INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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Original article text and available illustrations

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IUCR JOURNALS NEWS

A new vision for Acta Crystallographica Section A

Acta Cryst. (2013). A69, 533–534 (http://doi.org/qc9)



Simon Billinge



John Miao

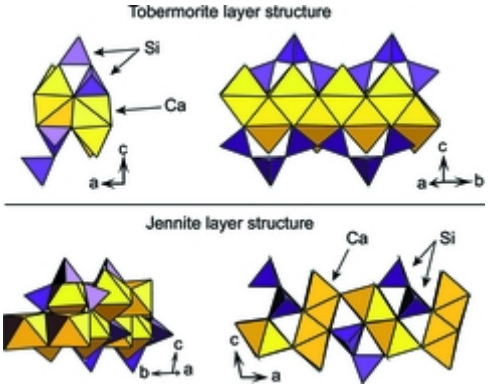
We are making some exciting alterations to Acta A to reflect the changing landscape of materials-structure research and emerging developments in the field. The subtitle will change from *Foundations of Crystallography* to *Foundations and Advances*, and a new *Advances* section will be created to accommodate articles describing original research of high potential impact. Manuscripts in this section will be 'fast-tracked', and certain of these will be promoted to a wider audience using commissioned viewpoint articles and press releases. Furthermore, *Advances* review articles will be invited, capturing the state of play in an emerging area of structure science.

S. J. L. Billinge and J. Miao

IUCR JOURNALS NEWS

X-ray diffraction: a powerful tool to probe and understand the structure of nanocrystalline calcium silicate hydrates

Acta Cryst. (2013). B69, 465–473 (http://doi.org/qdb)



Sketch of the layer structure from tobermorite (top) and jennite (bottom), two model minerals commonly used to describe C-S-H crystal chemistry. Yellow polygons and purple tetrahedra respectively symbolize calcium and silicon coordination spheres.

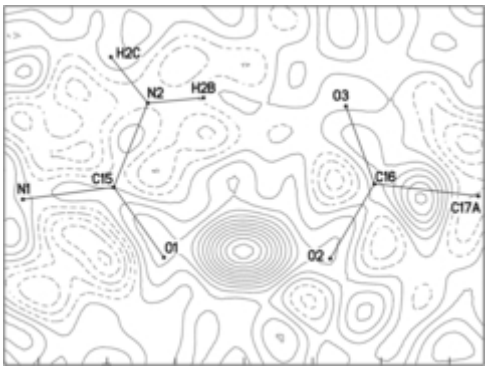
Nanocrystalline calcium silicate hydrate (C-S-H) is the main binding phase in concrete. Despite decades of studies, many aspects of its lamellar structure remain unknown, owing to its minute size and extreme structural disorder, both producing X-ray diffraction patterns often considered diagnostic for X-ray amorphous phase. However, closer investigation of these patterns strongly suggests that C-S-H resembles nanocrystalline defective tobermorite affected by turbostratic disorder and possibly interstratification, at least for calcium to silicon ratios lower than ~1.25.

S. Grangeon, F. Claret, Y. Linard and C. Chiaberge

IUCR JOURNALS NEWS

Methane-sulfonic acid salt forms of carbamazepine and 10,11-di-hydro-carbamazepine

Acta Cryst. (2013). C69, 1260–1266 (http://doi.org/qdc)



Difference Fourier map for the trifluoroacetic acid carbamazepine complex at 100 K showing the position of the acidic hydrogen at the mid-point between the acid and base; contour level = 0.05 e Å^{-3}.

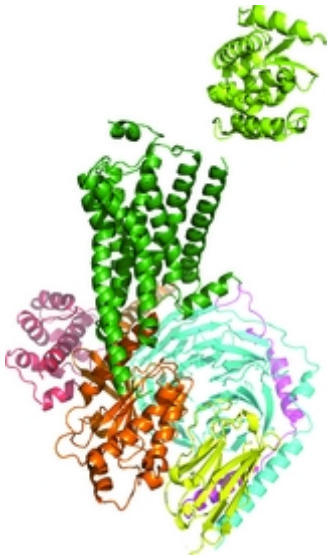
Methanesulfonic acid salt forms of carbamazepine and 10,11-dihydrocarbamazepine were characterized by single-crystal X-ray diffraction. The impact of salt formation on the carbamazepine framework is revealed through an examination of the C=O and C-N bond lengths. Similar analyses of 83 carbamazepine complexes from the CSD led to a re-examination of the trifluoroacetic acid complex, which was determined to be an intermediate-type complex with the acidic hydrogen at the mid-point between the acid and the base. This result has implications for the recent FDA guidelines on the development of pharmaceutical cocrystals. This paper forms part of the special issue on Pharmaceuticals, drug discovery and natural products.

A. R. Eberlin, M. D. Eddleston and C. S. Frampton

IUCR JOURNALS NEWS

Molecular replacements

Acta Cryst. (2013). D69, 2165–2166 (http://journals.iucr.org/d/issues/2013/11/00/isscontents.html)



The November issue of *Acta Crystallographica Section D* gathers contributions to the CCP4 Study Weekend, 'Molecular Replacements', held in January 2013 in Nottingham, UK. The proceedings recall the glorious past of molecular replacement (MR), confirm its present vitality, and point to a bright future for it: once a stucture is known for all known protein families, MR will become the technique of choice for future macromolecular crystal structures. Keep up the good work, structural biologists! And may MR always come to your rescue.

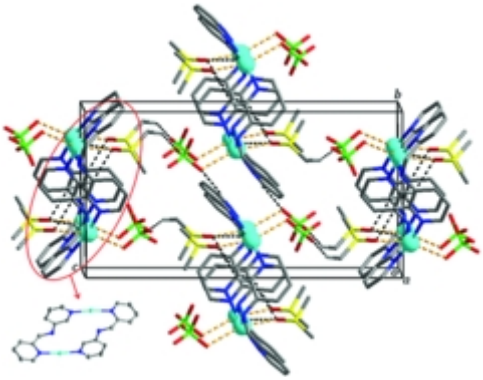
C. Ballard, P. Roversi and H. Walden

IUCR JOURNALS NEWS

Bis[μ-N-(pyridin-2-ylmethyl)pyridin-3-amine-κ2N:N’]disilver(I) bis(perchlorate) dimethyl sulfoxide disolvate

Bis[μ-N-(pyridin-2-ylmethyl)pyridin-3-amine-κ^2*N*:*N*’]disilver(I) bis(perchlorate) dimethyl sulfoxide disolvate

Acta Cryst. **(2013). E69, m575–m576 (http://doi.org/qdd)**



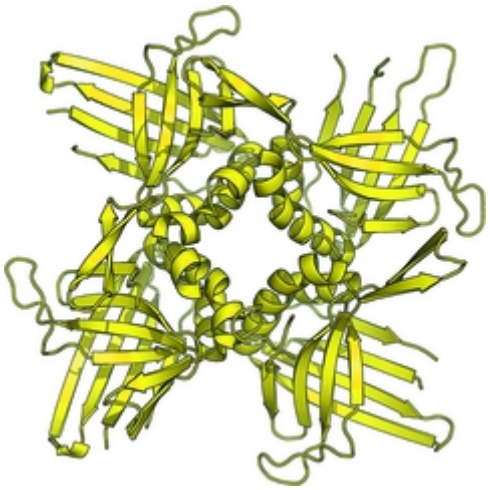
In the development of silver(I) coordination polymers, the investigation of Ag^{I} coordination polymers using unsymmetrical dipyridyl ligands with nitrogen donor atoms on different positions in the two terminal pyridines still remains lacking. A self-assembly of the unsymmetrical ligand *N*-(pyridine-3-ylmethyl)pyridine-2-amine with the silver ion afforded an unusual sixteen-membered metallamacrocyclic dimer. In the crystal, various intermolecular interactions such as Ag···O, N–H···O C–H···O, and C–H···π interactions between the metallamacrocyclic dimers and the anions or the solvent molecules lead to the formation of a three-dimensional supramolecular network.

S.-H. Moon and K.-M. Park

IUCR JOURNALS NEWS

A family portrait: structural comparison of the Whirly proteins from Arabidopsis thaliana and Solanum tuberosum

Acta Cryst. **(2013). F69, 1207–1211 (http://doi.org/qdf)**



Whirly proteins are mainly found in plants, where they localize to chloroplasts or mitochondria. These proteins bind single-stranded DNA with low sequence specificity. In the absence of the chloroplast-directed Whirly proteins, the chloroplast genome becomes unstable and accumulates DNA rearrangements. This article describes the crystal structures of the three *Arabidopsis thaliana* Whirly proteins. Comparison of these structures to that of a potato Whirly protein reveals strong structural similarity and suggests that all plant Whirly proteins bind single-stranded DNA in a similar manner.

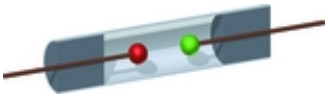
L. Cappadocia, J.-S. Parent, J. Sygusch and N. Brisson

IUCR JOURNALS NEWS

Capillary-based micro-battery cell for in situ X-ray powder diffraction studies of working batteries: a study of the initial intercalation and deintercalation of lithium into graphite

Capillary-based micro-battery cell for *in situ* X-ray powder diffraction studies of working batteries: a study of the initial intercalation and deintercalation of lithium into graphite

J. Appl. Cryst. **(2013). 46, 1537–1543 (http://doi.org/qdg)**



Sketch of the capillary-based micro-battery cell designed for *in situ* studies in transmission mode.

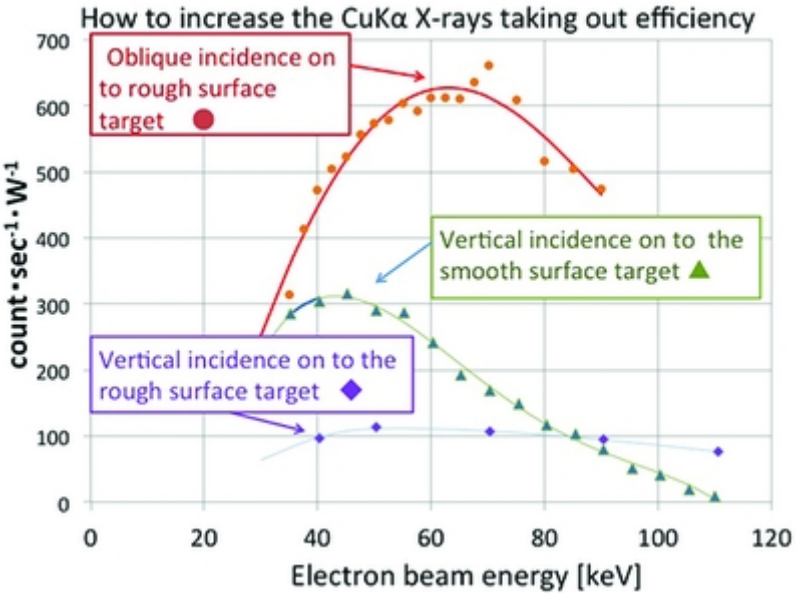
This paper reports the design of a novel capillary-based micro-battery cell for *in situ* X-ray powder diffraction studies of working batteries. The *in situ* cell makes it possible to obtain X-ray diffraction from a single electrode at a time, which facilitates detailed structural and microstructural studies of all types of crystalline electrode materials. The micro-battery cell was used to study the initial intercalation of lithium into graphite in a working Li–C battery. *DIFFaX+* was used to refine the stacking order/disorder in the graphitic phases.

R. E. Johnsen and P. Norby

IUCR JOURNALS NEWS

U-shape rotating anti-cathode compact X-ray generator: 20 times stronger than the commercially available X-ray source

J. Synchrotron Rad. (2013). 20, 829–833 (http://doi.org/qdh)



Take-off angle: 6°, through Φ 10 µm pin-hole, at 75 mm from the target.

A rotating anti-cathode X-ray generator, where the inner surface of a cylindrical annulus as target is irradiated, has been developed; we call this 'U shape'. A brightness of 129 kW mm^{-2} was obtained with this new generator. In addition, by using oblique incidence of the electrons onto a rough target, the efficiency of the X-rays extracted increased two times compared with that using with vertical incidence of the electrons onto a smooth target. Overall the new X-ray generator brightness is in total 20 times stronger.

N. Sakabe, K. Sakabe, S. Ohsawa, T. Sakai, H. Kobayakawa, T. Sugimura, M. Ikeda, M. Tawada, N. Watanabe, K. Sasaki and M. Wakatsuki

IYCR 2014

Ready, steady, go



Michele Zema



This video is also available with a description at www.iycr2014.org/about/video and now contains subtitles in English, Italian, Portuguese, Spanish and Russian. Please send translations in your own language to iycr2014@iucr.org.



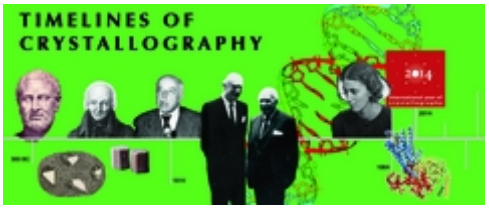
Some examples of media coverage following the IYCr2014 press conference. Full details can be seen at www.iycr2014.org/about/coverage.

The International Year of Crystallography has been formally launched with an online press conference on Thursday, December 12, 2013. Messages from the UNESCO Director General, Irina Bokova, IUCr President, Gautam R. Desiraju, and the science writer Georgina Ferry, author of famous biographies, including those of Dorothy Hodgkin and Max Perutz, introduced the release of the launching video of IYCr2014. The video 'What crystallography can do for you', created by Juanma García-Ruiz (U. Granada and CSIC) and Javier Trueba (Madrid Scientific Film), with the support of the IUCr staff, highlights the role of crystallography in different fields, from medicine and health to new materials, from farming to cultural heritage, and has already received more than 4,000 views since its release on the IUCr YouTube channel (www.youtube.com/user/theIUCr). After the screening of the video, journalists took part in a Q&A session moderated by Jonathan Agbenyega, the new IUCr Business Development Manager, and featuring Mike Glazer from U. Oxford. Extensive media coverage followed the press conference, with articles appearing, among others, in *El País* and on BBC News. All this material, some of which has been translated into different languages, is now available on the web site at www.iycr2014.org/about/media-kit.

As stressed by the President in his Letter, translation of documents into as many languages as possible is a fundamental vehicle to spread the knowledge of crystallography and fully exploit the efforts that are being made for IYCr2014. Everyone who can volunteer to help with translation is invited to contact the IUCr office (iycr2014@iucr.org).

Several new events celebrating crystallography and IYCr2014 have been added to the Calendar of events (www.iycr2014.org/events). Moreover, the IYCr2014 website has been enriched with a lot of new content, which we hope will help popularize crystallography and also provide useful tools for the expert.

Take some time to explore www.iycr2014.org, download new posters and calendars, and discover all its new sections and features.



A great project that has just been launched is the 'Timelines of Crystallography', developed by Marv Hackert (U. Texas at Austin) and Brian McMahon (IUCr): browse the different categories at www.iycr2014.org/timeline and discover how crystallography developed through the centuries and contributed to the advancement of science.



This video is also available on the IUCr YouTube channel at www.youtube.com/user/theIUCr.
The project of involving children worldwide in a crystal-growing experiment, coordinated by Luc Van Meervelt (Katholieke U. Leuven), is also expanding rapidly. New countries are now starting their own competitions, and new tools for newcomers are available at www.iycr2014.org/participate/crystal-growing-competition, including a downloadable brochure and a brand new video explaining step-by-step how to grow a single crystal.



Crystallography permeates our lives and is visible to the crystallographer's eyes in the objects of everyday life. The IUCr, in partnership with Agilent Technologies, has launched the photo competition 'Crystallography in everyday life'. Send your best photographs under this theme and do not miss the opportunity to win one of the two 1,000 US$ bursaries to go to Montreal for the IUCr Congress (August 5-12, 2014), where a special exhibition will be set up with the best photographs submitted. Find all details at www.iycr2014.org/participate/photo-competition.

The 23rd IUCr Congress (www.iucr2014.org) will be a special occasion for discussing and celebrating IYCr2014. A specific session will be dedicated to the Year and I would like to invite contributions about all the activities organized or planned at global, national or local level.

Michele Zema (mz@iucr.org), IUCr Project Manager for IYCr2014

IYCR 2014

IUCr-UNESCO OpenFactory



As part of the OpenLab project, already described in the previous issue of the *IUCr Newsletter*, the IUCr and UNESCO are implementing some special activities to be held in the factories of the main crystallographic instrumentation manufacturers. The aim is to provide young scientists from across the world with high-quality education opportunities, and to show a more complete picture of crystallographic research, which is brilliantly carried out not only in the universities and research centres. Moreover, workshops in the factories may also be focused on technical aspects and maintenance of crystallographic instrumentation, thus showing different possible job opportunities in our field.

The first of such projects, which will generally be referred to as IUCr-UNESCO OpenFactory, has already been planned and will be organized in partnership with the companies STOE, DECTRIS and Xenocs, and with the collaboration of the European Synchrotron Radiation Facility (ESRF). The STOE-DECTRIS-Xenocs OpenFactory will take place September 10-19, 2014. It will include a first part in Grenoble, where the students will spend significant time at the ESRF and will be trained in small-angle X-ray scattering at Xenocs' headquarters. Afterwards, the entire class will move to Darmstadt, where the workshops will focus on single-crystal and powder XRD at STOE's headquarters, with practical tutorials and hands-on experiments. The IUCr will supervise the educational activities, which will be done by scientists from the three companies, and guest lecturers selected by the IUCr.

A great networking opportunity is given to the students, who will join the STOE Users Meeting on September 18-19, 2014, thus interacting with highly experienced scientists and enabling the creation of their own network for possible future cooperation.

The program will be free of charge for all participants as STOE, DECTRIS and Xenocs will cover round-trip flights, accommodation, food and transport costs. Candidates are young scientists from all parts of the world. Applications, including a CV, recommendation letter and declaration of motivation, must be sent by March 30, 2014. For further information please visit www.iycr2014.org/openfactory.

Michele Zema

IUCR ACTIVITIES

New Business Development Manager for IUCr



We extend a warm welcome to Dr Jonathan Agbenyega, who has recently joined the IUCr staff in Chester, UK, as Business Development Manager. Jonathan completed his PhD in Materials Science at U. of Southampton in 1993 and also co-authored a book on Raman spectroscopy published by Wiley during this period. After a brief postdoc position at the Institute of Food Research, Norwich, UK, Jonathan began his career in scientific publishing. Jonathan has worked with leading publishers Wiley, Pearson and, more recently, Elsevier, where he was Editor-in-Chief and Publisher of *Materials Today* magazine.

Jonathan joins the IUCr at an exciting time in the development of the IUCr Journals, and will be reaching out to the wider science community, encouraging closer integration of the journals with the IUCr Commissions, developing a social media marketing strategy, boosting visibility of articles and authors by writing press releases highlighting the most significant papers, creating market research reports including citation and usage trend analysis, identifying subject trends and new journal opportunities, identifying target authors and encouraging them to submit to the journals, and exploiting opportunities arising from IYCr2014.

We hope you will join us in wishing Jonathan all the best in his endeavours and, if you have the chance, introduce yourself if you spot him at a meeting or workshop. Jonathan can be contacted at ja@iucr.org.

IUCR JOURNALS NEWS

1 January 2014 launch for IUCrJ



IUCrJ, the IUCr's new high-profile fully open-access journal, has got off to a flying start with scientific commentaries and research articles covering biology, chemistry, crystal engineering, materials, physics and FELs from leaders in the field in its inaugural issue. Launched in celebration of the International Year of Crystallography 2014 and overseen by expert editorial and advisory boards, the journal aims to become the natural home for reporting breakthroughs and 'full' structural science reports, rather than simply a structure or how it was determined. High-quality contributions with wide scientific appeal will be actively encouraged from chemists, biologists, physicists and material scientists, and the journal hopes to capture many of the spectacular results that are presented at IUCr Congresses and ACA, AsCA and ECA meetings.

For more information or to submit an article, please go to http://www.iucrj.org

IUCR ACTIVITIES

Twenty-Third General Assembly and International Congress of Crystallography

The Twenty-Third General Assembly of the IUCr and the Twenty-Third International Congress of Crystallography will be held at the Palais des congrès de Montréal, Canada, August 5-12, 2014, at the invitation of the National Research Council of Canada. Registration, the Opening Ceremony and the presentation of the Tenth Ewald Prize will take place on Tuesday, August 5, 2014.

The scientific programme will include invited lectures, microsymposia, a special IYCr2014 session, workshops and poster sessions. Exhibits of commercial and non-commercial equipment and books, as well as crystallographic software and database demonstrations, will also be held. Internet access will be available to all participants. J. Britten is Chair of the International Programme Committee (IPC) and A. Berghuis and M. Cygler are Co-Chairs of the Local Organizing Committee.

The Scientific Program announcement appeared in Volume 21, Number 3 of the *IUCr Newsletter.* More information can be found in this issue and at www.iucr2014.org/.

This announcement constitutes formal notice of the date and place of the General Assembly (Statute 5.3). The sessions of the General Assembly have been scheduled provisionally for the evenings of Wednesday, August 6, Thursday, August 7, Sunday, August 10, and Monday, August 11. The deadlines for proposals for amendments to Statutes, proposals for the agenda, receipt of reports and budgets from Commissions, *etc.*, which are laid down in the Statutes and By-Laws of the IUCr, are listed below.

General Assembly Timetables

Preparing for the General Assembly

February 6

Proposals for amendments to Statutes to General Secretary

March 6

Estimated budgets from Commissions to Executive Committee

April 6

Proposals for agenda of General Assembly to General Secretary

Proposals for amendments to Statutes to National Committees and Commissions

April 30

Reports of Commissions to General Secretary

May 28

Report of Executive Committee to National Committees and Commissions

Reports of Commissions to National Committees and Commissions

Budget to National Committees and Commissions

Agenda to National Committees and Commissions

During the General Assembly

'Before'

Notice by National Committees to General Secretary of names of delegates, alternates and chairs of delegations, and of distribution of votes if not one per delegate.

96 hours

Nominations by Executive Committee for Officers of IUCr

72 hours

Recommendations by Commissions to General Secretary for Chairs and members of Commissions

48 hours

Nominations by Executive Committee for Chair and members of Commissions

Notification of motion to amend or suspend By-Laws

36 hours

Notice to General Secretary of nominations by delegates for Officers of IUCr

24 hours

Posting of nominations by delegates for Officers of IUCr

24 hours

Notice to General Secretary of nominations by delegates for Chairs and members of Commissions

12 hours

Posting of nominations by delegates for Chairs and members of Commissions

Michael H. Dacombe (execsec@iucr.org)

MEETING REPORT

ECM28

Warwick, UK, August 2013
http://ecm28.ecanews.org/



The Quasi-Crystallites Quintet playing at the Opening Ceremony.



Crystallographers enjoying lunchtime at ECM28 in Warwick: from left Matteo Lusi, Simona Galli, Giulio Lampronti, Giancarlo Terraneo, Chiara Massera, Consiglia Tedesco and Marco Milanesio.

A total of 855 crystallographers from 50 countries met in Warwick, August 25-29, 2013, to attend the 28th European Crystallographic meeting, including almost 200 students and 74 exhibitors. Over the four days of the conference, 44 microsymposia and 16 keynote lectures presented the latest advances in all aspects of crystallography. The history of the ECA was covered in a very successful microsymposium. The Congress attendees were welcomed by the ECA President André Roodt, the Chancellor of the U. of Warwick, Richard Lambert, the Chief Scientific Adviser to the UK Government, Mark Walport, and the Editor-in-Chief of IUCr Journals, Samar Hasnain.

During the opening ceremony the 7th Max Perutz Prize was awarded to Randy J. Read, who illustrated the development and application of advanced statistical approaches to all stages of protein structure solution. A concert of brass music was provided by Warwick U. students playing in a specially formed quintet called 'The Quasi-Crystallites' (see photo). The conference closed with the beautiful lecture 'Quasi-Periodic Materials - Crystals Redefined' by the Nobel Prize laureate Dan Shechtman.

During the closing ceremony 17 Poster prizes were awarded.

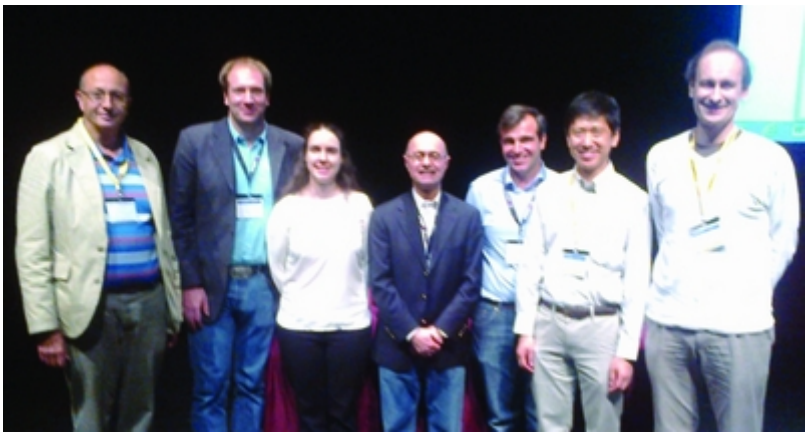


Crystallographers having a hard time following dancing instructions after the gala dinner.
Throughout the duration of the conference, all the participants had the privilege to visit the 'Two Braggs Exhibition', organized by Mike Glazer and Pam Thomas to celebrate the lives of W. H. and W. L. Bragg, bringing together a fascinating collection of historic equipment, notebooks, honours, letters, films and artwork never before seen in one exhibition. Along with this fascinating exhibition, a program of entertainment was offered to participants, with the showing of the movie 'Hidden Glory' - a play about Dorothy Hodgkin by Georgina Ferry - the film 'Driven to Diffraction', the film '50 years a winner' - made in 1965 to celebrate the 1915 Nobel prize awarded to the Braggs - the film 'El misterio de los cristales gigantes', the 'Celebration of a Centenary of Crystallographers', a special symposium to mark the Bragg Centenary, and a 'critical account on the discovery of X-ray Diffraction by Laue, Friedrich and Knipping'. The gala dinner was followed by a traditional Ceilidh dance.

In addition to the main conference, five well attended satellite meetings were held: a CIF Symposium, the European Young Crystallographers meeting, Crystallographic Information and Data Management, PDF Analysis, and Introduction to Software Development for Crystallographers.

Alessia Bacchi

Methods and Techniques



Speakers and Chairs in MS1: (left to right) John Helliwell, Lars Redecke, Catherine Dejoie, Abbas Ourmazd, Jose Trincao, Atsushi Nakagawa and Victor Lamzin.
In a session on Time-resolved Crystallographic Methods (MS1), L. Redecke (Germany) described how free-electron laser radiation and in vivo grown nanocrystals open new routes in structural biology and options for time-resolved experiments. Lars used very tiny (4 μm^3) *in vivo* grown crystals, of *Trypanosoma brucei* cathepsin B, a protein important in structure-based drug discovery aimed at sleeping sickness. The electron density map contained readily interpretable new features and showed no

serious disruption of X-ray scattering factors, a serious concern of applications of X-ray lasers in structural biology. A distinctive feature of this study was the use of femtosecond X-ray pulses. Previous studies of the time-resolved analysis of small changes in a protein crystal structure extend into the sub-nanoseconds regime using synchrotron X-ray radiation. X-ray lasers allow such studies to be extended into the femtosecond range. A. Ourmazd (USA) using mathematical techniques cogently argued that sparsely photon-populated diffraction patterns should be amenable to structure analysis. He postulated that 1012 X-ray photons per pulse would be adequate for structure analysis of most protein and virus structure studies with XFELs. This produced a vigorous discussion on the pulse fluxes required for biological FEL-based imaging. C. Dejoie (Switzerland) described using a monochromatic micro beam for serial snapshot crystallography. Laue methods allow efficient acquisition of more data at a lower X-ray flux pulse whilst preserving a strong diffraction pattern. J. Trincao (UK) described the strengths of the co-location of the Central Laser Facility, Dynamic Structural Science Consortium and the Diamond light source, and plans to form a consortium to build and access a nanocrystal beam line at the European XFEL in Hamburg. A. Nakagawa (Japan) talked about Coherent Diffraction Imaging of Spherical Biological Particles and the Japanese SACLA X-ray free electron laser studies of large spherically shaped virus single particles.

Chairs: John R. Helliwell and Victor Lamzi



Speakers and Chairs in MS3: (left to right) B. Klaholz, D. Wigley, G. Montoya, P. da Fonseca, P. Aller and J. Beale. (Missing: N. Galatanu).

The session on Hybrid Approaches (MS3) included oral presentations using crystallography and cryo-electron microscopy, novel approaches in SAXS, or *in situ* diffraction tests. D. Wigley (UK) combined crystal structures, electron microscopy and biophysical techniques to provide insight into the stoichiometry, architecture and molecular interactions between components of the chromatin remodeling complex and the nucleosome histone core. P. Fonseca (UK) presented the structural analysis of the human proteosome, a 2.6 MDa complex within which the 19S cap promotes substrate unfolding and translocation. The sub-nonmetric cryo-EM map of the complex was analyzed by fitting known and newly determined crystal structures, providing a full backbone model of the 19S caps. N. Galatanu (France) presented a SAXS setup comprising a low background camera and a micro-source coupled with multi-layer optics providing scatter-less collimation.

J. Beale (UK) described the extracellular domain of two peptide transporters of significant pharmaceutical interest due to their ability to bind a number of clinically important drugs. A combination of SAXS, crystal structures, *ab initio* modelling and ensemble organization provided insight into the mechanism of these membrane proteins.

P. Aller (UK) presented the in situ plate screening and data collection procedure where dehydration of crystals is achieved though replacement of the reservoir solution by an NaCl solution (0.5-1.5 *M*) and overnight equilibration. Examples were shown where the diffraction improved from the range of 2.9-2.6 Å to 2.8-2.3 Å under cryo conditions when freezing after dehydration without additional cryoprotectant, or improvement from 24 Å to 11 Å resolution for a membrane protein.



Speakers and Chairs in MS33: (left to right) Yaroslav Filinchuk, Elena Boldyreva, Scott McKellar, Iain Oswald, Kamil Dziubek and Francesca Fabbiani.

The session 'Molecular Compounds under High Pressure' (MS33) gave an overview of the latest trends in high-pressure studies of molecular materials. Elena Boldyreva (Russia) described multi-component crystals (including salts, hydrates and co-crystals) having industrial and crystal engineering significance. After a review of the motivation for high-pressure analysis, Elena presented case studies of amino acids and pharmaceuticals with examples from her work and what others have reported. The examples focused on pressure-induced phenomena, including mechanisms of phase transitions, proton transfer, order-disorder structural changes and tuning of hydrogen bonds, studied by a combination of single-crystal, powder diffraction and Raman spectroscopic methods.

A talk entitled 'Bonding and Phase Change in Ammonia Borane and Lithium Amidoborane under High Pressure' was given by J. Chen (USA). With the world's increasing fuel demands and limited fossil fuel resources, research on hydrogen storage is critically important. Ammonia borane is a very promising material for hydrogen storage but industrial applications are hampered by a slow and irreversible release of gas; reversibility of the decomposition reaction could potentially be promoted by the application of pressure. The phase diagrams of the title compounds were studied as a function of pressure and temperature, using a combination of powder diffraction and Raman spectroscopy. At 3.9 GPa opaque samples of lithium amidoborane turn transparent. The lack of dihydrogen bonding in this material, which is present in the hydrogenated parent compound and facilitates hydrogen release, may prove useful for optimizing hydrogen storage properties.

K. Dziubek (Poland) presented a historic perspective on 'Volumetric Measurements in High-Pressure Crystallography', including experiments on water by Sir Francis Bacon in 1620, J. Bramah's patent for a hydraulic pump in 1975, volumetric experiments by P. W. Bridgeman in the 19th century and the introduction of the diamond anvil cell in 1958. The speaker presented the design of the piston cylinder press in use at his home laboratory, which is capable of compressing liquid and solid samples up to *ca* 2 GPa. Direct compression experiments in the press provide precise information on volumetric properties and phase transition pressures complementary to diffraction experiments, as demonstrated by studies of chloroform and imidazole.

In 'Pressure-Induced Polymorphism in Small Molecule Acrylic Acids', I. Oswald (UK) described investigations on acrylic acid and methacrylic acid, monomers of two industrially relevant polymers. Using single-crystal X-ray diffraction and neutron powder diffraction (on the ISIS PEARL instrument), the phase behaviour previously inferred by Raman spectroscopy was extended and clarified. For acrylic acid, a phase transition at 0.75 GPa was identified, which is associated with pleating of molecular layers. Further compression to 7.0 GPa results in an increase of the puckering of the layers. For methacrylic acid, two-phase transitions could be identified at 0.4 GPa and 1.21 GPa, respectively. Compressing the sample further to 5.0 GPa appears to lead to polymerization.

The final talk was by S. McKellar (UK) on the effect of solvent and pressure on the post-synthetic modification of a metal organic framework. (MOF). Single-crystal compression studies of St. Andrew's

MOF revealed pressure-induced post-synthetic modification behaviour, in which exchange with a highly labile axial water molecule coordinated to Cu^{II} is observed. When methanol or acetonitrile are used, the exchange occurs at pressures below 0.3 GPa and hydrophilic channels are converted to hydrophobic pores. The post-synthetic modification phases are stable on releasing pressure. No ligand exchange is observed in the presence of isopropyl alcohol or ethanol, whilst exchange leads to a strain-induced collapse of the structure to an amorphous phase when using ethanol.

Chairs: Yaroslav Filinchuk and Francesca Fabbiani

Fundamentals



Speakers and Chairs in MS11: (left to right) back row: David Rae, Areej Abuhammad, Martin Lutz, Berthold Stoeger, Harry Powell; front row: Pietro Roversi and Loes Kroon-Batenburg.
The session on Twinning Problems and Advantages (MS11) saw a lively mix of theory and applications, both from the small-molecule and the macromolecular crystallography worlds: it was good to hear about aspects of twinning detection and modelling (Stoeger, Rae and Abuhammad), and software development to aid twinned data processing [H. Powell (UK) and M. Lutz (Netherlands)] and realise once more that (perhaps unsurprisingly) the two crystallography (sub) communities are facing very similar problems and have questions in common.

Moreover, after this session, and when dealing with twinned crystals, the question from Powell's talk will always come to mind: are the Thompson Twins in the Tintin stories really twins, or are they just very much alike and always found together? We shall never think of twinned crystals the same way ever again!

Chairs: Pietro Roversi and Loes Kroon-Batenburg



Speakers and Chairs in MS29: (Left-to-right) C. Lecomte, A. Mazzone, D. Sisak, O. Sobolev, M. Burla and M. Fronc. (Missing: M. Kubicki).

The session 'Getting More from your Electron Density' (MS29) had contributions on electron-density modification approaches to improve phase estimates from a given model, accurate electron-density modelling, and the importance of not over-restraining a model.

M. Burla (Italy) spoke about the *VLD* phasing algorithm, which is based on the properties of the difference Fourier synthesis and the joint probability distribution function. The efficiency of the algorithm was improved by introducing the *RELAX* procedure now implemented in *SIR2011*. Some applications include the combination of the *VLD* algorithm with the hybrid Fourier synthesis for *ab initio* phasing and its integration in a molecular replacement pipeline for automatic protein crystal structure solution.

D. Sisak (Switzerland) described a new approach for solving the structure of polycrystalline materials using a charge-flipping algorithm. Using a starting phase set for charge flipping, an approximate structure is obtained from direct-space optimization followed by a flowchart that indicates which approach is most suitable for a specific problem.

O. Sobolev (Russia) showed that large distortion of a residue in unrestrained refinement may suggest the presence of alternative conformations (ACs) for this residue. Analysis of atomic shifts in unrestrained refinement may reveal poorly ordered residues that should be checked first with electron-density maps to model in ACs.

M. Kubicki (Poland) described accurate electron-density modelling of 4-nitroimidazoles spore crystals, that revealed intermolecular interactions, (dipole-dipole, weak hydrogen bonds, H···H attractive contacts) and details of anharmonicity and dipole moment. Kubicki showed that these ultra-high resolution measurements can detect organic solid solutions such as $A_{(1-x)}B_x$ with x smaller than 4%.

M. Fronc (Slovakia) described electron-density modelling of $[Cu_2(\mu_2\text{-}I)_2(2,6\text{-dimethylpyridine})_2]$. This is a very ambitious project due to the presence of the very heavy atom, iodine, which bridges the two copper atoms.

Chairs: Annamaria Mazzone and Claude Lecomte



Speakers and Chairs in MS27: (left to right) Kirsten M. Ø. Jensen, Phoebe K. Allan, Antonio Cervellino, Arkadiy Simonov, Callum Young and Michela Brunelli. (Missing: Karena Chapman).
The 'Total Scattering' microsym. (MS27) opened with two presentations on in situ diffraction studies of the synthesis of nanoparticles (K. M. Ø. Jensen, Denmark) and the adsorption processes in functional porous materials for medical gas delivery (P. K. Allan, UK). Jensen, winner of one of the poster prizes, will start a post-doc position at Columbia U. (USA) in Simon Billinge's group, while P. K. Allan will soon be Junior Research Fellow at U. Cambridge.

Total scattering measurements now span X-ray, neutron and electron studies of powdered or single-crystal samples, with a growing range of tools including 'real-space Rietveld', reverse Monte Carlo (RMC) and whole particle modelling, and model-independent analysis of real-space features in the data. Other contributions in the session concerned a three-dimensional pair distribution function for comparing different local ordering models in single crystals (A. Cervellino, Switzerland), Jahn-Teller symmetry

switching in $LaMnO_3$ (A. Simonov, Switzerland) and a microstructure study of Fe_3O_4/γ-Fe_2O_3 nanoparticles (C. Young, UK)

Chairs: Michela Brunelli and Karena Chapman



Speakers and Chairs in MS30: (left to right) Simon Grabowsky, Joanna Bak, Regine Herbst-Irmer, Anna Hoser, Sander van Smaalen, Jozef Kožíšek and Birger Dittrich.

The microsymposium on 'Anharmonic Thermal Motion' (MS30) covered thermal motion and charge-density research in general. A talk by R. Herbst-Irmer (Germany) described a multi-temperature study of an interesting structure in which one of two independent molecules was affected by anharmonicity and the other was not, a fitting example to introduce the topic. A talk by J. Bak (Poland) exploited the combination of Hirshfeld-atom and X-ray wave function refinement, using the quantum crystallography program *TONTO*, which now treats anharmonicity. V. Smaalen (Bayreuth, Germany) showed that today's high-resolution protein data contain additional contributions to atomic displacements beyond thermal motion, thereby fundamentally affecting our ability to extract information on static and dynamic electron-density distributions. J. Kožíšek (Slovakia) focused on data quality for faithful modelling of charge density on a copper coordination complex, and A. Hoser (Poland) discussed structural energetic and charge-density investigations of triptycene and selective derivatives.

The ratio of male and female contributors favoured the latter.

Chairs: Simon Grabowsky and Birger Dittrich

Applications



Speakers and Chairs in MS8: (left to right) Jacqueline Cherfils, Marc Delarue, Aude Echalier-Glazer, Karin Kühnel, Valérie Campanacci, Saccas Savvides and Remy Loris.

In the microsym. 'Cell-Signalling Interactions and Allostery' (MS8) it was shown that in cells signals propagate between different biological active sites of a protein; and from protein to protein within cellular pathways. Allostery, a concept first devised 50 years ago by Monod, Wyman and Changeux, applies to many regulated signalling networks. Speakers in this session presented a variety of studies that illustrate signalling and allostery.

M. Delarue (France) presented crystal structures of pentameric ligand-gated ion channels, prototypical allosteric membrane receptors. He showed that ethanol stabilizes an open form of the receptor, suggesting a structural basis for neurological actions of ethanol in human receptors.

S. Savvided (Belgium) discussed how cytokines, extracellular signalling molecules, signal a receptor using a combination of biophysical, structural and computational approaches. Notably, he showed that Epstein-Barr virus intercepts a human cytokine (CSF-1) by allosteric competitive inactivation, rendering it unable to signal to its receptor.

V. Campanacci (France) presented a study of a bacterial effector that rewires membrane trafficking pathways in an infected host cell and uncovered a conserved enzymatic mechanism common to one class of toxins, which allows them to process diverse substrates.

K. Kuhnel (Germany) described a family of proteins that are crucial in an evolutionary conserved degradative pathway. She showed that these proteins have two phospholipid binding sites on a seven-bladed beta propeller structure that are adjacent but non-overlapping, suggesting how these proteins bind to membranes.

A. Echalier-Glazer (France) used crystallographic and in silico approaches to analyze the regulation of a large multi-protein complex implicated in various cellular functions through its role in the ubiquitin-proteasome pathway.

Chairs: Jacqueline Cherfils and Remy Loris



Speakers and Chairs in MS24: (left to right) Chick Wilson, Andrew Bond, Lee Brammer, Simona Galli, Colin Seaton, Pete Wood and Nikoletta Bathori.

In 'Organic and Inorganic Multi-component Crystals: Structure and Properties' (MS24), L. Brammer (UK) discussed studies of flexibility and chemical transformations in coordination with polymers and frameworks including gas and solvent sorption/desorption processes. Using single-crystal and powder diffraction, energy calculations and simulation of spectra, C. Wilson (UK) talked about controlling molecular assembly in the organic solid state, polymorph control and discovery from multi-component crystallization, and transferring crystal engineering to manufacturing environments. S. Galli (Italy) described using bipyrazolate ligands to construct porous coordination polymers. She showed that azole-based frameworks are chemically more stable than low density MOFs and can offer potentially comparable gas sorption properties. She also described how to use variable temperature PXRD to measure anisotropic thermal expansion properties. C. Seaton (Ireland) discussed the influence of the crystallographic environment on intermolecular proton transfer in multi-component molecular solids, using calculations on isolated molecules and clusters extracted from crystal structures. P. Wood's (UK) talk covered difficulties associated with crystal structure prediction for salts, and highlighted ways in which the Cambridge Structural Database might be used to approach some of these problems.

Chairs: Nikoletta Bathori and Andrew Bond



Speakers and Chairs in MS18: (left to right) Oleg Siidra, Biljana Lazic, Andrew Goodwin, Fernando Camara, Olga Yakubovich, Frederic Hatert and Xiaodong Zou.
The talks and posters in 'From Nature to Laboratory: Crystallography of Minerals and Mineral-related Materials' (MS18) covered mineral classification, structural prediction, modification of materials and new techniques for structural solution.

F. Camara (Italy) has classified Ti-silicate minerals into groups with different Ti-Si building blocks. The classification reveals relationships between structural topology and chemical composition and allows prediction of new minerals and crystal structures. F. Hatert (Belgium) showed a cation substitution mechanism occurring by oxidation in olivine-type phosphates that suggests development of new cathode materials. A. Goodwin (UK) reported on extreme negative linear compressibility (NLC) in a variety of framework materials and design principles for maximizing NLC of MOFs. O. Yakubovich (Russia) presented a polysomatic series of layered vanadates, arsenates and phosphates using the modular concept. X. Zou (Sweden) described new TEM techniques for solving three-dimensional structures of nanosized and/or intergrown zeolites and minerals.

Chairs: Oleg Siidra and Biljana Lazic



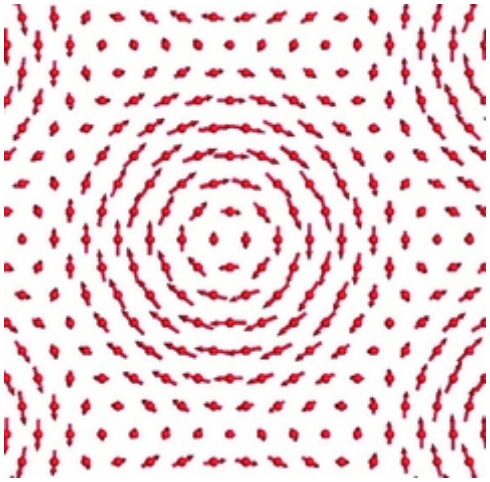
Speakers and Chairs in MS19: (left to right) Marie Colmont, Olga Yakubovich, Etienne Gaudin, Oleg Siidra, Vadim Kovrugin, Andrzej Grzechnik and Maria Wierzbicka-Wieczorek.
The session on 'Heavy Crystals: Structural Crystallography of Heavy-element Compounds' (MS19) began with invited lectures on the crystal chemistry and physical properties of intermetallic compounds (E Gaudin, France), and the influence of 'lone-pair' cations (Pb^{2+}, Tl^{+}) on geometry and dimensionality of oxosalt inorganic compounds (O. Siidra, Russia).

Three selected speakers discussed structures and stabilities of $LiCeF_5$ and $LiThF_5$ at high pressures (A. Grzechnik, Germany), novel silicates with the apatite crystal structure (M. Wierzbicka-Wieczorek (Germany), and structural variety of novel Pb and Bi selenites (V. Kovrugin, France and Russia).The broad range of these talks provided a general overview of the crystal chemistry of heavy elements.

Chairs: Olga Yakubovich and Marie Colmont



Speakers and Chairs in MS14: (left to right) H. Sharma, M. de Boissieu, K. Christensen, J. M. Perez-Mato, V. Petříček, R. David and H. Stokes.



Example of skyrmion-type spin ordering shown by H. Stokes.

The session 'Aperiodic Crystals: Structure, Dynamics and Magnetism' (MS14) focused on new types of research on quasiperiodic systems, epitaxial order in quasicrystals, and incommensurate magnetic structures. V. Petříček (Czech Republic) described a new option in *JANA2006* for the determination of commensurate and incommensurate magnetic structures combining representational analysis and magnetic symmetry. H. Sharma (UK) discussed the structure of ad-atoms on a five-fold surface of a quasicrystal where a quasiperiodic arrangement of Pb atoms is observed, in good agreement with preferential sites observed on the bare surface. Subsequently, H. Stokes (USA) presented new features of the program *ISODISTORT*, and showed that skyrmion-type spin configurations are simply obtained as incommensurate arrangements caused by the action of a single multi-*k* irreducible representation (see Figure). K. Christensen (UK) discussed the investigation of modulated molecular structures in a general service diffraction laboratory. R. David (France) described iron compounds that exhibit a complex interplay of commensurate and incommensurate structural and magnetic ordering.

Chairs: J. Manuel Perez-Mato and Marc de Boissieu



Speakers and Chairs in MS39: (left to right) Jose Gavira, Trixie Wagner, Terese Bergfors, Dominique Maes, Jindrich Hasek, Takashi Kumasaka and Elspeth Garman.

In the session 'Crystallization and Crystal Treatment', D. Maes presented atomic force and laser confocal microscopy images of growing crystal surfaces showing the dramatic effect of these impurities, and how

important it is to 'feed' crystals with pure protein. E. Garman, a.k.a. Auntie E, shared typical questions sent to her: 'I am in a polycrystalline relationship, and a loop has been hitting on me lately, how do I get out of this?' and 'I am experiencing embarrassing dryness and skins, what should I do?'. Auntie E gave wise advice to these crystals on how best to behave under stressful cryoconditions. J. Hasek showed how polyethylene glycol, polyethylene oxide type polymers, non-ionic detergents, and carboxylic acids could act as protein surface-active molecules. These 'sticky' molecules help form interactions on the protein surface that promote crystal contacts. Beamline scientist T. Kumasaka described the use of polyvinyl alcohol as a non-toxic sticky glue to stabilize the protein crystal under humidity control and subsequent cryocooling. Finally, T. Wagner presented GuideX, a database system to keep track of the 6000 or so small-ligand compounds that she manages at Novartis.

Chairs: Jose Gavira and Terese Berfors

Teaching, Art, History



Speakers and Chairs in MS40: (left to right) Davide Viterbo, Carl Schwalbe, Alicja Rafalska-Łasocha, Petr Bezdicka, Massimo Nespolo, Jordi Rius, and Laura Holland. (Photographed by Wiesław Łasocha).
Two invited lectures in 'Crystallography in Art and Archaeology' (MS40) examined artworks from the ground up. P. Bezdicka (Czech Republic) described how the powder diffraction pattern of the ground used to line an entire canvas clearly distinguishes among the five main sources of clay, widely used in Central Europe between the 16th and 19th centuries.

A. Rafalska-Lasocha (Poland) then discussed powder diffraction analysis of the origin and aging of the paint layer as a guide to conservation of art works. From 1750 to 1850, Naples Yellow contained lead antimony oxide mixed with potassium lead sulphate. In the late 1800s the second component was changed to zinc oxide. Green pigments usually are made from copper compounds, which may degrade over time. The identity of yellow and white pigments in two portraits of King John III Sobieski, who drove the Turks from Vienna in 1683, suggested they could be by the same artist.

J. Rius (Spain), described transmission micro-diffraction experiments on polished thin sections with synchrotron radiation. Typical samples were 15-30 μm thick, mounted on 1 mm glass slides, yielding discrete patterns or Debye rings depending on the number of grains struck by the beam.

L. Holland (UK) described the 'Light Reading' short story competition, www.light-reading.org, conceived by Diamond staff to draw parallels between the creative and scientific processes. The Diamond synchrotron building, science or scientists were to be mentioned in the story. The first competition in 2011 attracted over 70 entries from adults from around the world; in 2012 the competition was for 12 to 16 year olds.

D. Viterbo (Italy) discussed crystallographic themes in the writings of Auschwitz survivor Primo Levi (1919-1987). Levi's 1980 book 'The Search for Roots: a Personal Anthology' includes sections inspired by W. H. Bragg's book 'Concerning the Nature of Things', which also sparked Dorothy Hodgkin's interest in crystallography.

Chairs: Carl Schwalbe and Massimo Nespolo



Speakers and Chairs in MS41: (left to right) Santiago Garcia Granda, Anna Warren, Michele Zema, Annalisa Guerri, Jean-Louis Hodeau, Elena Boldyreva and Luc Van Meervelt.

In 'Crystallographic Teaching and Education' (MS41), crystallographers from France, Italy, Belgium, Spain and the UK described plans to celebrate the International Year of Crystallography. J.-L. Hodeau (France) described an exhibition called the 'Voyage dans le Crystal' (http://iycr2014.org/resource-materials/voyage-dans-le-cristal) that travels from prehistoric times to modern day, describing the beauty, mystery and modern applications of crystals.

L. Van Meervelt (Belgium) described a crystal-growing competition for high school students that has been held for the past 13 years in Belgium. Students grow crystals of alum and prizes are awarded at a public ceremony. In 2014 the contest will be open worldwide.

A. Warren (UK) gave a summary of the Big Bang Fair in London, where the Science and Technology Facilities Council, the BCA, Diamond, ISIS and YGG (Young Crystallographers Group) sponsored a Crystallography booth with hands-on experience for thousands of visitors. The YGG is very active in the dissemination of crystallographic science in Bristol (Kitchen Chemistry) and at Diamond Open Days. The audience was invited to build a unit cell with toothpicks and marshmallows.

The activities in Spain will include a crystal growth competition for students which began in Andalusia, Asturias, Catalonia and Aragon in 2008 and will extend to other regions in 2014. The programme 'Science, Crystals and Society' includes a short video showing 'What does a crystallographer do?', a 2014 'Crystallography diary and calendar' for 2014 (paper and virtual editions), a 'Postage Stamps exhibition' and a 'Virtual Geology Museum'.

M. Zema (Italy) described the long history of International Schools of Crystallography in Italy and announced the 'First European Crystallography School' supported by the ECA, which will be held in the IYCr 2014.

Chairs: Annalisa Guerri and Elena Boldyreva

In a microsym. on 'The History of the ECA' (MS42), A. Authier (France) discussed the emergence of crystallographic groups in many European countries in the 20 years following the founding of the IUCr in 1948. In 1972, despite complicating political challenges, many of these national groups formed the European Crystallographic Committee (ECC). There is general agreement that Authier's efforts to form these make him the progenitor of the ECA.

H. Fuess (Germany) described the 'Transition from a Committee (ECC) to an Association (ECA)'. Crystallographic meetings of the ECC improved cooperation between European researchers and soon led to a more structured organization. In 1997, the ECA was founded. Fuess registered as IM (Individual Member), number 1.

Santiago Garcia-Granda (Spain), past-president of the ECA, described the growth in size, scope and accomplishments of the ECA. He presented an elaborate and elegant exposition about many things related to the growth in size, power and achievements of the ECA. His presentation is available at the ECA website.

Jan Boeyens (South Africa) described how crystallography was first established in South Africa (around 1937). Soon after the birth of the ECA, the IUCr created the concept of 'Regional Associates', and the ECA accepted the responsibility for Africa as part of the Euro-African Region to cultivate crystallography in Africa. Though partly successful in Northern Africa, much remains to be done in central Africa.

William Duax (USA) drew upon his large collection of photos taken at ECM meetings to review the people (portraits, committees, social gatherings) and events (scientific meetings, official ceremonies, excursions, gala dinners) of ECA's history. Most of the photos are stored in the collection that has been organized chronologically on the IUCr website, thanks to the efforts of the talented staff in Chester.

Chairs: Sine Larsen and Paul Beurskens
The 29th Meeting of the European Crystallographic Association (ECM29) will be held in Rovinj, Croatia, August 23-28, 2015. Visit the website at http://ecm29.ecanews.org/.

MEETING REPORT

Meeting of ECM General Interest Group of Senior Crystallographers (GIG-SC) held at the U. of Warwick



Some of the attendees GIG-SC meeting. (Photo courtesy of Carlo Mealli).

Paul Beurskens (Netherlands) opened the meeting, presented the agenda and summarized the background for the establishment of the GIG-SC. The history of crystallography was the subject of a lively discussion. It was felt that although we are not historians we should record our reminiscences about important events and crystallographers for posterity, drawing upon written records in our own countries. The magnificent Bragg exhibition that Mike Glazer had created for ECM 28 was highly praised. Howard Flack had expressed an interest in editing a homepage for the GIG-SC. Herbert and Frances Bernstein offered help. Election of a new chairperson was discussed. Paul Beurskens did not want to continue as an officer but he was willing to maintain the mailing list. Sine Larsen might accept in about two years when her research grant expires. She promised to offer support to Svend Erik Rasmussen if he would assume the task of chairperson. He agreed to do so with the caveat that he might not be alive at the time of the next ECM in 2015.

Svend Erik Rasmussen

MEETING REPORT

ECM28 Satellite Meeting 'Introduction to Software Development for Crystallographers'



The first SIG9 computing school, an 'Introduction to Software Development for Crystallographers' was held at Warwick U., August 23-24, 2013. The school followed the general lines of recent IUCr Commission for Crystallographic Computing Schools; lectures were enhanced with in–depth tutorials and discussion among all participants.

Instructors were drawn from most areas of crystallographic application (e.g. protein, small-molecule and powder). An opening reception was held in Coventry at a West Midland Balti restaurant. Following a welcome from the organizers (H. Powell and A. Thorn), A. McCoy (UK) gave an introduction to 'Planning My Programming' and P. Emsley (UK) followed with his thoughts on 'Scripting and Automation of Existing Software'. E. Krissinael (UK) gave a tour round the 'Use and Usage of Libraries', using those from CCP4 as specific examples. R. Giordano (France) described 'Visualizing Statistics in *R*', a freely available statistical package which combines accessible statistical analysis functions with publication-quality plots and the ability to script together external programs. An afternoon of tutorials by the morning's speakers was followed by H. Powell's talk on fundamental guidelines of interface design.

On the second day, R. Neder (Germany) discussed computational aspects and the mathematical background for dealing with 'Matrices and Symmetry', and R. Cooper (UK) followed with 'Geometry and Space Groups' and methods to implement them in programs. L. Palatinus (Czech Republic) talked about 'Fourier Methods' and their implementation in code, while R. Read finished the lectures with how to deal with 'Structure Factors and Likelihood'. The afternoon was again given over to tutorials. Slides from the talks and some of the tutorials are available on the SIG's website at http://sig9.ecanews.org/sig9_warwick.html. Another workshop will be held before ECM29; details will be posted on the SIG's website.

MEETING REPORT

ACA 2013

Honolulu, Hawaii, July 2013
www.amercrystalassn.org/

Taken from ACA *RefleXions*, Fall, 2013

The meeting began with workshops on Biological SAXS - Theory & Practice; Getting the Most out of the Cambridge Structural Database, and on the *GSAS-II* Crystallographic Analysis System.

There were four Transactions symposia on various aspects of the Role in Crystallography of Neutron & Synchrotron Sources. TR.01, chaired by Richard Gillilan, was concerned with Small-Angle Scattering; TR.02, chaired by Christine Dunham, focused on Supramolecular Assemblies; TR.03, chaired by Antonio dos Santos and Jonathan Hanson, featured Emerging Characterization Facilities & Tools; and TR.04, chaired by Christine Beavers and Simon Teat, was about Chemical Crystallography.

Bau Award Lecture by Tom Koetzle



Thomas Koetzle

The inaugural 2013 ACA Bau Award for Exceptional Research Achievement in Neutron Diffraction was presented to Thomas Koetzle. In his talk entitled 'From Amino Acid Structures to Metal Hydrides: Four Decades of Single-Crystal Neutron Diffraction', Tom reviewed highlights of the research carried out together with his collaborators at Brookhaven National Laboratory (BNL) and at Argonne's Intense Pulsed Neutron Source (IPNS).

Koetzle noted that less than 1% of reported crystal structures used neutrons. A new generation of neutron sources and instrumentation have removed some of the obstacles to such analysis. Nuclear positions are determined directly, thereby removing any bias that may be introduced in X-ray work due to asymmetries in the electron-density distribution. More important, hydrogen and deuterium are located with precision similar to carbon. The neutron's magnetic moment can also be exploited to examine spin densities, *e.g.* in molecular magnets.

At BNL in the '70s Koetzle worked with neutron diffraction pioneer Walter Hamilton studying precise structures of the amino acids. From these studies they were able to discuss the strength of the hydrogen bonds that play a central role in molecular recognition in biology.

The second theme of Tom's work at BNL was studies of transition metal hydride complexes that established the details of bonding of hydrogen to metals. This work was done in collaboration with Bob Bau and his research group at USC. This 25-year collaboration resulted in more than 40 publications. They utilized H/D substitutions to confirm the absolute stereochemistry of enzymatic reaction products, and their work established precise *M*-H distances in a variety of bonding environments for a variety of metals. Following the closure of BNL's high-flux beam reactor, Tom moved to Argonne's IPNS and continued his work there for a decade with Arthur Schultz and his group.

Koetzle concluded his lecture by reviewing the new sources coming on line and how they will impact the practice of neutron crystallography, making it possible to use smaller crystals and much shorter data collection times.

Fankuchen Award to Richard Dickerson (Lecture by Alexander McPherson)



Alex McPherson

An overflow crowd attended a lecture by Alex McPherson honoring Richard Dickerson, recipient of the 2013 ACA Fankuchen Award. Dickerson sent a message expressing his appreciation to the ACA for the award.

McPherson treated us to a virtuoso lecture and placed Dickerson's many contributions to crystallography and structural biology in historical context. He showed vintage photographs of Sirs W. H. and W. L. Bragg, Lindo Patterson, David Harker, Linus Pauling, Dorothy Hodgkin, John Kendrew, Max Perutz, Francis Crick and Jim Watson. He reviewed milestones in the development of crystallization research, starting in 1840 with the crystallization of hemoglobin and leading up to the demonstration in the 1930's of diffraction from globular proteins by Bernal, Fankuchen and Hodgkin.

Dickerson was a graduate student in Bill Lipscomb's laboratory at Minnesota where he worked on boranes, receiving his PhD in 1957. He then worked with John Kendrew on the structure of myoglobin in England. He returned to the U. S. and at Caltech worked on the structure of cytochrome *c*. In 1969 Dick collaborated with the artist Irving Geis on 'The Structure and Action of Proteins'. This slim classic combined Geis's amazing illustrations with Dickerson's text and introduced generations of students to protein structure.

Alex concluded his lecture with a review of Dickerson's contributions to our knowledge of DNA structure. Dick's group was the first to obtain the atomic-resolution structure of B-DNA with the famous 'Dickerson dodecamer'. The Dickerson B-DNA model, together with Olga Kennard's model of A-DNA and Alex Rich's Z-DNA, undergirds much of today's explosive growth in nucleic acid structural research.

Dick Dickerson is a true giant in structural biology who was 'Present at the Flood', to quote the title of his 2005 book telling the story of how structural molecular biology came about.

Tom Koetzle

AW.03: Etter Early Career Award



Eric Ortlund

The 2013 Margaret C. Etter Early Career Award was presented to Eric Ortlund, Emory U, for elucidating structures of human nuclear receptors, pharmacological targets with high potential in a broad range of diseases. Eric described suppression of nuclear receptor signaling by a noncoding RNA. Noncoding RNAs are recognized as playing major roles in cell signaling and disease, yet the structural mechanisms driving

their evolution and function are poorly defined. Eric's work is shedding much-needed light on this process.

Albert Reger

Kenneth Trueblood Award



Tom Terwilliger

Tom Terwilliger received The Trueblood award for 'exceptional achievement in computational or chemical crystallography'. Terwilliger's lecture, 'Molecular replacement and model-building using distant homology models as templates', showed how to extend the reach of molecular replacement by using complementary information from the structure-modeling field and by using the local similarities of the search model to the structure to be determined. He presented a method he called 'morphing', in which a starting model is distorted (morphed) to improve its match to an electron-density map. He showed that a rather poor electron-density map can be used to morph a model with amazing accuracy, and to allow structures more distant from the target structure to be solved by molecular replacement.

Connie Rajnak

The 2014 meeting will be held May 24-28 in Albuquerque, NM. Details are available at www.amercrystalassn.org.

MEETING REPORT

Frolic Goats High-Pressure Diffraction

Poznań, Poland, April, 2013



Participants of the FgHp-6 (left to right): Michał Kaźmierczak, Mohamed Mahgoub, Szymon Sobczak, Kacper Rajewski, Ewa Patyk, Mathias Meyer, Kinga Ostrowska, Magdalena Sikora, Damian Paliwoda, Anna Maria Hernández Martin, Sławomir Domagała, Virginia Amate Padilla, Witold Zieliński, Marcin Stachowicz, Cristina Bosch Orea, Grzegorz Szklarz, Anna Olejniczak, Joanna Bąk, Marek Daszkiewicz, Mina Eshak, Maria Igartua Medina, Andrzej Okuniewski, Joachim Kusz, Michał Andrzejewski, Hanna Tomkowiak, Hanna Piotrowicz, Jędrzej Marciniak, Michael Hanfland, Weizhao Cai, Maciej Bujak, Hesham Alsoghier, Maria Nowak, Akram Behrooz, Marcin Podsiadło, Kamil Dziubek, Andrzej Katrusiak; absent from the photo are: Michalina Anioła, Jolanta Darul, Olga Ermakova, Katarzyna Kowalska, Paulina Pojawis, Małgorzata Ratajczak-Sitarz, Paulina Wawrzyniak, Zofia Dega-Szafran and Mirosław Szafran.

The 6th Frolic Goats High-Pressure Diffraction Workshop (FgHp-6), held at the Adam Mickiewicz U. in Poznań, April 14-16, 2013, welcomed 45 participants, representing 7 countries. The workshop is traditionally dedicated to the introduction to high-pressure research. The lectures included the subjects of 'Strain in materials' (A. Katrusiak), 'High-pressure experiments and data reduction with *CrysAlisPro*' (M. Meyer), 'Single-crystal diffraction at the ID09A beamline of the ESRF' (M. Hanfland), 'Pressure-induced conformational phase transition in 4,4’-bipyridine hydrobromide monohydrate' (M. Anioła), 'High-pressure crystallization of DL-mandelic acid' (W. Cai), 'Low-temperature and high-pressure behaviour of 1,2,4-trichlorobenzene. Melting-point differences in trichlorobenzene isomers' (M. Bujak), 'Comparative studies of 2-methyl-4-nitroanilinium hexachloridostannate(IV), bromide and two non-centrosymmetric chlorides' (M. Daszkiewicz), 'High-pressure diffraction study of toluene pursued in a collaborative project' (K. Dziubek) and 'HP experiments and data reduction with *CrysAlisPro*' (M. Meyer). For the first time the workshop included a poster session, for which *CrystEngComm* provided two poster prizes, awarded to Kinga Ostrowska for the poster entitled 'Menthol-mint racemate' and to Witold Zieliński for his work on 'Hydrogen bonds NH...N in compressed benzimidazole polymorphs'. The workshop included hands-on laboratory exercises in the DAC operation, alignment, loading, diffraction experiments, compressibility measurements in a piston-and-cylinder press, and computation and processing of high-pressure data.

The FgHp-6 Workshop was generously sponsored by the Faculty of Chemistry, Agilent Technologies and Bruker Poland, and was organized by the Team supported by the Foundation for Polish Science. On the first day of FgHp-6 the participants made a bicycle trip to the Morasko Meteorite Nature Reserve, where a rain of meteorites fell about 5000 years ago, and had a barbecue. On the next day after sessions, a tour was guided by Andrzej Muszyński through the museum at the Inst. of Geology, where several of the largest meteorites in Central Europe are exhibited, including one of 300 kg found in 2012 in the Morsko Reserve.

Andrzej Katrusiak

OBITUARY

Charles Caughlan (1915-2013)



Charles Norris Caughlan was born in Pullman, Washington, on January 20, 1915. While attending Grey's Harbor Junior College in Aberdeen, Washington, during the early 1930's, Charles observed the struggles and violence against the workers attempting to unionize the timber industry. The experience solidified his liberal political attitudes and he would work for peace and justice for the rest his life.

In 1941 he earned his PhD in chemistry at the U. of Washington, specializing in X-ray crystallography. From 1944-1946 he worked at Eastman Kodak Company in Rochester, NY, followed by a long and distinguished career as a chemistry professor at Montana State University, serving as head of the Chemistry Department for several years. Charles was a member of ACA, and served as local chair for the Bozeman ACA meeting in 1964. After retiring from the university, he was able to devote his time to his other passions: civil liberties and human rights, Scottish dancing, baking, gardening, music and travel. In 2006 the Montana ACLU awarded him the Jeannette Rankin Award 'for his tireless efforts to advance civil liberties and human rights and his steadfast commitment to peace and justice'.

The full article can be found in ACA *RefleXions*, Fall, 2013.

adapted from the Bozeman Daily Chronicle, May 5, 2013

OBITUARY

Ray Davis (1938-2013)



Raymond Edward Davis was born November 7, 1938 in Hobbs, New Mexico. At the U. of Kansas at Lawrence he was honored with a membership in Phi Beta Kappa and, in 1960, received a Bachelor Degree in Chemistry. He married his high-school sweetheart. He received his PhD in 1964 where he worked with Al Tulinsky at Yale U., and was a post-doc with David Harker at Roswell Park Memorial Inst. in Buffalo, New York. Ray accepted a position as an assistant professor in the Chemistry Department of the University of Texas at Austin in the fall of 1966.

Ray had a passion for teaching. He received the **Outstanding Teacher Award** given by campus freshman honor societies five times. In 1995, he was an inaugural member of the University of Texas's Academy of Distinguished Teachers, and was eventually made a University Distinguished Teaching Professor Emeritus. He coauthored *The Principles of General Chemistry* with Ken Whitten and completed the 10th edition of this textbook with George Stanley of LSU in 2012. Several editions have been translated into other languages. Ray also wrote high-school chemistry texts, and was an early proponent of hands-on undergraduate research projects.

Ray was Local Chair for the San Antonio ACA meeting in 2002. A paper on hydrogen-bonding analysis using graph sets by Ray and Joel Bernstein that was published in *Angewandte Chemie* has had more than 5500 citations.

Ray spent every day loving life, family, music, history and photography and simply learning something new. After moving to the country near Salado Village, Texas, Ray discovered a new love - watching and identifying hundreds of birds.

Ray's friends and former students created the Raymond E. Davis Endowment Scholarship in Chemistry and Biochemistry in his honor. Ray's passing has left a big empty hole in the lives and hearts of all who were privileged to love and know him.

The full article can be found in ACA *RefleXions*, Fall, 2013.

The Davis family and Vincent Lynch

OBITUARY

Jerome Karle (1918-2013)



Jerome Karle, who died on June 6th of liver cancer, was born Jerome Karfunkle on June 18, 1918, in Brooklyn, the son of immigrants from Eastern Europe. A precocious product of New York public schools, he completed high school at just 15 years old and went on to the City College of New York. He graduated in 1937 along with Herbert Hauptman (they did not know each other at the time) and Arthur Kornberg, another of City College's many Nobel laureates. He obtained a master's degree in biology from Harvard and pursued graduate studies in chemistry at the U. of Michigan.

At Michigan, he met his future wife Isabella Lugoski, on the first day of a physical chemistry lab. At the U. of M, Karle studied the diffraction patterns resulting from firing electrons at gases. After completing their dissertations in 1943, they moved to the U. of Chicago to work on the Manhattan Project. In 1946, they moved to the US Naval Research Laboratory (NRL) in Washington DC, where they remained until their retirement in 2009. Initially, Jerome and Isabella continued to focus on electron-diffraction experiments. In parallel, Jerome made a theoretical analysis predicting what diffraction patterns to expect from oriented hydrocarbons, and this got him wondering about applying his theories to the analysis of crystal structures. It was around this point that the Karles were joined by Herbert Hauptman.

Starting in 1950, Karle and Hauptman drew on fundamental knowledge about the nature of matter (specifically, that one cannot have negative electron density) to find mathematical relationships among the diffracted waves. Soon after, they established a probability theory, which they brashly announced in 1953 in an abstruse monograph entitled 'Solution of the Phase Problem'.

Early reception of the Karle–Hauptman work was at best muted. Quoting Karle himself, 'during the early 1950s ... a large number of fellow scientists did not believe a word we said'. The tide was turned by Isabella when she applied the work to challenging structures such as peptides. In 1966, Isabella and Jerome Karle published a landmark paper in *Acta Crystallographica*, which laid out step-by-step how to determine crystal structures. Others joined the venture with computer programs, and ever increasing numbers of ever more complex structures came to be determined through direct methods.

By the time Karle and Hauptman received the Nobel prize, Karle had become prominent in crystallography circles; Jerome served as President of the IUCr in the early 1980s, and was President of the ACA in 1972. He was elected to the National Academy of Sciences in 1976.

Karle's interests were broad, as suggested by the name he gave his unit at the NRL - the Laboratory for the Structure of Matter. The work there ranged from electron diffraction of gases to quantum chemistry of excited states, to the study of glasses and amorphous materials, and of course, crystals. Although these activities engaged several group members and were largely experimental, the Jerry I knew was a lone theoretician; he authored many papers alone and his main working interaction was with a computer programmer who tested his theories.

Ultimately, Karle's major contribution was to allow researchers to shift their focus from the intricacies and challenges of crystallography to molecules and biochemical mechanisms. He turned chemical crystallographers into crystallographic chemists.

The mathematical approaches that Karle and Hauptman established, known as direct methods, have helped researchers to elucidate the structure of key molecules such as vitamins and hormones, and to

gain insight into biochemical mechanisms. Karle and Hauptman shared the 1985 Nobel Prize in Chemistry for their work.

The awarding of the Nobel came as something of a surprise to Jerome. He was 39,000 feet over the ocean on a transatlantic flight when the pilot made an announcement over the loudspeaker. 'We are honored to have flying with us today America's newest Nobel Prize winner, and he doesn't even know it. In fact, the award is so new that Dr Jerome Karle, located in seat 29C, left Munich this morning before he could be notified that he was a recipient of the Nobel Prize in Chemistry'. In the cabin, he was feted with champagne.

Survivors include his wife Isabella; three daughters, chemists Louise Karle Hanson and Jean Karle, and geologist Madeleine Karle Tawney, and four grandchildren.

*Adapted from Nature, **499**, p. 410 (July 25, 2013) by Wayne Hendrickson, with some additions from the June 14th Washington Post article by Emily Langer*

REGIONAL NEWS

ACA History Portal Online



In January 2014 the ACA launched its new History Portal (www.amercrystalassn.org/history_home), which provides crystallographers, historians and curious science enthusiasts alike easy access to multimedia historical material gathered throughout the years by the Association.

Interested readers will be able to find fascinating, absorbing and inspirational stories of great men and women who contributed to the development of the science of X-ray crystallography. Audio and video recordings from ACA meetings and conferences will also be available for viewing.

This site provides an alternative, more convenient, path to the information: popping up with a simple Google search, it will contain the complete online versions of the personal memoirs, plus links to the videos hosted on the YouTube website.

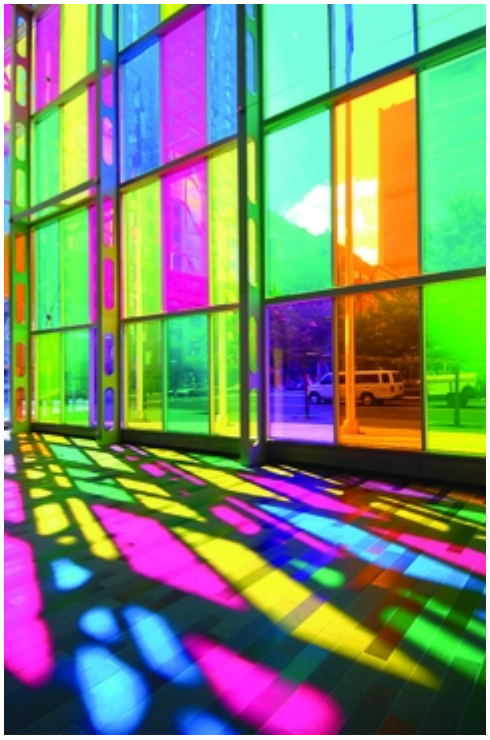
Timing could not be more perfect for its implementation: the History Portal debut coincides with the start of the International Year of Crystallography.

Comments and suggestions should be made to Virginia Pett (pett@wooster.edu).

Chiara Pastore, ACA RefleXions, Winter 2013

IUCR ACTIVITIES

IUCr 2014: Plans are beginning to … crystallize…



Montréal's Palais des congress: the beauty of aperiodicity.

A lot has happened on the IUCr 2014 front in the last couple of months. A full listing of microsymposia, workshops and confirmed keynote speakers is now available online and session chairs are being added every day. John Miao, Daniel Bish and Juan Manuel Garcia Ruiz have all accepted our invitation to deliver Plenary talks and we expect to be able to announce more very soon.

Of equal importance, the Call for Abstracts has been released and within days we received several completed submissions with many more listed as being 'in progress'. The success of each IUCr Congress hinges on the quality of the scientific program, and much of that depends on what you, the world's crystallographers, contribute. Although usually most of the abstracts are submitted closer to the deadline, in this case, February 11, 2014, we encourage you to do so as soon as possible. You should know that abstract reviewers will be actively working on the submissions as the abstracts arrive, so if you would like your abstract considered before the high-traffic period begins, please submit early. Your reviewers and organizing committee will most definitely appreciate it.

A variety of support options have now been posted and we expect more to come. The IUCr Travel Support Program will provide up to $1000 to successful graduate student and postdoctoral applicants. University-specific programs will also be available, and have started to be detailed on our website's Student Program page. And photographers young, old and in between can compete for two top prizes of $1000 each for submitting the best image of Crystallography in Everyday Life, thanks to a collaboration between the International Year of Crystallography 2014 (IYCr) and Agilent Technologies Inc. Many of the submitted photographs will be displayed during the Congress.

In addition to the core scientific program consisting of 112 microsymposia, up to 38 keynote lectures, 6 plenary talks and numerous poster presentations, several scientific and commercial workshops will also be offered on-site and have now begun to be detailed on our website. Space in the Congress Centre and in the Program is limited though, so if you have a side event you would like to schedule, please contact Michèle Bourgeois-Doyle (michele.bourgeois-doyle@nrc-cnrc.gc.ca) soon to see what options exist.

Great spaces are still available for exhibitors and sponsorship opportunities abound! Companies wishing to be a part of IUCr 2014 can select what options best suit their business needs by visiting our Sponsorship and Exhibitor Opportunities page.

Finally, only the most observant of you will have noticed that our Congress logo has been updated to acknowledge and echo IYCr. It is our pleasure and our honour to host the Congress during this important year and we do intend to celebrate it as fully as possible!

Important Dates and Deadlines

Early Bird Registration Deadline: Before and until May 1, 2014

Speaker/Poster Presenter Registration Deadline: May 1, 2014

Abstract Submission Deadline: February 11, 2014

Author Notification of Acceptance: Mid April 2014

Accommodations Deadline: Until blocks are sold out or June 25, 2014, whichever comes first

Tours Subscription Deadline: 48 hours before each tour but minimum needs to be reached by July 22, 2014 in order for the tour to take place

23rd Congress and General Asssembly of the International Union of Crystallography, August 5-12, 2014, Montreal, Quebec, Canada.
http://www.iucr2014.org/