INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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IUCR JOURNALS NEWS

The story behind the metrics



You can find no livelier debate amongst friends and colleagues than discussing the relative merits of the impact factor as a measure of an academic journal's importance. I did exactly this, to my peril, at our IUCr Congress in Montreal this summer. Over a chilled drink on the roof terrace of the convention centre, I happened to steer the conversation to metrics such as the impact factor, *h*-index and altmetric scores and how they are now commonplace in measuring research output from our universities and institutions of learning. Opinions varied widely amongst my colleagues and I can confidently say I heard comments from both ends of the spectrum in terms of whether they should be abolished immediately or enhanced with more sophisticated add-ons and supplemented with entirely new metrics.

The impact factor was probably the start of this crusade to provide some quantitative measure of performance in our research communities. The impact factor was devised by Eugene Garfield, the founder of the Inst. for Scientific Information. Little did Garfield know that nearly 40 years later we'd be still fiercely debating the merits of the impact factor as a measure of journal importance and the effect of policies of the journal editorial boards.

To add to this debate, Jorge Hirsch in 2005 introduced his *h*-index to the scientific community. The *h*-index is the number of papers by a particular author that receive *h* or more citations. The *h*, standing for highly cited, rightly or wrongly has already become one of the most widely used metrics for research evaluation. In describing what the *h*-index is, it is probably easier to talk about what some scientists do not like about it:

- It awards all co-authors on any one paper with the same measure.
- The older the author, the higher their score (in most instances).
- The *h*-index is used across disciplines, which is not measuring like for like.
- Books are given the same count as an article.

These are just a few of the criticisms, so it comes as no surprise that many scientists are lobbying for change to the *h*-index in order that it might emphasise different features. Whilst many of these proposed changes are themselves subject to fierce debate, the whole landscape is set to change yet again with a new player to the field simply called alternative metrics or altmetrics.

The growing interest and need to develop alternative measurements of scientific productivity resulted in the formation of a different way of analysis and the company called Altmetrics.

Altmetrics exploits the growing number of scholars moving their day-to-day work to the web. Google Scholar, Mendeley and ResearchGate all claim high levels of user sign-up. This trend is also witnessed across social media sites such as Twitter and to a lesser extent Facebook and LinkedIn.

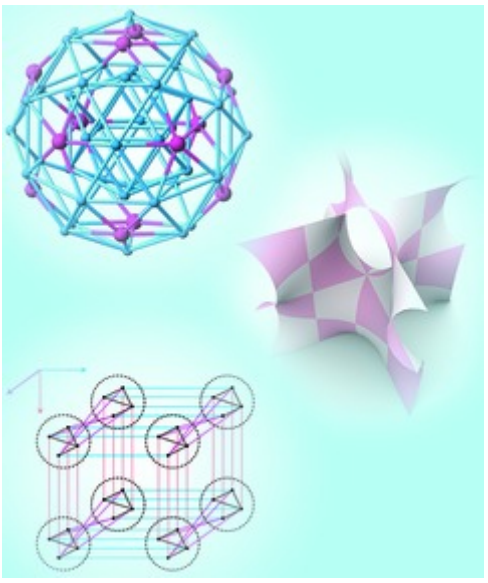
Altmetrics aims to expand our view of what impact looks like, but also comment on what is making the impact. What is making the impact is today as important as Eugene Garfield's world some 40 years ago. With the move to web we can now examine how raw data such as data sets, programs and code are being consumed, we can drill down to precise sections of a paper to determine what is making the impact, and comments posted on blogs, forums and social media platforms can be captured and tagged to papers to ensure we begin to understand the true value of research output. In 2010 Altmetrics published a manifesto that is well worth a read: http://altmetrics.org/manifesto/.

Whatever your conclusions when discussing this topic during your next dinner party, I will wager we will be still talking about its merits in another 40 years from now.

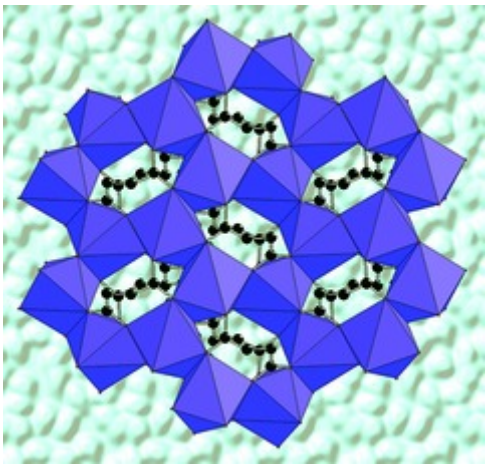
Jonathan Agbenyega, IUCr Business Development Manager (ja@iucr.org)

IUCR JOURNALS NEWS

Recent special issues

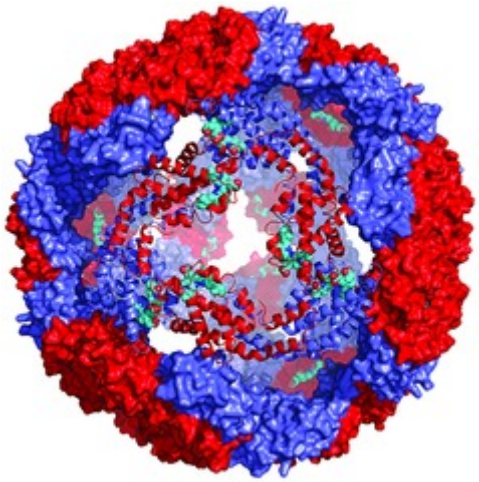


In their Guest Editorial (http://doi.org/whc) in this second special issue on **Mathematical Crystallography** in *Acta Crystallographica Section A: Foundations and Advances*, Massimo Nespolo and Gregory McColm describe the current activities of the IUCr Commission on Mathematical Crystallography. A recent and fruitful cooperation with US mathematicians has resulted in crystallographic special sessions at sectional meetings of the American Mathematical Society and specialized conferences of the Society for Industrial and Applied Mathematics (SIAM). In particular, the 2013 SIAM Conference on Mathematical Aspects of Materials Science in Philadelphia, USA, was the occasion to gather articles, partly arising from that meeting, for this issue. Perhaps befitting this digital age, this is a virtual issue, spanning three regular issues, but all appearing during the International Year of Crystallography. The result is a wide but necessarily incomplete selection from the panorama of research activities, which demonstrates the actuality and the importance of mathematical crystallography for every researcher interested in the periodic structure of matter, whatever the dimension and geometry.



A virtual issue featuring **Coordination Polymers**, with an introduction by Len Barbour, was published in *Acta Crystallographica Section C: Structural Chemistry* in July 2014 (http://tinyurl.com/coordinationpolymers). The past two decades have witnessed a veritable explosion of reports detailing the solid-state structures of coordination compounds consisting of conceptually infinite one-dimensional chains, two-dimensional nets and three-dimensional frameworks. The concepts involved are relatively simple; crystalline coordination polymers are most often formed from solutions containing metal ions and bridging ligands. The seemingly unlimited opportunities for preparing novel coordination polymers arise not only from obvious choices that influence structural topology (*i.e.* bridging-ligand geometry and metal-ion coordination mode) but also from a range of other factors, some of which can be quite subtle. The collection of articles selected for this virtual issue serves to showcase the amazing diversity of the field.





A collection of articles from the IUCr **Diffraction Data Deposition** Working Group (DDD WG) has been published in the October 2014 issue of *Acta Crystallographica Section D: Biological Crystallography* (http://tinyurl.com/diffractiondata). The DDD WG was commissioned by the IUCr in 2011 with John Helliwell as chair to examine the benefits and feasibility of archiving raw diffraction images in crystallography. The group initiated spirited discussions on this subject on the CCP4 mailing list, held workshops to gather input on the idea of archiving raw images, and encouraged wide analysis of the ideas and challenges. In this issue, several researchers in the field of macromolecular structure determination have written a collection of articles discussing the archiving of diffraction images, what it

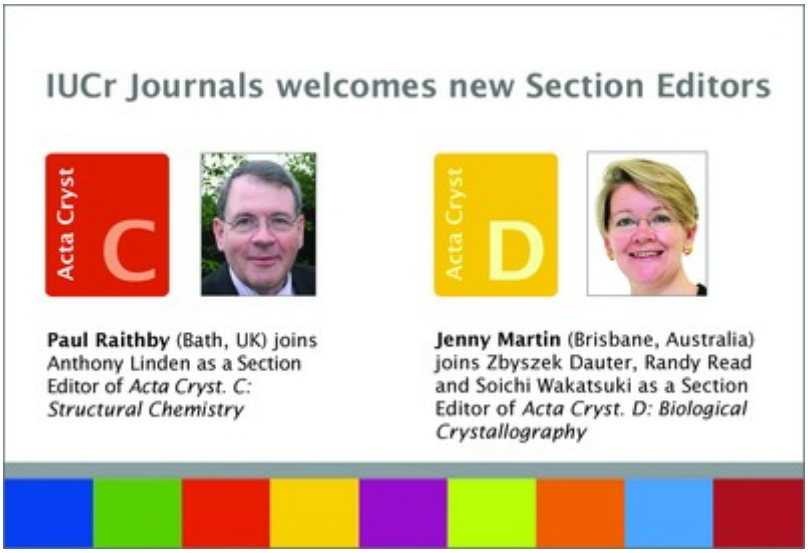
would make possible, and what challenges it poses. The DDD WG hopes that these articles will stimulate extensive debate and action in the crystallographic community.



The *Journal of Synchrotron Radiation*'s latest special issue (http://tinyurl.com/storagerings) explores **Diffraction-Limited Storage Rings (DLSRs) and New Science Opportunities**. Guest-edited by Mikael Eriksson and J. Friso van der Veen, the issue contains 22 articles connecting recent advances in accelerator technology with the new science that can be done at upcoming and future DLSRs. The cover illustration shows an artistic impression of the new MAX IV facility, currently under construction in Lund, Sweden, and one of a new generation of storage-ring-based synchrotron light sources employing a multibend achromat lattice to reach emittances in the few hundred pm rad range in a circumference of a few hundred metres. (Image courtesy of FOJAB arkitekter.)

Just some of the special issues in the pipeline: **Energy Materials** (*Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*), **CCP4 2014 Study Weekend - Two Way Street - Complementary Methods** (*Acta Crystallographica Section D: Biological Crystallography*), **Molecular Parasitology - Advances in Biology and Supporting Drug Discovery** (*Acta Crystallographica Section F: Structural Biology Communications*), **X-ray Radiation Damage to Biological Crystalline Samples** (*Journal of Synchrotron Radiation*) and **Free-Electron Lasers** (*Journal of Synchrotron Radiation*).

IUCR JOURNALS NEWS

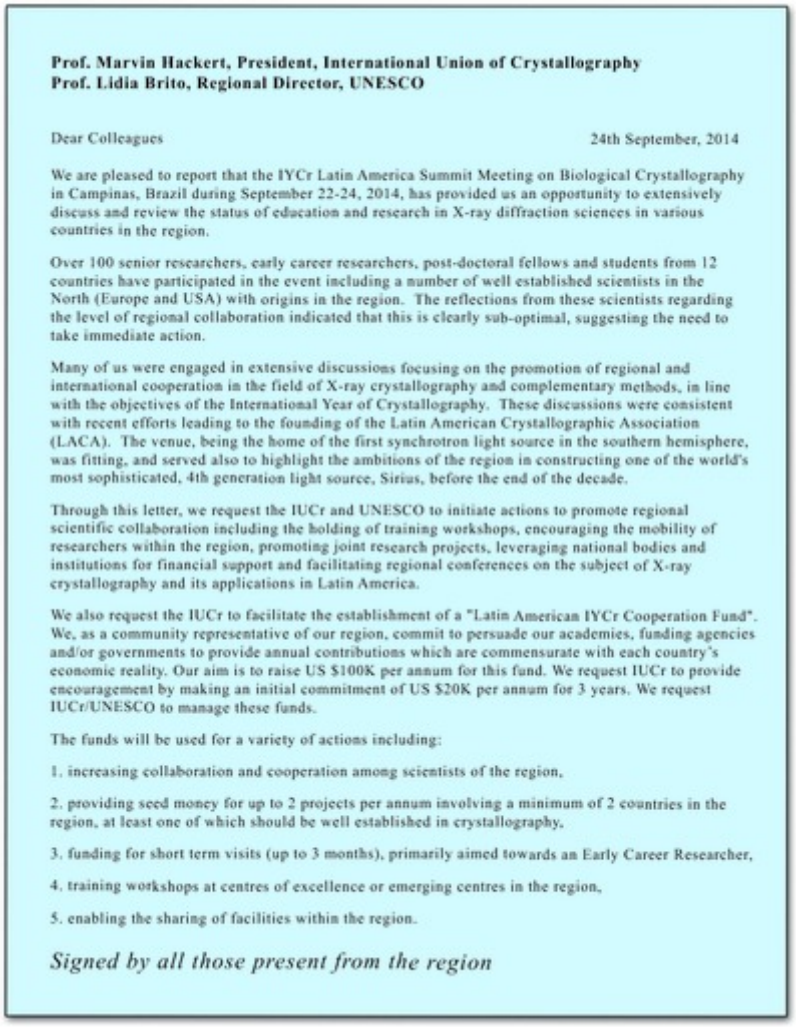


IYCR 2014

Latin American Summit a Success



Signing the petition.



Prof. Marvin Hackert, President, International Union of Crystallography
Prof. Lidia Brito, Regional Director, UNESCO

Dear Colleagues 24th September, 2014

We are pleased to report that the IYCr Latin America Summit Meeting on Biological Crystallography in Campinas, Brazil during September 22-24, 2014, has provided us an opportunity to extensively discuss and review the status of education and research in X-ray diffraction sciences in various countries in the region.

Over 100 senior researchers, early career researchers, post-doctoral fellows and students from 12 countries have participated in the event including a number of well established scientists in the North (Europe and USA) with origins in the region. The reflections from these scientists regarding the level of regional collaboration indicated that this is clearly sub-optimal, suggesting the need to take immediate action.

Many of us were engaged in extensive discussions focusing on the promotion of regional and international cooperation in the field of X-ray crystallography and complementary methods, in line with the objectives of the International Year of Crystallography. These discussions were consistent with recent efforts leading to the founding of the Latin American Crystallographic Association (LACA). The venue, being the home of the first synchrotron light source in the southern hemisphere, was fitting, and served also to highlight the ambitions of the region in constructing one of the world's most sophisticated, 4th generation light source, Sirius, before the end of the decade.

Through this letter, we request the IUCr and UNESCO to initiate actions to promote regional scientific collaboration including the holding of training workshops, encouraging the mobility of researchers within the region, promoting joint research projects, leveraging national bodies and institutions for financial support and facilitating regional conferences on the subject of X-ray crystallography and its applications in Latin America.

We also request the IUCr to facilitate the establishment of a "Latin American IYCr Cooperation Fund". We, as a community representative of our region, commit to persuade our academies, funding agencies and/or governments to provide annual contributions which are commensurate with each country's economic reality. Our aim is to raise US $100K per annum for this fund. We request IUCr to provide encouragement by making an initial commitment of US $20K per annum for 3 years. We request IUCr/UNESCO to manage these funds.

The funds will be used for a variety of actions including:

1. increasing collaboration and cooperation among scientists of the region,

2. providing seed money for up to 2 projects per annum involving a minimum of 2 countries in the region, at least one of which should be well established in crystallography,

3. funding for short term visits (up to 3 months), primarily aimed towards an Early Career Researcher,

4. training workshops at centres of excellence or emerging centres in the region,

5. enabling the sharing of facilities within the region.

Signed by all those present from the region

The IYCr2014 Latin America Summit Declaration took the form of an Appeal letter, with 67 signatories. The declaration from the IYCr2014 South Asia Summit and other IYCr2014 declarations can be viewed at www.iycr2014.org/declarations.

The IUCr-UNESCO Latin American Summit took place in Campinas, Brazil, September 22-24, with support by Funding Agencies CNPq, CAPES and FAPESP, sponsorship by Molecular Dimensions, Bruker, NanoTemper, Agilent, GE Healthcare, Rigaku/Dairix, Formulatrix, Astex, TTP Labtech and Incoatec, and Institutional Partnerships with CNPEM, LNBio, LNLS, ABCr and IFSC. This was the second summit meeting of the IYCr, where the scientific theme was biological crystallography and complementary methods. Over 100 senior scientists, young researchers, post-doctoral fellows and students from 12 countries met during the summit meeting held at the LNLS in Campinas.

Delegates enjoyed a mix of lectures on the history of Latin American crystallography, and examples of current cutting-edge research and the collaborative programs that are taking place in Latin America. We learnt how initiatives such as CeBEM have contributed to increased collaboration and strengthening of crystallography by providing funds for training courses, exchanges and sharing of facilities.

Marvin Hackert (President, IUCr) gave the opening lecture on IYCr2014 and the role and benefits of the OpenLabs and summit meetings. Lidia Brito, Regional Director for Latin America for UNESCO, spoke about the partnership of UNESCO with the IUCr for IYCr2014. Glaucius Oliva (IFSC/USP) presented an overview of the history of crystallography in Latin America, while Antônio José Roque da Silva (LNLS) presented a glimpse of the future with the construction of a fourth-generation synchrotron (Sirius) at Campinas. It became clear during the meeting how much progress has been made in biological crystallography in Latin America over the last 25 years, with dozens of groups where there were

previously none. The LNLS has had a central role in making this possible by giving access to equipment as well as financial support to groups spread around the region.

A memorable highlight was the keynote lecture given by Nobel Laureate Ada Yonath who discussed the progress to design better therapeutics from our understanding of the structure of the ribosome. She was given a standing ovation at the close of her talk. Another highlight was a round-table discussion mediated by Samar Hasnain (Editor-in-Chief of IUCr Journals) where the panelists reflected on the changes, opportunities and challenges facing the further development of crystallography in Latin America. At the close of the final session, a petition was presented and unanimously approved by those attending to ask for continued support from the IUCr and UNESCO to promote regional scientific collaborations in Latin America, with a pledge to partner in supporting these activities from regional resources. More information and a full description of the program can be found on the IYCr website under summits (http://www.iycr2014.org).

The summit was a clear success both scientifically and in generating the enthusiasm of working together for strengthening crystallography in Latin America. The success of the event was due to the positive spirit of the participants and the hard work of the local organizers Richard Garratt, Andre Ambroiso, Iris Torriani and Glaucius Oliva.

Marvin L. Hackert, President of IUCr, and Samar S. Hasnain, Editor-in-Chief of IUCr Journals

IYCR 2014

PANalytical OpenLab Ghana, June 9–12, 2014







The IUCr-UNESCO OpenLab Ghana, organized within the frame of the IYCr2014 in partnership with PANalytical B.V. and F. Malawi Engineering Co. Ltd, was held on June 9–12 at the Centre for African Wetlands on the campus of the U. of Ghana in Accra.

The event consisted of four days of training in X-ray powder diffraction, comprising presentations, hands-on sessions on software and practical sessions on the Empyrean, which was recently installed at the U. of Ghana in the Dept. of Physics.

Thirty powder diffraction enthusiasts were selected and attended the event celebrating IYCr2014, including PhD students, young and senior researchers and a few professionals from industry. Most of the attendees were from Ghana, though other West African countries were represented: Nigeria, Senegal, Liberia and Burkina Faso.

The OpenLab logistics and organization was carried out jointly by PANalytical B.V., F. Malawi Engineering Co. Ltd and the Dept. of Physics at the U. of Ghana in Accra.

The scientific lectures delivered by Gilberto Artioli (U. di Padova, Italy) included the nature of X-rays and their interaction with matter, basics of crystallography and diffraction, the experimental geometries for powder diffraction, data interpretation (including phase identification, available software and databases) and an introduction to full profile refinement. A few advanced applications were also shown, with a focus on materials science and mineral resources.

Marco Sommariva (PANalytical) covered most of the applied aspects such as the details of instrumental components, calibration and practical data collection. Quantitative phase analysis was also introduced.

Extensive hands-on laboratories involving data collection on the available instrumentation and demonstrations on data treatment and analysis were followed with extreme interest. All the attendees showed a real eagerness to learn and the participation was very interactive. Highly positive feedback was expressed during the whole event about both the lectures and the practical sessions.

Both lecturers promised to remain in contact to respond to further questions as a follow up to the course, although the delicate issue of freely available software and databases in developing countries is a general issue to be faced at the international level. A special effort was made during the OpenLab to present and operate freely available software, such as *GSAS*, and open-access databases, such as COD, in the attempt to direct the attendees towards independent crystallographic activities.

Overall it has been a highly rewarding experience, both for the lecturers and for the audience. The general impression is that the spirit and aims of IYCr2014 were perfectly targeted.

Gilberto Artioli, OpenLab Lecturer

IYCR 2014

Bruker OpenLab Uruguay, July 23–31, 2014



Participants Geraldine Hernández (Colombia), Andrea Naranjo (Brazil), Martín González (Brazil), Andrea Araya (Costa Rica) and Nilda Pinto (Perú) during a session of crystal selection and mounting in the lecture room.



Participants during a lecture.



A Type 1 OpenLab was held in Montevideo, Uruguay, this southern winter, motivated by the recent installation of the Bruker D8 Venture diffractometer at the Facultad de Química, U. de la República, Montevideo. The event, organized by the Laboratorio de Cristalografía, Estado Sólido y Materiales (Cryssmat-Lab), Cátedra de Física, DETEMA, and supported by the Facultad de Química, the Ministerio de Educación y Cultura of Uruguay, the Regional Office of Science for Latin America and the Caribbean of UNESCO and the IUCr, brought together 20 participants (young professors and advanced PhD students) from Argentina, Brazil, Costa Rica, Colombia, Perú and Uruguay who had the chance to learn the fundamentals and applications of single-crystal X-ray diffraction. From the 20 participants, 13 brought single crystals and were able to collect data and make the structure determination and refinement of

their own structures on site, and had the chance to follow the whole process from crystal mounting to CIF preparation with their own samples and results.

The OpenLab program included 14 hours of lectures and 12 hours of practical sessions on the history and fundamentals of crystallography, taught in Spanish, by the organizers Leopoldo Suescun, Álvaro W. Mombrú and Ricardo Faccio from the Facultad de Química, and the invited Javier Ellena from the Inst. de Física de Sao Carlos, U. de Sao Paulo. Additionally, it included 12 hours of lectures and 12 hours of practical sessions on the application of single-crystal diffractometry taught by Bruce Noll from Bruker. He also devoted a very significant number of hours to helping the participants select and mount their crystals, performing crystal evaluation and data collection set-up and guiding the data processing and structure determination process of organic, metal-organic, mineral and metallic samples.

One full day of the program (Sunday, July 27th) was devoted to collecting data to allow all participants to have their own data to work on practical aspects of refinement and CIF construction by themselves. Finally, the advanced participants enjoyed a special topic lecture on charge-density analysis given by Claude Lecomte, Vice-President of the IUCr.

During the official Opening Ceremony of the OpenLab, the official inauguration of the Single-Crystal X-ray Diffraction Laboratory of the Facultad de Química took place, in the presence of authorities or representatives from the U. de la República, the Facultad de Química, the Comisión Sectorial de Investigación Científica (CSIC), the Agencia Nacional de Investigación e Innovación (ANII) and the Programa de Desarrollo de las Ciencias Básicas (PEDECIBA), who provided the funds to purchase the instrument. Claude Lecomte introduced IYCr2014 to the participants and representatives from UNESCO and the Ministry of Education and Culture of Uruguay (co-sponsors of the OpenLab with Bruker), emphasizing the importance of the state-of-the-art equipment now available in Uruguay thanks to the synergic work by the IUCr, local Uruguayan agencies and Bruker.

The last morning of the event was devoted to presentations by the participants. Those who solved their structures showed their results, discussed their problems and received advice on how to finalize their work from other participants and lecturers. The last activity was the evaluation of the event. A round of comments from the participants suggested a unanimous positive view of the event when considered overall. Suggestions on the time distribution and an emphasis on different topics were received and will be used to adjust the program for future events of this kind. The list of participants, including contact information, and a summary of answers from a detailed and anonymous evaluation questionnaire are available from the web site of the OpenLab (http://cryssmat.fq.edu.uy/OpenLab/evaluationbyparticipants.pdf).

Leopoldo Suescun, Local Organizer

IYCR 2014

Agilent OpenLab Turkey, September 1–5, 2014





Following the United Nations declaration of 2014 as the International Year of Crystallography (IYCr2014), UNESCO and the IUCr have been planning scientific and public engagement events intended to increase the popularity and understanding of crystallography. The crystallography group in Dokuz Eylül University, being conscious that crystallographic teaching needs to educate students in the practical aspects of different areas of crystallography, organized an OpenLab meeting in partnership with IUCr, UNESCO and Agilent Technologies.

The IUCr-UNESCO OpenLab Turkey attracted about 56 applicants who were students, researchers and even some faculty from countries with close historical contacts with Turkey. The 45 selected delegates included post-docs, recent MSc and PhD graduate students, MSc students and one professor.

The scheduled dates of the courses in OpenLab Turkey were from September 1 to 5, 2014. Over the first four days of the workshop, fundamental aspects of a crystallographic investigation were presented in 11 lectures and 9 practical sessions. The international team of lecturers and instructors was composed of:

- Dinçer Ülkü (DÜ), Hacettepe U., Turkey;
- Ahmet Erdönmez (AE), Ondokuz Mayıs U., Turkey;
- Engin Kendi (EK), Hacettepe U., Turkey (former president of the Turkish Crystallographic Association);
- Orhan Büyükgüngör (OB), Ondokuz Mayıs U., Turkey (a Co-editor of *Acta Crystallographica Section E*);
- Daniel Baker (DB), Agilent Technologies;
- Horst Puschmann (HP), OlexSys Ltd;
- Stephen Astley (SA), Ege U., Turkey;
- Hasan Karabıyık (HK), Dokuz Eylül U., Turkey;
- Radek Kuzel, Charles U., Prague, Czech Republic (a member of the IUCr Executive Committee).

Details of the Scientific Program and the presentations of the meeting are available at http://iycropenlabturkey.org/.

The topics were carefully selected to cover the main aspects of crystallographic research, and were aimed at enabling each participant to independently solve and interpret a structure and to prepare a CIF file for publication. In the first two days, mostly intended for learning the fundamentals of crystallography, the main theoretical and practical characteristics of small-molecule single-crystal X-ray crystallography were covered. The principles underlying X-ray diffraction (AE), structure solution techniques (EK), data collection and reduction strategies (DB), structure determination on *OlexSys* (HP) and an introduction to supramolecular interactions (SA) were covered. The sessions in the subsequent two days concentrated on the applications of the principles given in the first two days. While doing these, structure refinement and details of reporting a structure (OB) were also taught, and the participants were informed about the Cambridge Structural Database and its applications (HK). The scientific program of OpenLab Turkey was concluded with an impressive and pleasurable presentation by Radek Kuzel.

During the meeting, the attendees took the opportunity to collect diffraction data from their own crystals and to prepare their structure reports in a computer laboratory. The final session, including a short oral exam, was organized to assess the level of understanding of the participants. In this session, succinctly prepared final structure reports were presented by participants in the morning of the last day of OpenLab Turkey. The success rate was highly encouraging. Certificates were awarded to the participants by the General Coordinator of OpenLab Turkey, Muhittin Aygün, and Radek Kuzel. The closing ceremony of the OpenLab Turkey was held on September 5 in the holiday resort of Dokuz Eylül U., enabling participants and lecturers to enjoy a good time together.

The successful development of the OpenLab Turkey was possible thanks to the full commitment of the lecturers, instructors and attendees, and the financial support provided by the IUCr, Agilent Technologies, the Turkish Atomic Energy Authority, Dokuz Eylül U. and the Turkish Crystallographic Association.

Muhittin Aygün, Local Organizer

IYCR 2014

STOE, DECTRIS, Xenocs OpenFactory: Contributing to the Spirit of IYCr2014; September 10–19, 2014



Twenty crystallographers, representing 15 nationalities, attended the IUCr-UNESCO OpenFactory, which was sponsored and organized by STOE, DECTRIS and Xenocs, and took place as part of IYCr2014.

The delegates received ten days of intensive training from STOE, DECTRIS and Xenocs staff and guest scientists in cooperation with the IUCr. The opening ceremony was held in Darmstadt on September 10th, where STOE offered a warm welcome to the participants. This was followed by the first lecture, in which DECTRIS took the delegates on an exciting journey through the instrumentation for X-ray analysis. From laboratory to synchrotron sources, advances in modern instrumentation were presented using several examples of difficult structures, whose solution was possible only owing to the features of MYTHEN and PILATUS detectors.

In Grenoble, after a fascinating introduction to the history of crystallography and today's challenges by Jean-Louis Hodeau, Directeur de Recherche at Institut Neel-CNRS and member of the IUCr Commission on Synchrotron and XFEL Radiation, the delegates received theoretical and practical training on small-angle X-ray scattering. Four different workshops were organized at Xenocs Headquarters so that the participants could get in-depth knowledge on Xenocs sources and optics, Xenocs SAXS/WAXS systems, and data treatment software, with experiments carried out on the Xeuss 2.0 SAXS/WAXS system.

The delegates also visited the European Synchrotron Radiation Facility (ESRF) and more specifically the ID02 SAXS beamline. A sunny weekend spent discovering Grenoble old town and a breathtaking view of Mont Blanc from the Bastille fortified site ended the first part of the OpenFactory very nicely.

In Darmstadt, the participants were trained in single-crystal and powder XRD at STOE's labs. The training involved one day of theoretical lectures, while two full days focused on hands-on workshops, from sample preparation to structure determination, for X-ray single-crystal as well as X-ray powder diffraction. As part of this, the participants performed measurements on the STOE IPDS 2/2T and STADIVARI single-crystal diffractometers, and STADI P and STADI MP powder diffractometers.

Thereafter, the participants joined STOE's Single-Crystal User Meeting, which included, among others, talks on 'Scaling, Indexing and Extreme Conditions Crystallography' by STOE's scientists. Furthermore, Dieter Fenske, Karlsruhe Inst. of Technology, gave an impressive talk on 'Nanosized Transition Metal Clusters; Synthesis, Structures and Properties', followed by Harald Krautscheid, U. of Leipzig, presenting his fascinating work on metal-organic frameworks.



As a highlight, Gautam R. Desiraju, Immediate Past President of the IUCr, gave his premier speech on '100 years of Crystallography: Seen through 15 small-molecule crystal structures', in which he illustrated some of the most fascinating developments over a timespan of a century.

The positive feedback from the participants was overwhelming. Next to all the knowledge being shared, it has been impressive how strong ties have been built among the participants, connecting young crystallographers from across the world in the spirit of IYCr2014.

Martin Fark, STOE Co-CEO and CFO

IYCR 2014

Calling all budding crystallographers!

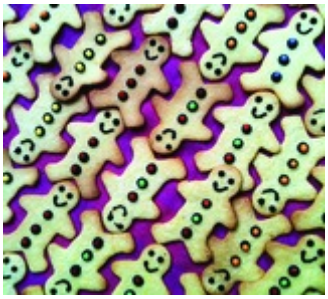


The Royal Society of Chemistry and the IUCr are offering young students worldwide the opportunity to participate in a global experiment to try to find the best conditions for growing the biggest crystals. Global Experiment 2014: The Art of Crystallisation, a project for IYCr2014, is aimed at students aged between 7 and 16 years, working in consultation with their teachers to learn how to dissolve samples of different materials, to grow large and regular crystals from saturated solution, and to test the effects of changing temperature, water softness or other environmental conditions. Students can post their results on a central website, and help in analysing the growing collection of data from all over the world.

The Global Experiment 2014 will remain open for the 2014-2015 academic year. For more information, visit www.iycr2014.org/participate/global-experiment-2014.

IYCR 2014

Crystallography in Everyday Life - IUCr/ Agilent Photo Competition







To celebrate IYCr2014, the IUCr and Agilent Technologies organized a photo competition in which amateur and professional photographers were invited to submit stunning images that capture the spirit of crystallography in the places, objects and experiences of everyday life.

The winning entries, chosen from 254 submissions, were announced at the IUCr Congress in Montreal. Two USD 1000 travel bursaries were awarded to: Mélanie Meyer (France) for her witty image 'When baking meets crystallography'; and Jens Preben Morth (Norway) for 'IceRowan', showing ice crystals forming on rowan berries.

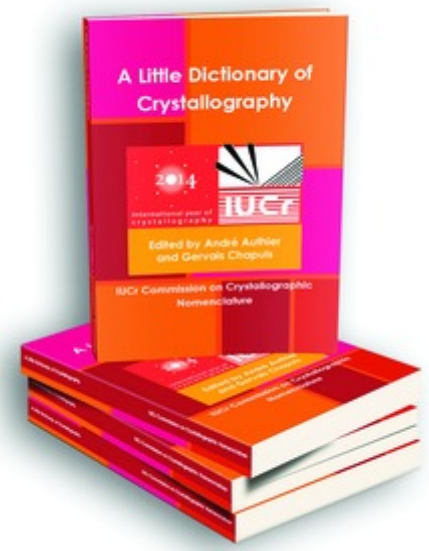
In parallel, an Australian satellite competition was held on April 22, 2014 at O'Reilly's Rainforest Retreat, Lamington National Park in Queensland. From the >130 images submitted to the international competition by that stage, 25 were shortlisted by a selection committee and these were displayed on poster boards at the conference mixer. Conference delegates were asked to select their favorite images. The winner of the competition was Graziano Lolli (Italy) for his image 'Romanesco broccoli' (see photo, courtesy of P. Walden). This event was organized with the assistance of P. Agrawal (Australian Academy of Science), M. Zema (IYCr Project Manager), and J. Archbold, P. Walden and J. Martin (all from the U of Queensland), and the prize of AUD 500 was sponsored by the Crystal29 conference. Selected images will be shown publicly at venues around Australia. (*by Bostjan Kobe and Jenny Martin; modified excerpt from SCANZ Newsletter, June 2014)*

The 3 winning and 13 most highly commended entries have been used in a celebratory Agilent/IYCr2014 Academic Calendar for 2014/2015. These and other noteworthy submissions were exhibited during the Montreal Congress and can be viewed in a special section of the IYCr2014 website at www.iycr2014.org/participate/photo-competition/result.

BOOK REVIEW

A Little Dictionary of Crystallography

Editors: André Authier and Gervais Chapuis
Publication date: 16 July 2014
Pages: xiv + 238



The lack of a compendium of crystallographic terms and the many questions related to matters of definitions and nomenclature led André Authier, Chair of the IUCr Commission on Crystallographic Nomenclature, to put forward the idea of an *Online Dictionary of Crystallographic Terms* at the 20th IUCr Congress in Florence (August 2005). The idea was received enthusiastically by the IUCr Executive Committee, and the website was soon established as a collaborative WiKi, using the same software that powers Wikipedia. Under the continuing guidance of its Editor-in-Chief, Gervais Chapuis, the system remains open to *bona fide* crystallographers wishing to correct or modify existing definitions, or to introduce new ones. The Nomenclature Commission carries collective responsibility for ensuring the quality of the definitions.

This special publication is a printed snapshot of the contents of the *Online Dictionary of Crystallography*. It was produced by the IUCr Commission on Crystallographic Nomenclature as a contribution to the educational outreach activities of IYCr2014.

Its dissemination in a handy pocket-sized format will encourage wide circulation and may be useful in classrooms and public libraries, as well as in laboratories and on individual scientists' book shelves.

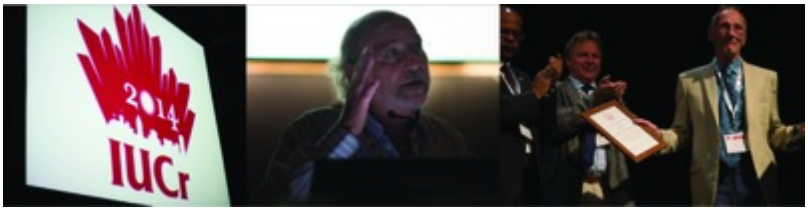
The most up-to-date version of the definitions in this book can be found at http://reference.iucr.org/dictionary.

The book is available for online purchase at http://tinyurl.com/little-dictionary. Order your copy now to take advantage of the special IYCr2014 discount: USD 13.80/EUR 11.00/GBP 9.00 + postage & packing (price from January 2015: USD 23.00/EUR 18.50/GBP 15.00 + postage & packing).

MEETING REPORT

XXIII IUCr Congress and General Assembly

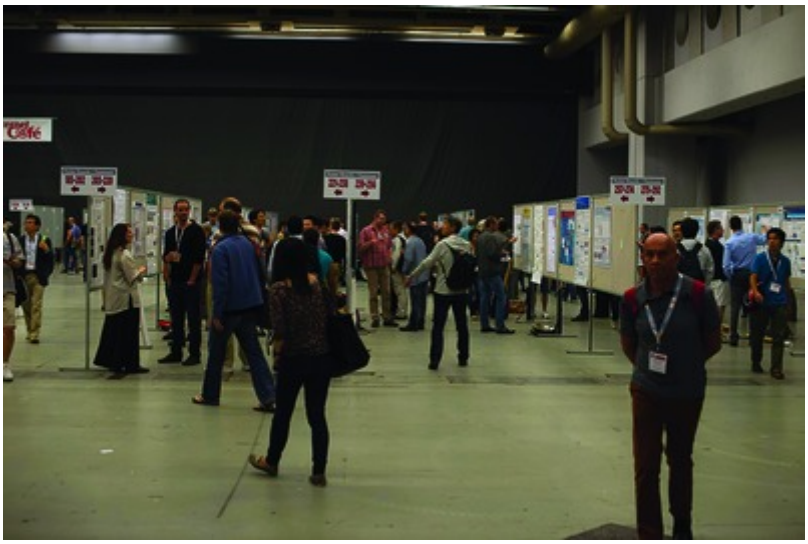
Montreal, Canada, 5-12 August 2014



The time has come to bid a final *adieu* to IUCr 2014 and all it entailed. It is with great pride and satisfaction that your Canadian hosts reflect on the summer's events and their special contributions to the International Year of Crystallography (IYCr). And none more so than the Congress's co-chairs, Mirek Cygler and Albert Berghuis, who look forward to actively participating in the Hyderabad Congress, albeit in a slightly more relaxed role!



Dan Schechtman





In total, IUCr 2014 attracted 2425 participants representing 67 different countries. Over 2300 abstracts were submitted, of which over 700 were presented orally. And everyone was treated to an authentic taste of Montréal life by experiencing the interconnectivity of its academic and scientific communities with its food, jazz and circus culture.

The International Program Committee, chaired by Jim Britten, delivered a scientific program packed with highlights. In the Opening Ceremony Ewald Prize lecture on superspace crystallography, Ted Janssen (top photo, far right) made a difficult subject as clear as the Montreal sky. On the following day, Nobel Laureate Dan Shechtman delivered the story of the discovery and acceptance of quasicrystals with passion and humor. In other Plenary Lectures we learned of self-assembled nanostructured materials from Juan Manuel Garcia-Ruiz (top photo, center), David Bish took us to Mars for some powder diffraction studies, and John Miao showed us the power of coherent diffraction imaging and electron tomography.

A series of 36 Keynote lectures, including the Gjønnes Prize lectures from Michiyoshi Tanaka and John Steeds, brought us the most exciting crystallographic research from the leaders in our field. The IUCr Commissions were well represented in talks on everything from charge density to HIV; from Li batteries to the most powerful X-ray sources developed to date; from minerals to MOFs, from mathematics to magnetics; from carbon to quasicrystals, from a Voyage dans le cristal to membrane trafficking.

The program committee would like to thank the over 220 microsymposium co-chairs who gathered together almost 700 speakers and put excitement into every day of the meeting. Attendance was terrific, if not overwhelming at times. These topics attracted enough additional science to fill almost 1500 posters in sessions organized by Alba Guarné, with a number of poster prizes awarded by our generous sponsors. Again, all of the Commissions were well represented, with aperiodicity and electron diffraction showing a significant increase in interest over previous congresses.

The tradition of a Software Fayre was continued, organized by Martin Lutz, allowing software developers to demonstrate the latest improvements to their programs. To round out the scientific offerings, seven on-site workshops were offered covering software (*USPEX*, *SHELX*, *OLEX2*), aperiodic crystals, XAFS and XFEL sources. A Rietveld refinement workshop was offered by PANalytical, and two well attended post-Congress satellite workshops were held at McMaster U. examining magnetic symmetry/structures and advanced electron diffraction.

Complementing the core program were special exhibits celebrating IYCr, organized by Louise Dawe and Michele Zema. A series of public lectures were held, movies were shown and posters were displayed, all with the intent to raise awareness and interest in this multi-faceted discipline. A photo competition and a virtual reality experience helped to round out the offerings.

This event will surely live on in the fond memories of both the organizers and the participants as one of the shining highlights of the IUCr congress series and of IYCr!

Keynote lectures

Combining neutrons with high-performance computing to understand complex biological systems



Paul Langan

The technique of neutron protein crystallography is currently available at only four facilities in the world: ILL (France), Oak Ridge (USA), FRM-II (Germany) and J-PARC (Japan). The keynote speaker Paul Langan, after receiving his PhD in Biophysics from Keele U., UK, conducted experiments at ILL, LANSCE, and Oak Ridge, where he became the director of the biology and soft matter division. Currently, he is a Program Advisory Committee member of J-PARC in Japan and a member of the Scientific and Technical Advisory Panel of NMX in ESS.

In his keynote lecture, Langan presented an overview of neutron facilities at ORNL and gave examples of applications in biological research. He then discussed how the future challenges in biology are driving further technological developments that will lead to new understanding in the emerging areas of dynamic functional assemblies, disorder and flexibility, biological membranes and associated complexes, and biomolecular function and ligand binding.

Nobuo Niimura

Structural genomics of chromatin regulators for biological discovery and epigenetic therapy



Cheryl Arrowsmith

Cheryl Arrowsmith (Canada) presented a program for developing inhibitors of protein modifiers of epigenetics, *i.e.* heritable changes in phenotype caused by mechanisms other than DNA sequence. Epigenetic modifiers place, interpret or remove modifications like methylation and acetylation on DNA and associated proteins, and may be useful targets to repurpose diseased cells into non-dangerous states. X-ray crystallographic structures and assays are used to find inhibitors which are potent, selective, cell-active and non-toxic. Exciting examples of inhibitors of different protein modifiers which use diverse modes of inhibition were presented: a small molecule which competes for the histone binding site in a SET domain of lysine methyltransferase was brought to market as a research tool. Other lysine methyltransferase inhibitors which target the SAM co-factor binding site feature high specificity.

An inhibitor acts allosterically against a dimeric arginine methyltransferase. A compound that prevents aberrant complex formation with fusion proteins in MLL-rearranged leukemia decreases the viability of these cancer cell lines. An inhibitor specific for the acetyl-lysine binding site in bromodomain-containing proteins is effective against a variety of cancer lines. A molecule specific for one malignant brain tumor protein family member acts by inducing protein dimerization. The program holds great promise for the production of molecules for the worldwide community for the investigation and treatment of a diverse set of diseases.

T. Martin Schmeing

Biological macromolecules

Crystallography of HIV/AIDS

The MS05 session entitled 'The crystallography of HIV/AIDS', chaired by A. Wlodawer (USA), was preceded by a keynote lecture given by E. Arnold (USA) in which he summarized his longstanding efforts aimed at characterization of HIV reverse transcriptase, a prime target for drug design. The studies of different classes of inhibitors bound to the enzyme were the key to creation of a number of successful anti-HIV agents. The failure of protease-directed drugs due to viral resistance and the methods of its prevention were discussed by C. Schiffer (USA). The two talks by P. Kwong (USA) and R. Diskin (Israel) dealt with anti-HIV vaccine design and the rational design of antibodies, respectively. While a vaccine is still not available, such studies go a long way to setting a path which may lead to its creation. A. Price (UK) gave an interesting talk on the interactions of the capsid protein with the host factors, while talks by K. Siu (Canada) and Y. Xiong (USA) dealt with structural investigations of other host proteins. The session provided an excellent summary of the state of the field 25 years after the first crystal structures of an HIV protein (protease) became available.

A. Wlodawer

Improving your crystallography: best practices and new methods



MS22 speakers and chairs (from left): L. Redecke, M. Gerstel, R. Read, P. Afonine, Z. Dauter, G. Evans and M. Yamamoto (co-chair); inset: W. Hendrickson.

In microsym. MS22, the first three speakers presented new methods of diffraction data collection and analysis in the context of the multi-crystal approach, and the last three described improvements in structure determination techniques leading to more accurate structural models. G. Evans (UK) presented the current status of the microfocus beamline and multi-crystal data collection facility at the Diamond Light Source. W. Hendrickson (USA) described their novel S-SAD structure determinations using long wavelengths and many crystals with a cluster analysis. The new serial crystallography approach using SR compared with XFEL-SFX was presented by L. Redecke (Germany). M. Gerstel (UK) introduced the new index *BDamage*, identifying the regions in structures most affected by radiation damage. P. Afonine

(USA) discussed the error sources of calculated electron-density maps and described the improved method of FEM (feature enhanced map), recently implemented in the *Phenix* software suite. In the last talk, R. Read (UK) presented modified likelihood functions concerned with tNCS applicable for molecular replacement and implemented in *Phaser*. The session was moved to a larger room after the first talk due to an overflow crowd.

Masaki Yamamoto

Small-angle X-ray scattering on biological macromolecules

Microsym. MS28 provided an impressive view of the state of the art in automation of data collection and analysis, together with recent results on complex systems. Recent developments in cryo-SAXS promise lower consumption of radiation-sensitive samples, enhanced automation and new options for time-resolved studies.

A study of cytokine:receptor interactions demonstrated the power of SAXS data and the seamless interface with other biostructural and biophysical techniques. A study of polyketide synthetases emphasized the need for expert sample preparation. A final problem elucidated bacterial protein:DNA packing. It was evident how beamline-based groups on both sides of the Atlantic have contributed to advance the field. Computational approaches to use the data for higher resolution modeling were discussed.

We wish to emphasize the importance of efforts to reduce ambiguity in data interpretation, through developing noise-independent fitting criteria, validation of data quality and three-dimensional models.

Bente Vestergaard and Zehra Sayers

Disease-related proteins

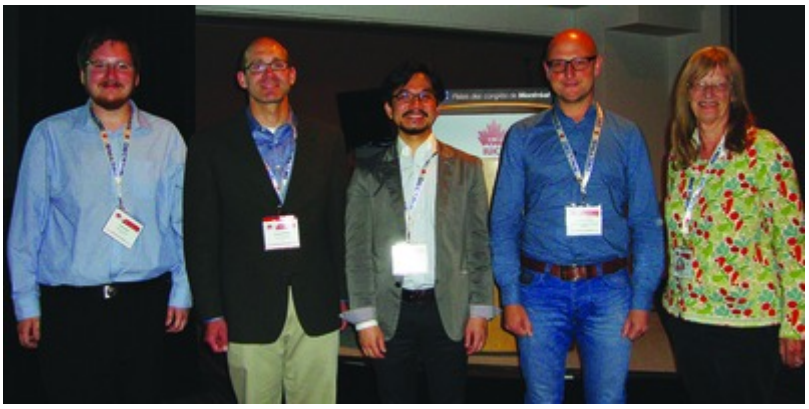


MS53 speakers and chairs (from the left): F. Van Petegem, M. Rizzi, S. Ribeiro, B. DeLaBarre, M. Banfield, M. Miyano and J. Cherfils.

The microsym. MS53 gave an up-to-date view of how crystallography can be crucial for understanding the role played by specific proteins in the pathogenesis of neurodegenerative disorders, cancer and cardiovascular diseases. Examples of the use of structures for the development of pharmaceuticals endowed with either a spectacular specificity or a loose one that results in efficacious multi-targeting was illustrated, together with their use in understanding the molecular bases of mutations that cause a disease. Moreover, the fascinating interplay at the host-pathogen interface was covered with examples from diseases affecting humans or plants. D. Eisenberg (USA) showed how a conserved self-assembly mechanism affecting different proteins is at the base of different pathologies, and how crystallography is contributing to the elucidation of the structure of amyloid fibers and toxic oligomeric intermediates. Evolutionary links between different disease-related proteins were also illustrated.

Menico Rizzi and Sandra Ribeiro

Structure of metal compounds mimicking protein active sites



MS91 speakers and chairs (left to right): J. Hall, G. Rohde, J. Kondo, C. Fischer and C. Cardin.

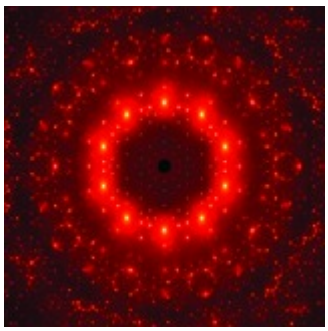
In microsym. MS91, C. Fischer (Germany), a synthetic chemist, described both expected and unexpected results in the model chemistry of molybdenum and tungsten oxidoreductase enzymes, highlighting the difficulties of emulating nature. G. Rohde (USA) described the challenging syntheses of methane monooxygenase intermediates. The work required low temperatures to study the dibridged Fe^{IV}-O-Fe^{IV} system, using crystallography and XAFS, and featuring the very short Fe-O distance of 1.8 Å. He described the highly reactive open-core structures of the form (Fe=O)-O-(Fe=O). A. Višnjevac (Croatia) described work on hydrophobic cavities created using a calixarene-type methodology to produce 'bowl' systems, which could contain Cu^{I}, Cu^{II} or Zn^{II}.

The remainder of the session concerned mercury complexes of oligonucleotide duplexes (J. Kondo, Japan) and the interactions of ruthenium polypyridyl cations with nucleic acids (J. Hall, UK).

Christine Cardin and Pat McArdle

Physical and/or fundamental

Recent advances in quasicrystal research



False-color image of the high-energy integrated precession pattern from icosahedral Tb-Cd taken on the 6-ID-D beam line at the Advanced Photon Source. Credits: Diffraction pattern taken by A. Kreyssig, M. Ramazanoglu and A. I. Goldman. Samples grown by T. Kong and P. Canfield. All researchers from Ames Lab and Iowa State U. Publication: A. I. Goldman *et al.*, *Nature Materials* **12**, 714 (2013).



MS02 speakers and chairs (left to right): An-Pang Tsai, S. Forster, S. Thiem, J. Wolny, H.-R. Sharma, A. Goldman; inset: T. Seki. Missing: F. Eriksson.

Microsym. MS02 entitled 'Recent advances in quasicrystal research' reported the state of the art of quasicrystals. A. Goldman (USA) reviewed progress in understanding the magnetic properties of rare-earth metal (*R*) containing icosahedral quasicrystals. Interesting results included: the discovery of a series of binary $Cd_{88}R_{12}$ quasicrystals, which exhibit short-range magnetic order, and the observation of long-range antiferromagnetic order in Cd_6R approximants. The speaker reviewed Zn-Mg-*R* systems and

described the new understanding of Cd-*R* systems. The magnetic properties of all *R*-containing quasicrystals are very similar, indicating the common feature of cluster-based intermetallic compounds. An open question is why long-range anti-ferromagnetism is present in the Cd_6R approximants and not in $Cd_{88}R_{12}$ quasicrystals. Structure analysis of the quasicrystals may answer the question.

An-Pang Tsai

Electronic and magnetic phenomena at extreme conditions

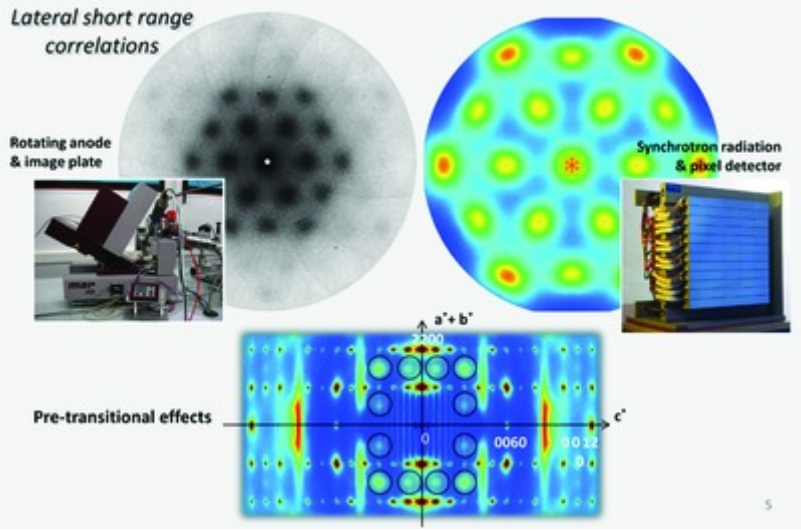


MS41 speakers and chairs: (from left, lower row) T. Yamanaka, G. Saleh, H. Nojiri, J. Attfield, S. Madson and K. Friese (co-chair); (from left, upper row) K. Prokes (co-chair) and K. Prassides.

Non-ambient pressure, temperature and/or magnetic fields often lead to novel electronic and magnetic states. In microsym. MS41 it became apparent that the term 'extreme conditions' is relative. J. Attfield (UK) showed that our ambient world could constitute extreme conditions for systems that were prepared under high pressure and temperatures and quenched. Unusual orbital order or giant negative thermal expansion phenomena can be stabilized. Novel field-induced magnetic phases can be studied most directly with scattering techniques. However, fields in excess of ~17 T are achievable only in pulsed fields. The contribution of H. Nojiri (Japan) nicely summarized such techniques. K. Prassides (UK) described how superconductivity emerges under pressure from insulating antiferromagnetic alkali fullerides. Other talks focused on maximum entropy reconstruction of electron densities from precise X-ray diffraction data under pressure (T. Yamanaka, USA), X-ray and Mössbauer spectroscopy under pressure (S. Madsen, Denmark), and the theoretical study of *ab initio* prediction of the stability of Na_2He compound under extreme pressure (G. Saleh, Russia).

K. Prokes

Diffuse scattering and partial disorder in complex structures.



Diffuse scattering in urea inclusion compounds (Rabiller).

Topics covered in MS42 included complex incommensurate structures in urea inclusion compounds by P. Rabiller (France), perovskite-based ferroelectrics by M. Pasciak (Czech Republic) and J. Pacaud (France), the disordered structure of crystalline sodium fluorosilicate by E. Stronks (Switzerland) and intergrowth zeolitic materials by W. Slawinski (Norway). In addition, Simonov (Switzerland) presented a new method for analyzing diffuse scattering involving the use of three-dimensional pair distribution functions (3D-PDF). The studies involved the use of X-ray scattering (both laboratory-based and synchrotron sources), neutron scattering and energy-filtered electron scattering.

Richard Welberry

XAFS

X-ray techniques for innovation in industry



MS38 speakers and chairs (left to right): T. Kawaguchi, W. Łasocha, S. Monaco-Malbet, F. Gozzo, K. Lawniczak-Jablonska, J. Cutler, T. Wroblewski and A. Phillips.

Utilization of X-ray techniques in material characterization is increasingly important in development, innovation and commercialization. Topics in microsym. MS38 ranged from life science to materials science, and illustrated how dedicated support programs at light sources facilitate industrial engagement.

F. Gozzo (Switzerland) described how powder diffraction is important for drug development, including the detection of contamination at sub-percent level. T. Kawaguchi (Japan) presented work on improving our understanding of lithium nickel oxide battery material by applying site-selective diffraction anomalous fine-structure (DAFS) spectroscopy. W. Łasocha (Poland) described the development of various polyoxometalate catalysts for application in green chemistry and the production of adipic acid from

cyclohexane. A. Phillips (UK) gave an example in metal-cyanide framework chemistry where neutrons and X-rays coupled with DFT calculations characterized metals in a framework. Along with industry examples, T. Wroblewski (Germany) and S. Monaco-Malbet (France) highlighted industrial liaison programs and how they have benefited small enterprises and large multi-national corporations.

Krystyna Lawniczak-Jablonska and Jeffrey Cutler

Instrumentation, techniques and/or computation

Recent advances in quasicrystal research

Small-angle scattering for magnetism and magnetic structures

In MS08, topics in magnetic SANS research were discussed including vortex and skyrmion lattices, 3He spin filters, Nd-Fe-B permanent magnets and perpendicular magnetic recording media. M. Eskildsen (USA) discussed vortex lattices in type-II superconductors. For Sr_2RuO_4, it was shown how the magnetic SANS technique could provide information on superconducting anisotropy and the nature of the pairing mechanism. SANS experiments on MgB_2 in the presence of a small-amplitude AC magnetic field revealed the existence of dual power-law correlations, which drive the system to the ground state. The recently discovered skyrmion lattices in B20 compounds can be considered as a novel particle-like state of matter. S. Mühlbauer (Germany) outlined the potential use of skyrmion textures in spintronics applications. Nd-Fe-B magnets are an extremely important class of energy materials, which are used in hybrid electric vehicles and wind turbines. T. Ueno (Japan) showed how magnetic SANS can contribute to the understanding of the coercivity mechanism in this class of materials. ^{3}He spin filters for polarizing and analyzing neutron beams are gaining popularity at neutron sources. P. Jiang (USA) reported on the properties and advantages of ^{3}He spin filters (large acceptance angle and broad wavelength range) over conventional single-crystal or supermirror polarizers. The use of the SANS technique for studying the magnetic microstructure of perpendicular magnetic recording media and the magnetization-reversal process was demonstrated by S. Lee (UK). Polarized SANS provides a powerful means to separate weak magnetic signals that are on top of a large nuclear background.

Andreas Michels

Meso- and nanostructures developed *via* heterogeneous interfaces



MS39 speakers and chairs (left to right): W. Tremel, H. Bernstein, J. Cambedouzou, M. Schmiele, K. Edler, E. Rosseeva, U. Vainio, D. Schwahn.

Microsym. MS39 covered topics ranging from biomineralisation, core-shell nanoparticles and protein function to small-angle scattering data analysis of aligned carbon nanotube forests. Highlights included invited presentations by W. Tremel (Germany) and E. Rosseeva (Germany) and a contributed one by U. Vainio (Germany). Both invited talks presented experiments on nanostructuring and self-assembly of calcium carbonate using a range of organic templates. Tremel also presented novel sample environments in levitating droplets. Stabilization of amorphous mineral polymorphs as a precursor of

mineralization was described. Vainio's talk dealt with orientation distribution of shape-anisotropic materials determined by a generalized normal distribution function related to Kohlrausch's stretched exponential decay. The function is broadly applicable across a wide variety of materials, including those that form glasses.

Karen Edler

Materials or minerals

Structure determination from low-resolution data: when the going gets tough



MS11 speakers and chairs (left to right): A. Meden, A. Edwards, K. Shankland, H. Gies, S. Smeets, P. Whitfield and I. Evans.

Diffraction data of limited resolution make structure solution difficult. The speakers of the MS11 microsym. presented various aspects of this problem and outlined different ways of solving it. K. Shankland (UK) and H. Gies (Germany) described the approach of using prior knowledge of the molecular geometry or building blocks for organic and inorganic (zeolite) structures, respectively. S. Smeets (Switzerland) described the use of complementary sources of information like electron microscopy. Two contributions elucidated the examples of applying Laue (A. Edwards, Australia) and TOF (P. Whitfield, USA) neutron diffraction for structure solution. In the discussion, the question of possible future development of a computer program for the automated simultaneous treatment of data from various sources, *e.g.* powder and electron diffraction or NMR or other spectroscopic data, was raised and the answer was positive.

Ivana Evans and Tone Meden

Role of defects in crystal structure formation, organization and stability



MS15 speakers and chairs (left to right): S. Schorr, C. Ling, J. Hadermann, P. Ferreira, I. Richardson and S. Pereira.

Microsym. MS15 concerned the importance of defects in crystallography and materials science. Two contributions were particularly noteworthy. P. Ferreira (USA) showed deformation of nanoparticles observed *in situ* under phase contrast in conventional and aberration-corrected TEM. Evidence for nucleation of dislocations and dislocation motion was observed during *in situ* nano-indentation, but upon unloading the dislocations were no longer visible. J. Hadermann (Belgium) examined new modular oxide structures using lone pair cations as chemical scissors. She addressed the role of lone pair cations such as Bi^{3+} or Pb^{2+}. Their flexibility reduces the strain that would otherwise be present at the interfaces

separating structure modules. Hadermann showed that this concept allowed the introduction of crystallographic shear planes into a perovskite structure, a feat that was considered highly unlikely before.

Sérgio Pereira

Reports to be continued in Volume 22, Number 4

MEETING REPORT

IUCr poster prize winners



Poster prize winners at Congress were (left to right), front row: A. Kupka, D. Braun, E. Bykova, M. Pillon, L. Gallington, A. Mitropoulouv, M. Walden, C. Price, J. Leung, and A. Guarné; back row: N. Tsutsumi, A. Almawi, B. Trastoy, and A. Bazin; insets: J. Lübben (left), A. Bitra (right); missing: J. Santos, D. Batuk, F. Almeida and C. Tsuboi.

IUCR ACTIVITIES

New IUCr Executive Committee



Back row: M. J. Cooper (Convener, IUCr Finance Committee), M. H. Dacombe (Executive Secretary). Executive Committee: J. M. Guss, R. Kuzel, M. Takata, W. Depmeier and S. Garcia-Granda. Front row: H. Dabkowska, L. Van Meervelt (General Secretary and Treasurer), M. L. Hackert (President), A. M. Glazer (Vice-President) and G. R. Desiraju (Immediate Past President).

At the XXIII Congress, Marvin L. Hackert was elected as the new President of the IUCr. The photograph shows the new Executive Committee for the triennium 2014-2017.

AWARDS AND PRIZES

Recipients of 2014 Gjønnes Medal



John Steeds and Michiyoshi Tanaka receive the 2014 Gjønnes Medal.

John Steeds (UK) and Michiyoshi Tanaka (Japan) received the 2014 Gjønnes Medal for their outstanding contributions to convergent-beam electron diffraction that has revolutionized electron crystallography. The work of Steeds, Tanaka and colleagues at Bristol and Sendai has had a major impact on the design of transmission electron microscopes. Steeds was a pioneer of dislocation imaging and wrote a monograph on the anisotropic elasticity theory of dislocations.

In his lecture entitled 'A Convergence of Beauty and Utility', Steeds highlighted his involvement in the development of the technique of CBED. This work had a crucial role in placing convergent-beam electron diffraction (CBED) on a firm experimental and theoretical footing. He analyzed Bloch wave propagation through crystalline material and interpretation of CBED patterns. Technical advances in EM provide the ability to form small convergent electron probes that have allowed exploration of the symmetry of patterns and their relationship to crystal symmetry, as detailed in the 'Buxton Tables'. CBED became a technique that is widely used for lattice parameter determination, strain determination and point and space group determination, and for the evaluation of charge-density distributions at a sub-atomic level. CBED is now used by almost all electron microscopists who study materials. Steeds pioneered the use of TEM as a versatile and controlled way to introduce point defects into wide band gap semiconductors.

Elena Orlova

MEETING REPORT

Workshop on Hot Topics in Contemporary Crystallography

Šibenik, Croatia, May, 2014

www.hazu.hr/kristalografi/HotTopics/



Participants at the workshop on Hot Topics in Contemporary Crystallography in Šibenik, Croatia.

The Croatian Association of Crystallographers, supported by the IUCr and ECA, organized a workshop to mark the International Year of Crystallography in Croatia. The workshop was organized to promote excellence and innovation in crystallography and to transfer state-of-the-art knowledge to the talented PhD students and postdocs in crystallography and related disciplines. The participation criteria were based on the students' CVs, recommendation letters and abstracts submitted. In addition to an intensive program (daily from 9 am to 10 pm), the participants presented 16 posters. The five most interesting abstracts were chosen to be presented in the form of short lectures. The invited lectures were: 'Hot topics in macromolecular crystallography' (E. Garman, U. of Oxford, UK), 'The whole is more than the sum of its parts' (H.-B. Bürgi, U. of Bern, Switzerland), 'Charge density' (D. Stalke, U. of Göttingen, Germany), 'Absolute structure and absolute configuration' (H. Flack, U. of Geneve, Switzerland), 'Twinning in crystallography' (R. Herbst-Irmer, U. of Göttingen, Germany) and 'Advanced solutions from the Cambridge Structural Database' (P. Wood, CCDC, UK). The selected topics are of great importance in structure determination and interpretation of data.

E. Garman told the story of her 18 years of research on TBNAT protein, published in *Science* **343** (2014), and described how to improve protein models through refinement of the electron-density map. Elspeth also gave a fine historical reminiscence on the 100 year anniversary of X-ray crystallography. Determination of the absolute structure of a molecule is of critical importance in pharmacology, biotechnology and enantioselective synthesis in organic chemistry. H.-B. Bürgi described dynamic crystallography based on analysis of displacement parameters with data collected at different temperatures to understand difficult examples of disorder. Residual density studies based on characteristics of electron structure and its modification provide information on the nature of intra- and intermolecular interactions that are essential in materials design. Knowledge gained from residual density studies used in syntheses of low-valent silicon compounds, accompanied by electron transfer, was presented by D. Stalke. R. Herbst-Irmer demonstrated how the problems of twinning can be overcome. P. Wood (CCDC) demonstrated the use of the CSD in polymorph analysis, crystal engineering and supramolecular chemistry.

Sixteen lectures and five intensive hands-on practical sessions made a high impact on the audience; discussions revealed a very sound level of knowledge and interest on the part of the young crystallographers. The inspiring atmosphere of the workshop was also supported by the presence of A. Roodt, the president of ECA. Thanks to donations, lodging and board expenses were covered for twenty participants.

The organizing committee of the workshop comprised A. Višnjevac, Chair, J. Popović, Co-Chair, M. Đaković, Program Coordinator, A. Šantić, Fund-raising Coordinator, and D. Matković-Čalogović and B. Kojić-Prodić, Scientific Advisors.

Biserka Kojić-Prodić

MEETING REPORT

Crystal 29

Queensland, Australia, April 2014



Participants at Crystal 29.

The 29th meeting of the Society of Crystallographers in Australia and New Zealand (SCANZ) was held at the Lost World Conference Centre, O'Reilly's Rainforest Retreat, Lamington National Park in Queensland from April 22-25, 2014. Over 100 delegates attended, including ten exhibitors and sponsors. Anyone invited to speak at any of the last three meetings was not eligible for an invitation at this meeting.

The program included 59 speakers and 31 posters. The speakers included four keynote speakers [J. Etheridge (Monash U.), A. Goodwin (Oxford U.), A. Vrielink (U. of Western Australia - UWA) and V. Arcus (U. of Waikato)], two SCANZ medalists [Matheison Medal: M. Kvansakul (La Trobe U.); Bragg Medal: S. Hall (UWA)] and six rising star awardees [J. Busby (U. of Auckland), J. Aickett (U. of Sydney), A. Stewart (Cardiac Research Inst.), V. Chang (Cardiac Research Inst.), S. Broughton (St. Vincent Inst. of Medical Research, Melbourne), T. Ve (U. of Queensland) and S. Thomas (UWA)]. The 1987 speaker was P. Fromme (Arizona State U.), who gave an inspirational presentation on the groundbreaking technology of serial femtosecond nano-crystallography.

Jenny Martin and Bostjan Kobe (excerpted from SCANZ Newsletter, June 2014)

AWARDS AND PRIZES

CODATA Prize 2014 awarded to Sydney Hall



Sydney R. Hall

Sydney R. Hall, now Emeritus Professor at the U. of Western Australia in Perth, Australia, through life-long leadership has resoundingly produced outstanding achievements in the world of scientific and technical data. His efforts have reached beyond crystallographic data and into many other science disciplines. He devised a universal self-defining text archive and retrieval (STAR) file format that evolved into the Crystallographic Information Framework (CIF), a momentous contribution in the area of data characterisation, and well known to structural chemists and biologists in particular as both a data and publications standard. It enables data validation for articles published by IUCr journals, an approach pioneered by Prof. Hall in his role during the 1990s as Editor of *Acta Crystallographica Section C: Crystal Structure Communications.* The CIF standard has been adopted by journals publishing crystal structure results. It also forms the essential core for data in prominent databases such as the Cambridge Structural Database (>half a million entries, growing by more than 40,000 each year) and the Protein Data Bank (>100,000 entries, growing by ~10,000 per year). These databases are widely used by researchers from many science disciplines. In addition, the STAR File approach is being applied to such diverse applications as botanical taxonomy, quantum chemistry, chemical informatics and biographical databases.

Sydney Hall will receive the Prize at SciDataCon 2014 (www.scidatacon2014.org/), the International Conference on Data Sharing and Integration for Global Sustainability, in New Delhi, India, November 2-5, 2014. This is the continuation of the CODATA Conference series, now co-organised with CODATA's sister organization, the ICSU World Data System.

From the CODATA website:

> The CODATA Prize is a major biennial award which acknowledges outstanding achievement in the world of scientific and technical data. The work of Professor Sydney Hall certainly meets these criteria and the CODATA Prize Committee is very pleased to recognise his outstanding contribution. It is particularly fitting that a crystallographer should be so recognised during the International Year of Crystallography.

John R. Helliwell and Brian McMahon

AWARDS AND PRIZES

ACA 2015 Awards

The American Crystallographic Association has announced its 2015 award winners



Greg Petsko

G. Petsko (Weill Cornell Medical College and Brandeis U., USA) has been selected to receive the **2015 Martin J. Buerger Award**. Petsko has used X-ray crystallography, molecular biology, yeast genetics, organic synthesis, enzyme kinetics and molecular dynamics calculations to understand enzyme structure and function. With D. Ringe, his long-time collaborator at Brandeis, he has developed new diffraction techniques that allow the recording of entire macromolecular data sets in milliseconds and which, combined with low-temperature experiments, can be used to capture snapshots of catalytic intermediates. Recently, he has focused his attention on neurodegenerative diseases, such as Alzheimer's, Parkinson's and Lou-Gehrig's diseases, using structure-based drug design techniques to develop possible therapeutics against what he defined as the 'coming neurological epidemic'.



Laurence Marks

L. Marks (Northwestern U., USA) is the recipient of the **2015 B. E. Warren Award**, which recognizes an important recent contribution to the physics of solids or liquids using X-ray, neutron or electron diffraction techniques. His research focuses on achieving more efficient catalysis using controlled oxide nanoparticles, improving solid oxide fuel cells to produce electricity directly from hydrocarbons, studying the wearing process caused by friction of metallic surfaces to improve prosthetic devices, and engineering a new type of concrete/cement with a cheaper energy production cost.



Yan Jessie Zhang

Y. J. Zhang (U. Texas, Austin, USA) is the recipient of the **2015 Margaret Etter Early Career Award**. The ACA established this annual award in 2002, to recognize the work of scientists at the earlier stages of their independent careers in crystallography. Zhang received her BS from Tsinghua U. in 1997, working in the field of medicinal chemistry. She earned an MS in crystallography with B. Matthews at the U. Oregon in 2000, and a PhD from the Scripps Inst. for Biological Studies in 2004 with I. Wilson. She conducted post-doctoral research on enzymes involved in transcription and oncogenic pathways with the guidance of J. P. Noel. As a grad student she solved the crystal structure of the glycinamide ribonucleotide formyltransferase. In the fall of 2008 she joined U. Texas at Austin, where her main focus

is to understand the mechanisms of transcriptional regulation and their impact in neuronal stem-cell differentiation.

Excerpt from ACA Summer Newsletter, 2014

AWARDS AND PRIZES

ACS 2014 Gordon Hammes Biochemistry Lecture



Thomas Poulos

T. Poulos (U. California, Irvine, USA) is being recognized for his outstanding contribution in scientific research at the interface of chemistry and biology, particularly in the realm of biochemistry, biological chemistry and molecular biology. Poulos' research focuses on the structural biology of heme enzymes. He solved the first heme enzyme crystal structure, cytochrome c peroxidase, and the first cytochrome P450 crystal structure. In collaboration with R. Silverman (Northwestern U., USA), the Poulos group is also working in the area of NOS structure-based drug design in an effort to develop therapeutic agents for neurodegenerative diseases. Poulos' lecture will be delivered at the American Chemical Society national meeting in the fall of 2014.

Excerpted from ACA RefleXions, Summer 2014

AWARDS AND PRIZES

Crystallographers in the news

		
Yingong Shi	Randy Read	Robert Von Dreele

The Royal Swedish Academy of Science presented the **2014 Gregory Aminoff Prize** to **Y. Shi**, (U. Beijing, China), recognizing the significance of his studies of protein complexes involved in programmed cell death.

R. Read (Cambridge U., UK) received the **Max Perutz Prize for 2013** from the European Crystallographic Association, for the development and application of statistical analysis at all stages of protein structure determination.

R. Von Dreele (Argonne National Lab., USA) received the **2013 Hanawalt Award** from the International Center for Diffraction Data (ICDD) for his insight and creativity in bringing the power of powder diffraction analysis to the study of macromolecules.

Excerpted from ACA RefleXions, Winter 2013

AWARDS AND PRIZES

2015 Aminoff Prize



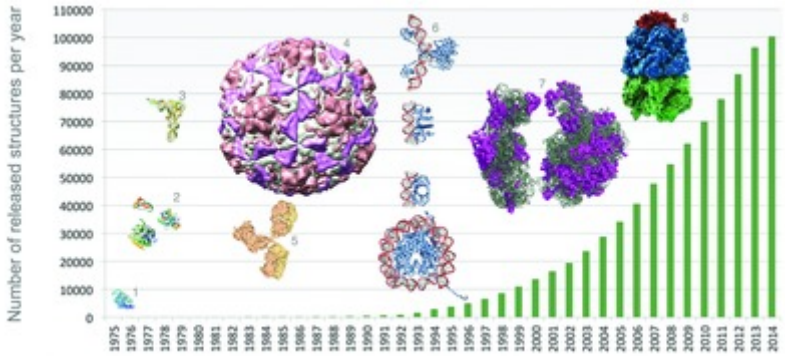
Ian Robinson

The 2015 Aminoff Prize will be awarded to Ian Robinson of the London Centre for Nanotechnology at University College London and the Research Complex at Harwell, Didcot, UK. The English page of the website is: www.kva.se/en/pressroom/Press-releases-2014/Gregori-Aminoff-Prize-2015/ and the Swedish one: www.kva.se/sv/pressrum/2014/aminoffpriset-2015/. This award is especially timely as the 2015 Nobel symposium will be on the free electron laser and next year has been designated the International Year of Light. The latter will once again be celebrated with a virtual issue in *Physica Scripta*, on this occasion to be organized by Professors Skulley, Schleich and Glauber.

The virtual issue on the Aminoff series, to which many are contributing, is growing slowly but steadily (http://iopscience.iop.org/1402-4896/page/Crystallography-Virtual-Issue, although obtaining the relevant copyright and permissions for figures has proved to be something of a nuisance for some papers. Ivar Olovsson's article on Gregori Aminoff will be published within the next couple of weeks, as will Jack Dunitz's paper, and Gérard Férey and Jean-Louis Hodeau's on E. F. Bertaut.

NOTICE

Protein Data Bank: 100,000 structures



The Worldwide Protein Data Bank (wwPDB) released to the community its 100,000th structure on May 14, 2014. Established in 1971, this central public archive of experimentally determined protein and nucleic acid structures has reached this important milestone thanks to the efforts of structural biologists throughout the world.

Excerpted from ACA RefleXions, Summer 2014