Alan Tennant (Hahn-Meitner Institut): *Patterning of Sodium Ions and the Control of Electrons in Sodium Cobaltate*

The full scientific programme and further details about the conference 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 (LANSCÉ) 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 RMCProfile 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).

PCG-SCMP AGM

The PCG-SCMP Annual General Meeting will be held during the BCA Spring Meeting in York, on Wednesday, 9th April at 11:45. Elections for positions of the Committee Chair and Vice-Chair will be held at the AGM.

YOUNG CRYSTALLOGRAPHERS

YC Meeting, 7-8th April 2008, York

The Young Crystallographers satellite will be held 7-8th April 2008, prior to the main meeting in York. It will follow the familiar format of sessions starting with a plenary lecture, followed by 15-minute contributed talks.

Further details of the satellite and the full scientific programme can be found at the group web pages via: www.crystallography.org.uk.

NEWS

Beamline News

Diamond Beamline I11: High-Resolution Powder Diffraction

Beamline I11 is a dedicated powder diffraction instrument at Diamond Light Source. An in-vacuum undulator placed inside the SR machine will provide an intense and highly collimated X-ray source and with the necessary optics, a high purity beam of low energy-bandpass X-rays in the range 5 - 30 keV will be delivered at the sample. The double-crystal monochromator (Si111), harmonic rejection mirrors, white beam slits and other auxiliary components are housed in the optics hutch. In the experimental hutch a large heavy duty 3-circle diffractometer (θ -, 2θ - and δ -circle) has been installed for the mounting of two detection systems to collect high quality diffraction data, i.e. multi-analysing crystals for high angular resolution experiments ($\Delta d/d \sim 10^{-3}$ - 10^{-4}) and a fast position sensitive detector for time-resolved studies ($\Delta t \sim$ ms-s). Powder specimens in capillaries, flat-plate holders or small sample cells can be attached onto a small xyz-table which is mounted on the inner θ -circle. Larger sample cells and stages are mounted on a large moveable sample table. High sample throughput (200 samples, capillary) is available via robotic arm.

When operational, the beamline will be a powerful user facility for high resolution (d -space and time) diffraction studies of polycrystalline materials under ambient and non-ambient conditions. At present the commissioning of beamline components with X-ray beam is underway and it is on schedule to receive users in the next beamtime allocation period, AP4 (October 2008 - March 2009). Please refer to the website

<http://www.diamond.ac.uk/ForUsers/Welcome> for information regarding application procedures.

More technical details about the beamline can be found at

<http://www.diamond.ac.uk/Beamlines/Beamlineplan/111/default.htm>.

I11 Beamline Scientists are: Chiu Tang (c.c.tang@diamond.ac.uk), Steve Thompson (s.p.thompson@diamond.ac.uk) and Julia Parker (j.parker@diamond.ac.uk).

Chiu Tang, Diamond

Diamond Beamline I16: Materials and Magnetism

During the past 15 years, UK researchers with interests in magnetic X-ray scattering and studies of weak electronic ordering phenomena have had to travel to the ESRF in Grenoble to carry out experiments using the high-flux X-ray beams available from Third Generation Synchrotron Light Sources. Now the UK has its own world-class Third Generation Source, in the form of Diamond, which celebrated its completion, on-time and budget, when it welcomed its first users in January 2007.



Professor Brian Tanner (Durham University Physics Department) on Diamond Beamline I16 in January 2007

One of the first ('Phase-I') beamlines is I16, which is optimised for high-resolution studies of weak resonant and non-resonant scattering arising from magnetism, charge and orbital ordering, and other exotic processes which occur at spacegroup-forbidden settings.

The beamline can provide X-ray beams of intensities similar to those of ESRF undulator sources, with a focus size of less than 50 × 200 microns, tunable from 3 - 15 keV. A large, high-resolution six-circle kappa diffractometer provides a very open geometry and can support a range of sample environments, including several cryostats with a temperature range between 4 and 800 K. Polarisation can be

manipulated with a diamond phase retarder to produce either horizontal (linear) or circular beams. A linear polarisation analyser is also available to study the polarisation state of the scattered or transmitted beam.

The potential applications of the beamline are actually far wider than its name would suggest. Typical projects carried out and planned for the near future include some of the current 'hot topics' such as multiferroics, along with studies ranging from new resonant phenomena in X-ray physics (thermal motion induced scattering, resonant Borrmann effect), coherent diffraction, polymer films and strain scanning.

For more information on the beamline see the Diamond web site: <http://www.diamond.ac.uk> or contact steve.collins@diamond.ac.uk. The next proposal deadline is 1st April 2008.

Steve Collins, Diamond

Diamond Beamline I19: Small-Molecule Single-Crystal Diffraction

The method of choice for determining the structure of a crystalline solid is single crystal diffraction. Accurate structure determination is vital for understanding the properties of a material and the way in which it functions. Any material which can yield single crystals of sufficient quality and size can be probed using this method. As sources become more powerful and as the methodology and instrumentation become more advanced, it is possible to study crystals of decreasing quality and size, thus making the technique viable to an increasing number of systems which were previously very difficult, if not impossible, to study with single-crystal techniques.

The use of synchrotron radiation for single crystal diffraction is necessary when structures are too complex, or crystals are of insufficient quality or size to allow structure determination from the relatively low intensity of a laboratory X-ray diffractometer. The advantages of synchrotron radiation have been amply demonstrated by station 9.8, and latterly 16.2, at the SRS Daresbury Laboratory where structure determinations have been achieved from samples that would have previously proved intractable on conventional laboratory sources. Building on this achievement, a successful bid was made in 2003 for the construction of a dedicated small-molecule single-crystal X-ray diffraction beamline at the Diamond Light Source (the new synchrotron facility at the Harwell Science and Innovation Campus), and since

then the design and development of the beamline, designated I19, has been moving apace.

The station has been designed to have an optics hutch and two experimental hutches, set up in tandem. The first experimental hutch (EH1), which will be operational from October 2008, is designed for more conventional structural studies and will have a high-throughput mode of operation. The hutch will house a diffractometer with a conventional CCD detector and a robotic sample changer to allow a rapid cycling of samples. It is envisaged that there will be a high-degree of automation in the screening of samples, data collection and the subsequent data analysis. However, this mode of operation will not be fully implemented until the robot is fully commissioned by early 2009. There will be limited scope for specialised sample environment equipment with the EH1 diffractometer, although it will be possible to use small sample cells such as diamond-anvil cells, and most studies will be limited to the use of open-flow cryo-devices either using nitrogen or helium. To increase the scope of structural science supported by I19, the second experimental hutch (EH2) will house a larger diffractometer and will be available during the following allocation period (from April 2009). It is this diffractometer, with its greater flexibility, that is likely to be of more interest for physical crystallography experiments. The EH2 diffractometer will be initially equipped with a conventional CCD detector and a purpose-built fast area detector will be provided as a later upgrade. The EH2 diffractometer will take a range of heavy environmental cells either provided by DLS, such as a closed cycle cryostat, or designed by the user. Equipment for excited state crystallography experiments is currently being designed for commissioning in this larger hutch next year. The two hutch system will allow complex experiments to be set up in the second hutch while allowing the beam to be used in the first hutch, thus optimising beamtime allocations.

Beamline I19 is included in the next call for direct access mode applications, which is now open with a deadline of 1st April 2008. This will be for the fourth allocation period AP4 (period October 2008-March 2009). Proposals can be discussed in advance with the Principal Beamline Scientist Dave Allan (david.allan@diamond.ac.uk) or Beamline Scientist Harriot Nowell (harriott.nowell@diamond.ac.uk).

Dave Allan, Diamond

RECENT EVENTS

Magnetic Structure Workshop, 14-17th January 2008

The challenge faced by researchers, both new and experienced, to studies of magnetism and magnetic structures are considerable. The drive to ordering can lead to unexpected structures that lie at the heart of a material's magnetic properties. Many are captivated by systems that possess competing interactions - these are said to be frustrated, or the coupling between magnetic and electric dipole ordering in multiferroics. Such delicate plays between energies may be first evidenced and characterised by phase diagrams decorated with equally subtle magnetic structure.

The biannual PCG/ISIS workshop on magnetic structure determination provided a rare opportunity to go through the basics of what magnetic structures are, their different types and how they can be described and determined. The language follows that of the physicist because descriptions built from the relevant physics lead to an underlying elegance of the mathematics and the clearest reflection of the physical processes involved. There could be no apology for the sessions being filled with terms such as Bloch waves, propagation vectors, representations and basis functions, as these form the foundation of what magnetic structures are.

The international make-up of the participants affirms the interest and the importance of the subject. The tutors were Juan Rodriguez-Carvajal (ILL), Paolo Radaelli (ISIS), Laurent Chapon (ISIS), Aziz Daoud-Aladine (ISIS) and Andrew Wills (UCL). The workshop began with a summary of the different types of diffractometer available (PR) and the mathematics of the diffraction process (PR, ADA) before the first practical workshop on the indexing the magnetic reflections (JRC). Use of FullProf Studio (LC) allowed simple visualisation of different magnetic structures and an opportunity to become familiar with the Fourier summations that express their language.

The second day took representations from the world of molecular spectroscopy to crystals (LC and ADA) and then to magnetic structures (ASW). These symmetry calculations are daunting to most researchers, not because they are particularly complex, but because they can be long. As programs such as SARAh (ASW) and BasiReps (JRC) perform them in a matter of seconds, care was taken to introduce concepts that will become clear when the participants begin to study their own systems. Introductions

to these programs and using them to aid refinements with GSAS and FullProf were also given.

The third day explored the use of Shubnikov space groups (PR). These symmetries are an extension of the space groups familiar to crystallographers and offer opportunities to visualise the interplays between the different symmetries in magnetic structures. The reader is cautioned that they are a limited symmetry description and representational theory if far more general: a statement that was repeated many times at the workshop (!), and exemplified by an example of a refinement using both GSAS and the results of representational theory (ASW).

Andrew Wills, UCL

Magnetic Structure Workshop, 14-17th January 2008: From a Student Perspective

In the second week of January, (probably most peoples first week back after the Christmas break), approximately 25 participants arrived at Cosener's House, Abingdon for the 3rd workshop to be held there on "Magnetic Structure Determination from Neutron Diffraction Data", organised by the Physical Crystallography group of the BCA and the ISIS facility. The group consisted of just under 50% UK based participants, a small handful of US researchers, with the remainder being made up of European researchers. This brought a wide range of different levels of experience in magnetic Rietveld refinement to the course, with a rough 50:50 split of GSAS and FullProf users (the two most widely used magnetic Rietveld refinement programs).

The first morning saw a leisurely introduction to the basic strategies of data collection for magnetic Rietveld, basic formulae and why people often choose powder over single crystals, (or more to the point why they often have no choice). The afternoon consisted (after a smallish introduction) of solving solutions without symmetry using simulated annealing and visualising these with FPStudio program (Laurent Chapon).

The second day of the course had some of us wondering if we would be getting wet feet from the rather high Thames at the bottom of the Cosener's House gardens, but crack on we did with symmetry concepts and representational analysis. A particularly useful tool of SARA h (Andrew S. Wills) was introduced which from first experiences seemed to make things a lot easier!

In the evening several participants took the opportunity to present flash presentations of what they are studying in their research.

The final day of the course saw the introduction of Shubnikov symmetry and how it can be implemented in the GSAS program. The afternoon was then spent devoted to the students' own problems brought with them, before a formal dinner was held (less formal than previous nights, but with wine provided...) at Cosener's. The remainder of the evening was spent by many in the local pub, mainly glad that the following morning had a leisurely start due to the commencement of the Physical Crystallography Group Winter Meeting.

Overall the course proved a great success, despite the clear gulfs in experiences of the different refinement software between the European and UK/US split. As was announced at the end, it is a rare opportunity that both heads of the diffraction groups of ISIS (Paolo Radaelli) and ILL (Juan Rodriguez-Carvajal) are available to pass their experience to students on a course.

Adrian Hill, Edinburgh University

PCG Winter Meeting, 17th January 2008

The PCG Winter Meeting took place on the final day of the Magnetic Structure Workshop. The participants heard a collection of talks that expanded on the concepts introduced in the workshop, showing some of the challenges faced by the modern researcher.

Starting the day Oleg Petrenko (Warwick) gave a summary of recent work on the kagomé staircases $\text{Ni}_3\text{V}_2\text{O}_8$ and $\text{Co}_3\text{V}_2\text{O}_8$. As well as giving an excellent overview of the diffraction and specific heat studies required to build a picture of the complex magnetism in these materials, his talk served to introduce the subject of frustration that was continued by the following speaker Tom Fennell (UCL), this time detailing the fantastic intricacies of the spin ice pyrochlores.

A key take-home message for the meeting is that magnetic structures are subtle, and that thought and care needs to go into their study. This was beautifully shown in a presentation by Jane Brown (ILL) and outstanding introduction to Spherical Neutron Polarimetry, as realised by CRYOPAD. Her tour through its use showed well how even the simplest of systems can still hold

questions that may only be answered by considered and careful experiment.

The meeting was closed by Alessandro Bombardi (Diamond) and a moment away from the dominance of neutron diffraction as a tool for the study of magnetic structures. Alessandro introduced the use of resonant and non-resonant X-ray scattering in V_2O_3 and $HoMn_2O_5$ showing how the orbital and spin contributions of the transition metal and rare earth can be probed through the different resonances. The final of many inspirational talks that were comfortably before the next set of proposal deadlines!

Andrew Wills, UCL

ACKNOWLEDGEMENT

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

Ivana Evans, Durham

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BCA Spring Meeting

8th - 10th April 2008, York

“Structure, Property & Function”

Plenary: Paul Attfield

Charge Order in Oxides - Putting the Fun into Functional Materials

Local Structure and Disorder in Crystalline Materials

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Martin Lees: *Magnetic Order in $\text{Ca}_3\text{Co}_2\text{O}_6$*

And much more.....

Further information and registration at: www.crystallography-meetings.org.uk

