INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

Volume 22 · Issue 1

Collected archival edition
Original article text and available illustrations

Contents

> Extraction incomplete: missing article positions 1.

IUCr journals news

IUCr Journals Open to SESAME 3

Small-Angle Scattering (SAS2012) – special issue 4

What's so special about Acta Crystallographica Section C? 5

Special Issue on Crystal Engineering 7

You've published your article; now who's going to read it? 42

IYCr 2014

Launch of the International Year of Crystallography 8

Commemorative stamps 13

IYCr2014 Opening Symposium in Japan 14

Presentation and answers to a few questions about 3D printing of crystallographic models 15

IYCr Down Under 18

Feature article

Crystallography in North America 20

Meeting report

News from Latin America 24

Frontiers of Crystallography 28

HEC 16 30

First School of Crystallization and Polymorphism 31

Regional news

Latin American Crystallographic Association (LACA) 27

ACA History Portal 32

Awards and prizes

IUCr Ewald Prize to Janner and Janssen 33

Book review

Review of Authier's 'Early Days of X-ray Crystallography' 35

Editorial

Editorial 38

Special report

Start planning your travel to Montréal today! 39

IUCR JOURNALS NEWS

IUCr Journals Open to SESAME



SESAME (Synchrotron light for Experimental Science and Applications in the Middle East; www.sesame.org.jo), a third-generation synchrotron light source under construction in Allan, Jordan, is scheduled to come into full operation in late 2015/early 2016.
As part of the celebrations of the International Year of Crystallography 2014, the International Union of Crystallography (IUCr) is pleased to support the SESAME project by providing free online access to IUCr Journals for the period 2014 to 2016, inclusive. This will allow access to

- *Acta Crystallographica Section A: Foundations and Advances*
- *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*
- *Acta Crystallographica Section C: Structural Chemistry*
- *Acta Crystallographica Section D: Biological Crystallography*
- *Acta Crystallographica Section E: Structure Reports Online*
- *Acta Crystallographica Section F: Structural Biology Communications*
- *IUCrJ* (a new open-access high-influence journal launched in 2014)
- *Journal of Applied Crystallography*
- *Journal of Synchrotron Radiation*

Full details of these journals can be found at http://journals.iucr.org.

On receiving the news from the IUCr, SESAME Scientific Director, Giorgio Paolucci, commented 'On behalf of the SESAME community, I am very grateful to the International Union of Crystallography for providing access to these journals. I am sure that at this point in time scientific programs at SESAME will benefit greatly from this generous opportunity.' Samar Hasnain, Editor-in-Chief of IUCr Journals, added 'The availability of these nine journals to the SESAME staff as part of the International Year of Crystallography activities is a positive contribution from the Union to this very special project.' Chris Llewellyn Smith, President of the SESAME Council, said 'SESAME greatly appreciates and needs the goodwill and support the project is receiving from round the world, at a time when political turbulence in the Middle East is making scientific collaboration across borders harder but even more desirable'.

IUCR JOURNALS NEWS

Small-Angle Scattering (SAS2012) – special issue



This virtual special issue comprises a selection of rigorously peer-reviewed papers based on work presented at the 15th International Conference on Small-Angle Scattering in Sydney, Australia. This special issue has been edited by Elliot Paul Gilbert and Andrew J. Allen of the Bragg Inst., ANSTO, Kirrawee DC, NSW, Australia, and National Inst. of Standards and Technology, Gaithersburg, USA, respectively. Also assisting were guest co-editors Andrew Jackson, Yoshiyuki Amemiya, Charles Dewhurst, Dmitri Svergun and Aldo Craievich.

The meeting has been running for almost 50 years and *Journal of Applied Crystallography* is proud to have provided a home for some of the most cutting-edge research in the field of small-angle X-ray and neutron scattering during this time.

It is worth noting the importance and rich history behind the small-angle scattering community events, especially during IYCr2014.

The first of these meetings was held in Syracruse, USA, 26 years on from André Guinier's effective inception of the technique. The aim of the SAS meetings has always been to promote interaction among scientists who use X-ray and (already by the second meeting, which took place in Graz, Austria, in 1973) neutron small-angle scattering to study a variety of materials, such as liquids, solids, alloys, glasses, polymers, gels, liquid crystals, proteins in solution, biopolymers etc. The papers published in this issue of *Journal of Applied Crystallography* represent just a small selection of those papers presented at the conference, each paper having successfully passed through a rigorous refereeing process.

The compilation provides an excellent walkthrough of some of the history and current state of the art across small-angle X-ray and neutron scattering, covering fields of application, theory, methods of analysis and instrumentation.

The application of scattering methods in food science is brought up to date, and papers in the area of tissue engineering and drug delivery highlight nicely how small-angle neutron scattering (SANS) is being used to understand and improve the properties of the materials being applied. Other areas covered touch on the increasing role of scattering across a diverse range of materials and disciplines as we continue to witness growth in the theory, computation and instrumentation.

The special issue will provide must-have information to all crystallographers and related researchers with interests in current research and future trends in the area of small-angle X-ray and neutron scattering.

The next meeting will take place in Berlin, Germany, in September 2015 and will mark the 50th anniversary of the SAS conference series.

This special issue, which has been sponsored by PANalytical (http://www.panalytical.com), is available at http://journals.iucr.org/special_issues/2014/sas2012/.

IUCR JOURNALS NEWS

What's so special about Acta Crystallographica Section C?



The International Year of Crystallography in 2014 is a perfect opportunity for the International Union of Crystallography to refurbish all of its journals and publishing activities. Not least, significant changes are under way at *Acta Crystallographica Section C* (http://journals.iucr.org/c). The subtitle of the journal has been changed to *Structural Chemistry* and the scope widened to reflect the fact that small-molecule crystallography undeniably plays a crucial role in most aspects of the chemical sciences. *Section C* now specializes in the rapid publication of articles that highlight interesting science and research enabled by the determination, calculation or analysis of small-molecule crystal and molecular structures, with a view to how the structural observations help the understanding of a chemical, physical or structural question being investigated.

In order to inaugurate the new scope of the journal and demonstrate to readers and potential authors the types of papers that the journal is keen to attract, the journal has published **four special issues** over the last few months and we are very excited about the quality and breadth of papers in these issues.

The first issue was on *Scorpionates* (Guest Editor: Glenn P. A. Yap, Dept. of Chemistry & Biochemistry, U. of Delaware, USA; September 2013) and included contributions from some of the best authors in the field of this chemically important family of prolific and work-horse ligands wherein the structure has a palpable effect on reactivity.

The next special issue was titled *Pharmaceuticals, drug discovery and natural products* (Guest Editor: Christopher S. Frampton, Pharmorphix, Cambridge, England; November 2013) and addressed and discussed the timeless questions of polymorphism, stereochemistry and H-atom position. The structural data presented originate not just from X-ray analyses, but also from NMR and computational studies, thus demonstrating the widened scope of the journal.

The effort on refocusing the journal in 2013 culminated in the third special issue, on *Interplay of crystallography, spectroscopy and theoretical methods for solving chemical problems* (Guest Editors: Larry Falvello, U. de Zaragoza, Spain, and Alberto Albinati, U. degli Studi di Milano, Italy; December 2013). This issue presented research articles and scientific comments demonstrating that the vast utility of structure determination is manifest in other techniques in addition to single-crystal diffraction analysis, and that a description of structure can derive immense leverage from physical measurements and computational modelling.

The turn of the year saw the move to full electronic publication for *Section C* and the journal launch fully into its science-facing mission as an outlet for research in structural chemistry in its broadest sense. The most recent special issue, on *Computational materials discovery* (Guest Editor: Artem Oganov, Center for

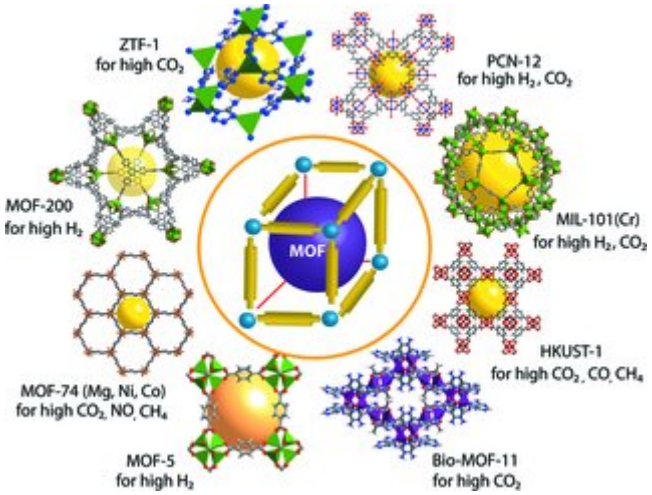
Materials by Design, State U. of New York, USA; February 2014), highlights the two most important breakthroughs of this field, i.e. crystal structure prediction and electronic structure calculations, and their applications to specific problems of materials science.

These four exciting special issues contain excellent papers covering a variety of topics in structural chemistry and herald a new identity for *Acta Crystallographica Section C*, one underpinned by structural work but with interest in and eyes on all chemical fields where this work plays a significant role. The papers are expected to be highly cited and you are now invited to continue the surge of *Section C* to the forefront of structural chemistry by submitting your own papers in the style of those represented in these special issues.

Anthony Linden, Section Editor

IUCR JOURNALS NEWS

Special Issue on Crystal Engineering



Acta Crystallographica Section B is also publishing a series of special issues in celebration of IYCr2014 and, having extended its subtitle to *Structural Science, Crystal Engineering and Materials* last year, it is fitting that the first of these should highlight the fundamentals of crystal engineering. Guest-edited by Andrew Bond (U. Copenhagen, Denmark), the issue gives a clear indication of two main areas where crystal engineering is now being applied, namely pharmaceutical solids and metal–organic frameworks (MOFs), emphasising the commitment of IUCr Journals to publishing cutting-edge research in crystal engineering through *Acta Crystallographica Section B*.

The issue is available free online at http://journals.iucr.org/b/issues/2014/01/00/isscontents.html.

IYCR 2014

Launch of the International Year of Crystallography

Paris, France, January 20-21, 2014

From SCANZ Newsletter, No. 63, Feb 2014 (abridged version)



The Monday morning audience.

The Opening Ceremony of the International Year of Crystallography was held on Monday, January 20 and Tuesday, January 21 at UNESCO headquarters in Paris. Over 800 people attended the opening sessions that included a collection of welcoming remarks – a recorded video welcome address from Ban Ki-moon and an address by the UNESCO Director-General who formally opened the meeting, followed by welcoming speeches from the President and Vice President of the IUCr, a representative of the Moroccan government (that Kingdom put the case to declare 2014 as IYCr), the President of the Centre National de la Recherche Scientifique (CNRS), and Presidents or Past Presidents of the International Union of Pure and Applied Chemistry, European Physical Society, International Mineralogical Association, and the International Union of Biochemistry and Molecular Biology. Some of these talks reminded the audience that 2011 was the International Year of Chemistry and 2015 will be the International Year of Light. There were remarks on the history of crystallography, and on the history of the IUCr. The UNESCO speakers seemed to show particular interest in the contribution that crystallography might make to sustainable development. The IUCr Vice-President described the IUCr-UNESCO program of OpenLabs in Africa, South and Central America, and South Asia.



Mankind's fascination with crystals was stimulated by the discovery of naturally occuring clusters of rock crystal (quartz). (Photo by J.-L. Hodeau)



Public exhibition 'Voyage into the Crystal'. (Photo by M. L. Hackert)



Participants in the 'Young crystallographers' panel.

Following coffee Jenny Glusker talked on the history of crystallography, including very early speculation (*e.g.* by Robert Hooke, 1665) that the regularity of crystal forms must imply a regular arrangement of the internal constituents. Of course the history of crystallography since the discovery of X-ray diffraction is more familiar to most of us, and Jenny took us through the usual highlights in a most professional manner. Immediately after this there was a session entitled 'Talented young crystallographers of the world' chaired by freelance science writer Philip Ball. In his introductory remarks Philip dipped into history a few times – he showed William Bragg and Max von Laue together at a Solvay Conference in Brussels in 1913 (however national rivalries were apparent at that time), mentioned the history of success of women crystallographers (for example Hodgkin, Lonsdale, Franklin), and remarked on a recent high-resolution study (Umena *et al.*, *Nature*, 2011) that throws light on the splitting of water at the membrane-protein complex photosystem 2. Then eight 'talented young crystallographers' – not all so very young and some well established – gave their presentations by pre-recorded video. They sat on stage along with a similar number of perhaps younger and less well established crystallographers, and after the videos engaged in discussion under Philip Ball as chair. They raised familiar issues – short-period funding, intense pressure on young scientists to teach and publish – as well as issues relating to lack of resources in some countries and the difficulty of pursuing unequal collaborations.

After lunch we moved from young crystallographers to a Nobel Laureate. After training as a physician, Brian Kobilka realized that crystallography would enable him to 'see' his favorite molecules. His interest is the system of message transmission through cell walls. This involves a stimulant (agonist) outside the cell, a receptor that is embedded within the membrane and a protein inside the cell wall. The protein is known as a G-protein and the receptor as a G-protein-coupled receptor. He shared the Chemistry Prize in 2012 for his high-resolution crystallographic studies of the active ternary complex comprising the agonist, the β_2-AR (adrenergic, *i.e.* responsive to adrenaline) receptor and the G-protein. The work was challenging at every turn – extraction of complex from membrane and expression, purification and crystallisation, diffraction studies at the APS and ESRF, and the need for tricks such as the use of antibodies to stabilise the conformation. The crystallography suggests that the action of the agonist on the receptor is amplified through the membrane by the receptor geometry. The structural details of the

receptors are of great pharmaceutical interest because they are often the targets for drugs. Comments were made on both the years devoted to the project, and the extent of collaboration involved.



The Russian delegation. (Photo by M. L. Hackert)

The final session on Monday was given to a review of crystallography in the BRICS countries – Brazil, Russia, India, China and South Africa. I had not previously encountered this grouping, and am not sure of the basis for it. In opening remarks, UNESCO reiterated hopes that crystallography might provide a vehicle for promoting sustainable development, for encouraging women into science, and for north–south collaboration. The BRICS countries were represented variously by ambassadors, government science bureaucrats and crystallographic association chairs. A number of these countries appeared to be persuaded of the nexus between scientific research and economic growth – I am unsure that the Australian government is persuaded of such a link – and were increasing their investments accordingly. Brazil in particular was ramping up science support as a fraction of GDP, had 7.2 million students enrolled in tertiary education (maybe not just science), and was 13th in publication output, with increasing citation impact. This investment was considered to have enhanced activities in the petroleum industry, aerospace (3rd in world), and agriculture (Brazil now a net exporter). Brazil is also a leader in the use of bioethanol for vehicle fuel. Brazil established the first synchrotron radiation source in the southern hemisphere in 1997, and was building its second synchrotron to come on line in 2016. It was claimed Brazil has 3,000 PhD crystallographers. It will play a leading role in the recently established Latin American Crystallographic Association. South African crystallography started in 1937 in Cape Town with R. W. James (who had worked with Bragg), and then developed through his students and his students' students. It is evidently quite strong in supramolecular chemistry, but short on macromolecular crystallography, which I would attribute to lack of access to synchrotrons. India also has a good tradition in crystallography, again with an emphasis on supramolecular chemistry and crystal engineering, with some good protein crystallography but that perhaps limited by limited access to synchrotrons. I am moved to reflect that protein crystallography in Australia benefitted from good arrangements for synchrotron access well before the commissioning of the synchrotron in Melbourne. Russia has great traditions dating back to the 19th century, while China has been opening up its activities (*e.g.* two-way traffic of scientists) as well as constructing new facilities. Current Chinese activities encompass metal-organic-framework systems, molecular ferroelectrics, molecular nanomagnets and, in the macromolecular field, the structures of light-harvesting proteins and the SARS virus.



John Spence on X-ray lasers.



Juliette Pradon: 'Crystallographic research in the developing world'. (Photo by R. Kuzel)

On Tuesday, John Spence (Arizona State) opened with a fascinating talk on X-ray lasers and their use in crystallography. These give very short (femtosecond) pulses of great intensity. The breakthrough realisation was that while one pulse was guaranteed to destroy any crystal, the process of destruction was so slow that the pattern could be captured before this occurred. The strategy is one of 'diffract then destroy'. Data are collected by directing the X-rays through a jet containing tiny crystals. There is the possibility of obtaining X-ray patterns from single particles, such as viruses, and with this technique the phase problem might be circumvented. A current interest is the study of photosynthesis by time-resolved crystallography. Martijn Fransen (PANalytical) brought us back onto the laboratory scale with a review of the impact of (mostly powder) X-ray diffraction in the cement industry, ore analysis, pharmaceuticals, microelectronics and crystal deformation. Juliette Pradon (CCDC) spoke on research involving collaboration between CCDC and a group in the U. of Kinshasa (DRC) – this involving two-way visits of students and staff. David Bish (Indiana) and David Blake (NASA) gave an account of research carried out using the (very) portable X-ray diffraction (XRD)/X-ray fluorescence (XRF) device, developed over twenty years, and now carried on Mars by the Curiosity rover. It returned its first X-ray diffraction patterns in October 2012. The first analysis from a sand dune showed amorphous content, no hydrated minerals, no clay, feldspar, and was generally similar to the basaltic soil found on the flanks of the Mauna Kea volcano in Hawaii. The second sample was from a drilling rig – this now contained both clay minerals and a hydrated mineral, bassanite. Mars is now a dry environment, but it seems it was wet in the past. The next talk was from Frank Burgäzy (Bruker) on the history of crystallographic technology. He covered X-ray tubes (first commercial tube produced by Siemens just three months after Roentgen's discovery), optics, detectors and software. The latest laboratory X-ray source is based on a liquid metal jet, as a means to overcome the problem of power dissipation. The final talk in the pre-coffee session was from Philippe Walter (CNRS, Paris) on the applications of X-ray diffraction in the study of art and historical artefacts. The approaches are to take a very tiny sample, when permissible, for evaluation at a synchrotron, or to take a portable X-ray diffractometer (*cf.* the Mars probe) to the painting or artefact of interest. The studies of art depend on the fact that most pigments are crystalline – *e.g.* $PbCrO_4$ commonly used for yellow. The composition and shapes of crystallites can be analyzed with diffraction to reveal such things as the fact that da Vinci used 2 μm layers of glaze. The methods can be used to check authenticity, trace the trade in pigments and assist in conservation. I derived some personal satisfaction in seeing that quantitative phase analysis, *via* the Rietveld method applied to X-ray powder patterns, in the development of which I played some personal part (Hill & Howard, *J. Appl. Cryst.*, 1987), was showing up in the laboratory (Fransen), on Mars (Bish) and even in the world of art (Walter).

After coffee, we moved gently from the study of art to art itself, namely Islamic art, firstly in the hands of Abdelmalek Thalal (Marrakech) and Emil Makovicky (Copenhagen). Certain Islamic art is strong on the symmetries of constellations and of periodic tilings. Many of the tilings have symmetries that can be identified with the plane groups that are reported in our *International Tables*. There are also instances of quasi-periodic tilings with five- or ten-fold motifs. Certain architectural features show an 'under and over' character and are better described using layer groups (with which I am not familiar). Makovicky showed examples of mistakes in periodic tilings, amounting to twin boundaries and the like – maybe not so surprising if one considers that there would be many workmen involved in the process. Peter Lu (Harvard) gave the final rather mathematical account of Islamic tilings. The building blocks of quasi-periodic Islamic architecture are, he claimed, the five Girih tiles, as appear in the Topkapi scroll. Peter indicated a connection of Girih with Penrose tiles, and finally a connection to the Fibonacci sequence. Fascinating stuff, but it would take me much more time to digest it.



Visitors to the IUCr stand, manned by Jonathan Agbenyega, Mike Hoyland and Peter Strickland. (Photo by M. L. Hackert)

This brought us close to the end of the meeting. Samar Hasnain (Liverpool), Editor-in-Chief of IUCr journals, gave an account of the role of those journals in the international development of crystallography. There followed a talk by Chris Llewellyn Smith (Oxford) on the development in Jordan of an international synchrotron source, SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East). Chris had been Director at CERN, and I learned that CERN had been set up after WW2 by UNESCO in an effort to encourage cooperation between previously warring nations as well as to further science. SESAME will be a 2.5 GeV third-generation light source. The current members are Bahrain, Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, the Palestinian Authority and Turkey. The dual purposes of encouraging cooperation between warring nations and furthering science are evident. Maciej Nalecz (UNESCO Basic Sciences) gave a short closing speech.

All in all, an interesting day and a half, and I think worth the hours of travel involved. As to the International Year of Crystallography itself, it behooves us all to try to make it a success. A number of activities have been planned to celebrate the International Year of Crystallography; contact the organizers of these projects if you wish to help out with any of these activities at iycr2014@iucr.org.

Chris Howard

Footnote: Another excellent comprehensive review of the opening in Paris, written by Carl Schwalbe, the editor of the BCA newsletter, appeared in the spring edition of Crystallography News.

IYCR 2014

Commemorative stamps



Stamps from Belgium, India, Israel, Moldavia, Poland, Slovakia and Switzerland.
Several countries have issued postage stamps to celebrate IYCr2014 and bring the importance of crystallography to the attention of the public. For more information, please visit http://www.iycr2014.org/events/postage_stamps.

IYCR 2014

IYCr2014 Opening Symposium in Japan

The IYCr2014 opening symposium held in the Auditorium of the Science Council of Japan (SCJ), on January 23, 2014, was attended by 149 participants from Japan.

The 'IYCr2014 Japan Initiative' was launched on September 16, 2013, to celebrate the birth of modern crystallography and to showcase the role of crystallography in past, present and future research and technology in Japan. A total of 37 Japanese Societies and Associations are partners of the IYCr2014 Japan Initiative.



Sumio Iijima, Charman of IYCr2014 Japan Initiative.

In his opening address Sumio Iijima, Chairman of the IYCr 2014 Japan Initiative, described the history of crystallography in the world and in Japan, and discussed the present state of the art of crystallography. Takashi Onishi, Chairman of SCJ, talked of 'Prospects for the IYCr'.



Five lectures covering bioscience, chemistry, crystal engineering, science, materials science and physics were presented. The lecturers were: Yoshinori Fujiyoshi (Nagoya U.), 'Crystallography for understanding human beings at the atomic level and drug discovery'; Masahiro Irie (Rikkyo U.), 'Molecular crystals that respond to light'; Gen Sazaki (Hokkaido U.), 'New behavior of melting of ice: Two kinds of liquid below zero degrees Celsius'; Kei Hirose (Tokyo Inst. of Tech.), 'Crystal structures deep in the earth'; and Jun Akimitsu (Aoyama Gakuin U.), 'The discovery and crystallography of high-temperature superconductivity'.

In closing, Kazue Kurihara (Tohoku U.) announced that the IYCr2014 Initiative will provide many opportunities to engage diverse science and technology communities, reaching out and building bridges to new partners in academia and industry, and building public awareness of crystallography.

The meeting was organized jointly by the IUCr group, Chemistry Div., Science Council of Japan, and the Crystallography group, Chemistry and Physics Div., Science Council of Japan, and co-organized by the IYCr2014 Japan Initiative, the Crystallographic Society of Japan and the Japanese Association for Crystal Growth.

Eiji Nishibori, Chair of Public Relations Committee for the Crystallographic Society of Japan

IYCR 2014

Presentation and answers to a few questions about 3D printing of crystallographic models



Figure 1: J. L. Hodeau, former president of the Association Française de Cristallographie (left) and T. David (right) examined 3D models and posters [2] at the grand opening of IYCr 2014. (Photo by D. Chateigner)

A collection of 3D printed models of molecules and cubic packing of spheres and crystals (Fig. 1) was displayed at the IYCr 2014 opening ceremony in Paris by P. Moeck, W. Kaminsky and D. Chateigner (International Advisory Board of the Crystallography Open Database, COD [1]), and T. J. Snyder (Trevor.snyder@3dsystems.com).

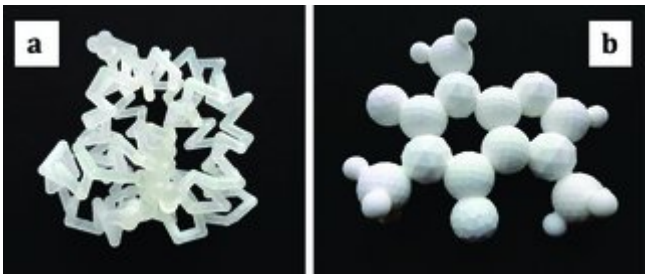


Figure 2: 3D printed models of (*a*) a myoglobin and (*b*) a caffeine molecule. Note that the representations of the nitrogen atoms (inside the rings), ketonic oxygen atoms and carbon atoms have distinctly different surfaces, and that the smaller size spheres represent hydrogen atoms in (*b*).

Models exhibited included back-bone representations of hemoglobin and whale sperm myoglobin (Fig. 2*a*); atomic (ball and stick) representations of herapathite, sucrose, buckminsterfullerene and caffeine (Fig. 2*b*); polyhedron models of sucrose and a Japanese α-quartz twin (Fig. 3*a*); as well as unit-cell representations of the cubic primitive, body-centered and face-centered packings of equal-sized spheres. The last was complemented by an 'opened up' piece with exposed intersites (Fig. 3*b*), intended for demonstrating structural prototypes, *e.g.* halite and fluorite, which are prototypical to copper with additional spheres of fitting sizes. All of these models had dimensions of several centimetres.

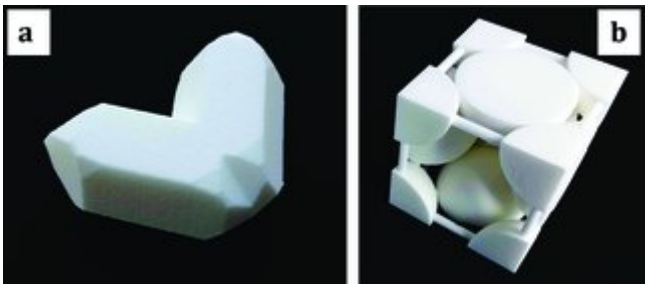


Figure 3: 3D printed models of (*a*) a Japanese α-quartz twin and (*b*) an 'opened up' unit-cell representation of the cubic densest packing of equally sized spheres that can be used to demonstrate derived structures by the filling of the various intersites.

One *may* infer from the observation that most of these models had 'evaporated' from the exhibition desk in Fig. 1 by the end of the meeting (and presumably 'condensed' into some briefcases and ladies' purses) that crystallographers see value in the 3D printing of the objects with which they are professionally concerned. This may entice the manufacturers and vendors of X-ray crystallography equipment and software to offer suitable 3D printers to crystallographers and the wider scientific community.

All of our crystallographic models were printed from *.stl files, *i.e.* the worldwide standard 3D printing format that was developed by 3D Systems. (The STL file format is also known as the Standard Tessellation Language.) Employing the freeware packages *Cif2VRML* and *WinXMorph* [3] developed by W. Kaminsky, the corresponding 3D printing files were created directly from *.cif files. Beginning at their 'educational COD offspring' website [4], the friendly people from the Crystallography Open Database will put 3D printing files of molecules and crystals into open access [5]. Other news from the COD [1] is that the Crystal Eye project [6] and the Crystallography Open Database have joined forces and there are now more than 260,000 entries in this database, of which more than 70,000 are Simplified Molecular-Input Line-Entry System (SMILES) compliant.

Selective Laser Sintering (SLS [7]) was used to print out the 3D models in Figs. 2*b*, 3*a* and 3*b*. The models that were semitransparent (*e.g.* Fig. 2*a* and arrow in Fig. 1) were made with the MultiJet Printing (MJP) technique. Color models can be made with the ColorJet Printing (CJP) technique. 3D crystallographic models and other parts can be ordered through 3D Systems Corporation's Quickparts Solutions for on-demand printing in the cloud [8]. Our mini-poster in Paris [2] also showed one of the newest 3D 'personal printers' called the Cube 3 [7], which utilizes the plastic jetting technique. This printer will be available for under $1,000 later this year.

The 3D printing technology used and the size of a crystallographic model will determine its production time and cost. In most cases, it may take a contemporary 3D printer from tens of minutes to tens of hours to complete a job. Models printed by the SLS, MJP and CJP techniques are of higher esthetic appeal and quality, but cost more compared with plastic jetting models from a Cube [7] printer. The price to 3D print today is as low as a few US dollars per crystallographic model, but can also be hundreds of US dollars when printed on an industrial high-end production machine. Prices will come down significantly as the technology develops and are only limited by the cost of the material (order of magnitude $1 per 50 gram). A Cube printer [7] will suffice for many needs of crystallographers.

The authors [9] are committed to further optimizing the printing of crystallographic models and are very happy to answer questions from the community.

[1] http://crystallography.net; mirrors in Lithuania: http://cod.ibt.lt, France: http://cod.ensicaen.fr, Spain: http://qiserver.ugr.es/cod, and North America: http://nanocrystallography.org

[2] http://nanocrystallography.research.pdx.edu/media/mini-posterIYCr 2014.ppt

[3] http://cad4.cpac.washington.edu

[4] http://nanocrystallography.research.pdx.edu

[5] N. Jones, *Atomic Secrets: 100 years of Crystallography*, *Nature* **505** (issue 7485) 602-603 (2014)

[6] http://wwmm.ch.cam.ac.uk/crystaleye

[7] SLS and Cube are registered trademarks of 3D Systems Corporation

[8] http://www.3dsystems.com/quickparts

[9] http://nanocrystallography.research.pdx.edu/nano-crystallography-group/recent-senior-collaborators

Peter Moeck and Werner Kaminsky (on behalf of the International Advisory Board of the COD) and Trevor J. Snyder (on behalf of 3D Systems Corporation)

IYCR 2014

IYCr Down Under

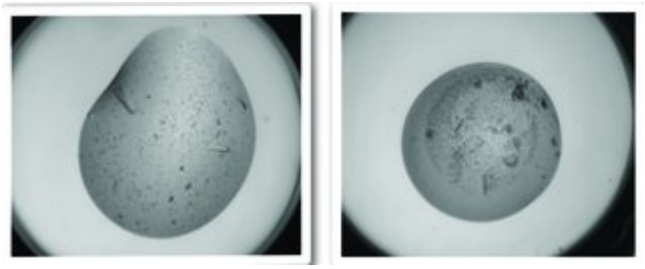
From SCANZ Newsletter, No. 63, Feb 2014



SCANZ has allocated $20,000 to support various activities to celebrate the International Year of Crystallography (IYCr):

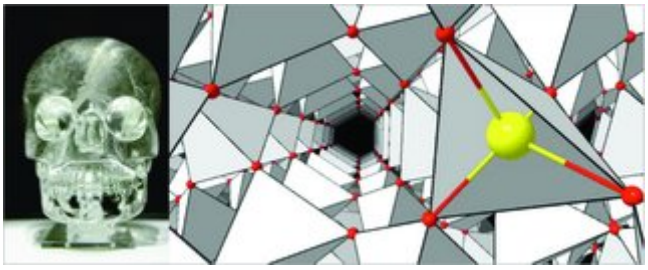
Crystal growing competition: SCANZ, the Australian Academy of Science and the Royal Australian Chemical Inst. are supporting a National Crystal Growing Competition. States and territories that run individual competitions will send their winning entries for selection of national winners (jennyjonesdr@gmail.com).

Remote data collection: At the Australian Synchrotron (U. of Queensland) researchers will demonstrate remote data collection (coordinated by Brett Collins).



With the help of Citizen Scientists, Janet Newman hopes to develop software that can distinguish between drops containing crystals (left) and those without (right).

Citizen Science Crystal Drop Evaluation: Janet Newman is leading a citizen science project for ABC Science's 'National Science Week' to evaluate the results of crystallization trials to develop a robust computer algorithm that could identify subsets of trials that are interesting enough to require human examination. Participants will match dozens of images to a set of 10 standards. These data will be a training set for a machine-learning program to classify images into sets (www.scienceweek.net.au/abc-sciences-national-science-week-citizen-science-project-2014).



Left, crystal skull from the British Museum - picture taken by Rafal Chalgasiewicz. Right, the crystal structure of quartz, representation generated using *Diamond* (www.crystalimpact.com/diamond/). The images are from Hubert Chevreau's post on quartz (http://crystallography365.wordpress.com/2014/01/14/quartz-dear-indi-let-me-in-next-time/).

Crystallography365: Crystallography365, led by Helen Maynard, is an attempt to blog a crystal structure each day in 2014: http://crystallography365.wordpress.com. The goal is to draw attention to crystal structures useful to society. Anyone interested in writing entries for crystallography365 contact helen.maynard-casely@ansto.gov.au.

'**Crystals in the City**' is being planned by Neeraj Sharma for August 9-30, 2014 (National Science Week in Australia). A dozen 6 ft tall structural models will be exhibited in cities in Australia. The structures will 'reflect' their surroundings and inform the public of crystallographic achievements, with hands-on activities and an opening event organized by Chris Ling at the Verge Gallery (U. of Sydney).

FEATURE ARTICLE

Crystallography in North America

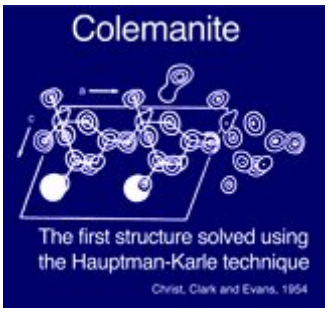


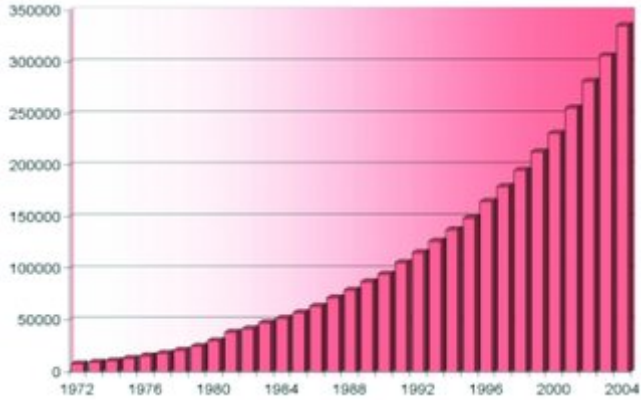
In 2013, Richard Dickerson received the ACA's Patterson Award in recognition of his ground-breaking atomic resolution structures of DNA oligomers. Alex McPherson accepted the award on Dickerson's behalf at the ACA meeting in Hawaii in 2013. Alex reviewed Dickerson's significant contributions to science, and on the eve of the International Year of Crystallography, he gave a splendid review of the history of the field. In that presentation Alex expressed the opinion that David Harker's significant contributions to the field deserved greater recognition than he had received. Alex noted Harker's major contributions, which included the Harker section heavy-atom method that made crystallography a versatile tool that hundreds could use to determine structures, the application of inequality relationships to get phases from intensities to solve one of the first boron-containing compounds and understand its chemistry, the determination of one of the first protein structures, fostering development of one of the first automatic diffractometers and probing the use of color in multi-dimensional symmetry analysis, a concept that remains to be fully exploited.



Dorita Norton and David Harker.
Harker's achievements were vital, perhaps essential, to the work that earned over a dozen Nobel Prizes. Herb Hauptman was so cognizant of his debt to Harker that David was the first of the five individuals that Herb invited to accompany him to Stokholm in 1985.

In his editorial preface to the inaugural issue of *Acta Crystallographica* in 1947, P. P Ewald wrote: 'Crystallography was transformed into an effectively new science by the discovery of X-ray diffraction in crystals in 1912. In the following two decades, an enormous development took place, forging into a practical tool what had originally been a physical experiment, and the atomic structures of hundreds of substances of ever increasing complexity were established. No second spectacular crystallographic discovery has since been made of consequences comparable with those of the original discovery of X-ray diffraction, but general progress in methods has been such as to result in opening up many new possibilities for research in the immediate future.'





Although crystallography was in its infancy in the United States, the seeds of the second spectacular crystallographic discovery were already evident on page 7 of that first volume of *Acta Cryst.* in Harker and Kasper's paper entitled 'Phases of Fourier coefficients directly from crystal diffraction data'. It was this work that inspired Hauptman and Karle to embark on their development of 'Direct Methods'. The first decades of that odyssey were met by the skepticism of the entire community, including David Harker, who warned ominously and incessantly of the dreaded homometric solution. But when the method was successfully applied to determine a structure previously too complex to tackle, the skeptics became true believers and exponential growth in the number of structures determined ensued (see figure).



Dorothy Hodgkin with Linus Pauling in Asilomar, CA, in 1977.

Although US crystallographers were relatively late coming to the field, the first volume of *Acta* included papers on studies of crystal chemistry by Linus Pauling (CalTech), W. H. Zacharias (U. of Chicago), Rob Burbank, Howard Evans and Martin Buerger (MIT), Charles Fenimore (Johns Hopkins), and Rose Mooney (Tulane U.). Ralph W. G. Wyckoff (National Inst. of Health) published his first electron micrographs of viruses and R. E. Rundle of Iowa State College was looking at interstitial compounds. I trace my crystallographic roots to Rundle *via* Norm Baenziger, who published his first inter-metallic structure in Volume 2 of *Acta Cryst.*

Milestones in Canadian Crystallography have included significant contributions to programming instruments for data collection and techniques for structure refinement by crystallographers in Ottawa, including Eric Gabe and Yvon Le Page; mineral structure characterization and mineral data bank

assembly by Jose and Gabrielle Donnay at McGill; the creation of the Inorganic Structure Data Bank by I. David Brown and Guenther Bergerhoff; and the completion of the first protein structure in Mike James's laboratory in Alberta. The Nobel Prize in Physics 1994 was shared by Canadian Bertram N. Brockhouse and Clifford Shull for their pioneering work on neutron and electron diffraction, respectively. A more detailed account of Canadian crystallographers and their accomplishments appeared in Volume 18#2 of the *IUCr Newsletter*. US pioneers in crystallographic software development included Bill Busing, Henry Levy and Carroll '*ORTEP*' Johnson.



Ned Seeman, Joel Sussman, Helen Berman, and Sung-Hou Kim in front of MIT. (Photo courtesy of American Crystallographic Association)

Another benchmark in our US crystallographic history was the creation of a Dept. of Crystallography at U. of Pittsburgh by George Jeffrey. Jeffrey trained more than one generation of crystallographers, developed collaborations with industry and launched a series of annual meetings to celebrate the accomplishments of crystallography. It was in Pittsburgh that three young crystallographers, Helen Berman, Ned Seeman and Sung Ho Kim, collaborated on the determination of a challenging DNA structure. Helen Berman went on to develop and eventually direct the Protein Data Bank, Ned Seeman single-handedly created the field of nanocrystallography and earned numerous awards including the 2012 Kavli Prize in Nanoscience, and Sung Ho Kim became a leader in the community of Protein Structural Biology. Recent Nobel prizes have honored determination of some of the most complex and important macromolecular structures. Tom Stietz shared the award for the ribosome determinations with the UK's Ramakrishnan and citizen of the world Ada Yonath, and Arther Kornberg was honored for his determination of the structure of RNA polymerase II.

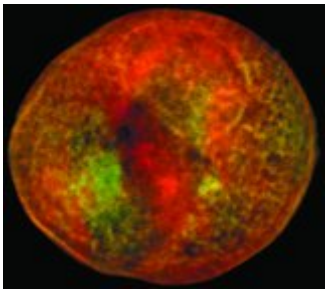


Seated: J. Kendrew, C. Shull, B. Brockhouse, W. Lipscomb; Standing: J. Karle, H. Deisenhofer, H. Hauptman, H. Michel.
David Harker established the Crystallographic Center at Roswell Park Cancer Inst., another incubator for new crystallographic ideas and leadership. Philip Coppens founded the field of electron density analysis, and Eli Shefter was an early advocate of using crystallographic analysis to foster rational drug design. Harker and Kartha determined the crystal structure of ribonuclease at the same time that Perutz and Kendrew completed the structures of hemoglobin and myoglobin in the UK. Nobel Prizes were awarded to Perutz and Kendrew in 1962.

Much later Alex McPherson, more than any other crystallographer, demonstrated that crystal growth was neither magic nor mystical, but a science to be pursued with care and creativity. He, too, struggled for years to gain appreciation for his methods. But once he demonstrated that crystallography was more science than art, his brilliant workshops and lectures drew standing room only crowds.



Henk Shenk and David Sayre at ECM-20, Krakow, Poland, in 2001.



Two-dimensional image of a yeast cell (scale bar 1 μm). Hue represents the phase and brightness the amplitude of the X-ray exit wave. (D. Sayre, Crystallography Across the Sciences 2, p. 33-35)
Another US leader in the field of crystallography was David Sayre, whose tangent squared formula was crucial to the implementation of direct methods. David's brilliant mind also contributed to the development of Fortran at IBM and his vision of using X-ray diffraction to study individual cells led to the development of the X-Ray Femtosecond Electron Laser (XFEL) technique, the most recent spectacular crystallographic discovery. Certainly the names and work of other US crystallographers belong in this list and readers are encouraged to offer their prime candidates.

I have previously suggested that the future of crystallography lies in Africa, South America and South Eastern Asia. The IUCr regional affiliate, the Asian Society of Crystallography (AsCA), has already been a catalyst extending the technologies to new countries in the area. The European Regional Affiliate (ECA) has generously held meetings in South Africa and Morocco. The impending formation of a Latin American Regional affiliate of the IUCr also bodes well for the future. It may well be that the next hundred years will see spectacular crystallographic discoveries in the Southern Hemisphere.

William L. Duax

MEETING REPORT

News from Latin America

First Latin American Crystallography Meeting

Córdoba, Argentina, October, 2013
From ACA RefleXions, Winter 2013



(Front) Iris Torriani and Mario Suwalsky, (back) Claude Lecomte, Joel Bernstein, Hugo Monaco and Jordi Rius.



Silvia Cuffini, Natalia De Vincentis, Iris Torriani, Aldo Craievich, Miguel Delgado, José Solís and J. R. Santisteban.



Alexander Briceño and Mauricio Fuentealba, Middle: Viviana Dabbene and Raúl Carbonio, Back: Daniel Vega, Aldo Craievich, Edilso Reguero and Oscar Piro.



Diego Lamas, Raúl Carbonio and Gautam Desiraju.



Graciela Punte, Daniel Vega and Diego Lamas.

The Primera Reunión Latinoamericana de Cristalografía was held in conjunction with the Ninth Annual Meeting of the Argentinean Crystallographic Association (AACr) at the U. Nacional de Córdoba (UNC), Córdoba, Argentina. The meeting was preceded by the second workshop of the AACr dedicated to Neutron Diffraction Techniques for Materials Characterization. Alberto Podjarny (IGBMC, France), Gabriel Cuello, Mónica Jiménez-Ruiz (ILL, France) and Javier Campos (ICMA, Spain) participated as instructors. The fifth school of the AACr followed the meeting November 4-8. The theme of the school was Structure Solution and Microstructural Analysis from Powder Diffraction Data, and it was led by Jordi Rius and Carlos Frontera (ICMB, Spain) and Ernesto Estévez-Rams (ICTM, Cuba). Raúl Carbonio (UNC, Argentina) coordinated the local organizing committee. The scientific program included 11 plenaries, 8 semi-plenaries, 13 short presentations and about 130 poster presentations. Participants came from Latin American countries (Argentina, Brazil, México, Chile, Colombia, Cuba, Perú, Uruguay and Venezuela) and from the US, Canada, Spain, France, Italy, Germany, UK, United Arab Emirates, South Africa and India. Invited speakers included Joel Bernstein, Claude Lecomte, Robert Dinnebier, Mino Caira and Bill Duax. An Honorary Doctorate from U. Nacional de Córdoba was conferred on Gautam Desiraju, IUCr President. Major equipment manufacturers (Agilent, Bruker and Rigaku), as well as the ICDD, were represented at the exhibit. Financial support for the event was provided by CONICET (Argentina), U. Nacional de Córdoba, IUCr and ICDD, among others. At the Latin American assembly it was decided to hold the Latin American meetings every year, except in the same year as an IUCr Congress. Brazil will host the 2015 meeting, and for 2016 it will be decided between Venezuela and Cuba.

Graciela Díaz de Delgado

REGIONAL NEWS

Latin American Crystallographic Association (LACA)

A major accomplishment during the meeting in Córdoba was the formation of the Asociación Latinoamericana de Cristalografía (Latin American Crystallographic Association, LACA). A committee composed of representatives from each Latin American country with active crystallographers will work on the proposal to become a Regional Associate of the IUCr. J. Sabino (Brazil), D. Lamas (Argentina) and L. Bucio (Mexico) were elected as provisional President, Vice-President and Secretary, respectively. The newly formed LACA will encourage collaboration within the American continent and the formation of crystallographic societies and committees in Latin America.

Graciela Díaz de Delgado

MEETING REPORT

Frontiers of Crystallography

Novosibirsk, Russia, October 2013

The Novosibirsk State U. (NSU) Institutes of Geology and Mineralogy and Solid-State Chemistry and Mechano-Chemistry, Russian Academy of Sciences (SRAS), and the IUCr supported the Advanced School organized in Novosibirsk, October 2-6 2013, and dedicated to the International Year of Crystallography. Agilent organized a satellite seminar on instruments for high-pressure diffraction. Stoe maintained instruments (Stoe STADI-4 equipped with Ag tube, IPDS2T, IPDSII, STADI-MP) that were used during the school. The principles of the diamond anvil cell (DAC) operation were explained using different models produced by Almax-Easy Lab [H. Ahsbahs (Marburg), R. Miletich (Wien) and A. Kurnosov (Bayreuth)].



A group of participants and lecturers at the Inst. of Geology and Mineralogy Siberian Branch of the Russian Academy of sciences.

The school hosted 37 young participants from Russia, Germany, Japan, Nigeria and the United Kingdom. There were no attendance fees and 10 participants received partial or complete support for travel and lodging from the IUCr. 13 lecturers from Russia, the UK, Germany, Spain, Austria, Italy, Canada and Sweden presented lectures, tutorials and demonstrations in the multi-faceted and coherent program. Most of the lecturers covered their own expenses. The IUCr visiting professorship programs supported two of the lectures and partial support came from the NSU.



At Secondary School No. 162 after the lecture by Professor Juan Manuel Garcia Ruiz.

Events for the general public and children were also organized. J. M. Garcia Ruiz gave evening lectures at the Science Café 'Eureka' and a lecture on crystallography for school children. The movie 'The mystery of giant crystals' was shown and awards for the best questions and answers following the lectures were given.

The three main topics of the School were crystal growth in nature, the laboratory and industry, high-pressure crystallography and aperiodic structures.

The first topic included lectures on mineral growth patterns (J. M Garcia Ruiz, Spain); magnetic oxides (H. Dabkowski, Canada); crystal growth of minerals at high pressure (A. Shatsky, Russia); high-pressure synthesis of super-hard nano polycrystalline diamonds (K. Litasov, Russia); artificial diamonds (Y. Palyanov, Russia); and 'Where do diamonds grow?' (R. Angel, Italy). The attendees visited the Mineralogical Museum of the Inst. of Geology and Mineralogy (SRRS), as well as the facilities used to grow large single crystals of artificial minerals (BARS, a multi-anvil large volume press).

E. Boldyreva (Russia) discussed supramolecular systems, and C. Pulham (UK) addressed energetic materials. R. C. Miletech (Austria), R. Angel (Italy), C. Hejny (Austria), K. Friese (Germany) and A. Grzechnik (Germany) presented lectures, demos and tutorials on all aspects of high-pressure diffraction techniques, including creating and measuring pressure in the diamond anvil cell, sample preparation, data collection, data processing, structure solution, structure refinement, precise measurement of cell parameters and preparing data for publication. A. Kurnsosov (Germany) gave a lecture on the combination of high-pressure X-ray diffraction with Brillouin spectroscopy, and B. Zakharov (Russia) spoke on combining high-pressure X-ray diffraction with Raman spectroscopy. R. Angel lectured on elastic tensors and bulk moduli and the effect of non-hydrostatic stress on cell parameters.

The topic of twins and aperiodic structures studied at ambient and high-pressure conditions featured a presentation on twin structures and super space by K. Friese (Germany). N. Bolotina (Russia) introduced *JANA* and held tutorials, during which some of the students determined the crystal structures of their own samples! S. Lidin (Sweden) lectured on modulations in intermetallics and powder refinement of modulated structures. Many participants will long remember that 'reciprocal space is the best place to stay' and 'the dark ages of crystallography' were those when people did not care to look at their structures in reciprocal space.

The week was filled with intensive learning, making new scientific contacts, cultural events and peaceful walks in the autumn forests of Akademgorodok.

Elena Boldyreva

MEETING REPORT

HEC 16

Hipping, Austria, September 2013
www.mfpl.ac.at/research/research-networks/hec16

The complete version of this article is available here.

The 2013 Heart-of-Europe Bio-Crystallography (HEC) conference, a series begun in 1998, was organized by K. Djinovic-Carugo (Vienna, Austria) in the village of Hipping near lake Attersee.



Participants of the 16th Heart of Europe Bio-Crystallography Meeting. (Photo by Jae-Geun Song)

This year's meeting attracted 114 participants from 26 research groups. The 2013 HEC lecture on 'Intrinsically Disordered Proteins' was given by P. Tompa (Brussels, Belgium). Because some proteins do not have a defined structure in solution, or in the absence of a binding partner, it is of importance for crystallographers to learn about the current state of the art in the field of intrinsically disordered proteins. The scientific program included 35 short presentations in 6 sessions, and commercial presentations by the sponsors of the meeting. On Friday afternoon the attendees enjoyed a lovely but rainy boat ride on the Attersee.

The prize for the best student lecture was a ticket to the opening ceremony of IYCr 2014 in Paris, which was donated by the IUCr with some travel support. The winning talk, entitled 'How Pre-Crystallization Analysis Can Save Your Project', was given by J. Pisackova (Prague, Czech Republic).

M. Jaskolski gave a talk on the 15-year history of HEC Meetings. A publication of the same title, edited by Jaskolski and M. Sikorski (Warsaw, Poland), summarizes all previous meetings, including posters, programs, reminiscences of organizers and numerous photographs.

U. Mueller and M. Weiss (Berlin, Germany) will organize the next HEC Meeting, September 25-27, 2014, in Berlin.

Manfred S. Weiss and Uwe Mueller

MEETING REPORT

First School of Crystallization and Polymorphism

Costa Rica, January 2014



Participants at the first School of Crystallization and Polymorphism.

With the support of the IUCr, the First School of Crystallization and Polymorphism was held at the University of Costa Rica (UCR) in San José de Costa Rica, January 27-31, 2014. The school was organized by G. Madrigal (UCR) and A. Araya (UCR). The School attracted 52 participants from universities and companies from Costa Rica, Panama, Guatemala and Mexico. The international team of lecturers was composed of S. Cuffini (SC), U. Federal de São Paulo of Brazil, A. Moreno (AM), U. Nacional Autónoma de México, J. Bernstein (JB), Ben-Gurion U. (Israel) and NY U. (Abu Dhabi), and J. Manuel García-Ruiz (JMGR), U. de Granada (Spain).

The School opened with a presentation on the International Year of Crystallography and an overview of the importance of crystals in science, technology and art (JMGR). The second day covered the fundamentals of nucleation, crystal growth and crystal morphology (JMGR) and the basic aspects of polymorphism and case studies that illustrated the importance of crystal forms in the pharmaceutical industry (JB). The third day was devoted to the technical aspects of crystallization, including proteins (AM), polymorphs and co-crystals (SC), and to solid-state characterization techniques (SC). Thursday covered combined lectures and hands-on demonstrations of crystallization techniques (JMGR, AM), with lectures on the thermodynamics of polymorphism, enantiotropism and monotropism (JB). The last day of lectures was on the legal aspects of polymorphism (JB), methods of preparation of novel crystal forms and habits (SC) and (AM), and analysis of the experiments performed the previous day (AM, JMGR). The closing session featured a colloquium following the public screening of the movie 'The mystery of the giant crystals'.

This successful school, the first ever organized in Central America, was facilitated by the sponsorship of INIFAR, LABIOFAR, INBOX (PANalytical), the U. of Costa Rica and IUCr.

Juanma Garcia-Ruiz and Joel Bernstein

REGIONAL NEWS

ACA History Portal

http://www.amercrystalassn.org/history_home
From RefleXions Spring 2014



In the winter issue of ACA RefleXions the launch of the History Portal, the new ACA website, was announced. A brainchild of V. Pett and J. Flippen-Anderson, the History Portal collects multimedia material about notable scientists who contributed to the development of crystallography, and branches off from the Living History series that has been featured in several issues of RefleXions.

A brief text in the 'History Home' page explains the idea behind the History Portal. In the 'People' section, readers can browse the written contributions of different scientists and a panoply of other biographical material, while through the 'Videos' page they can watch 'Award' and 'Historical' videos hosted on YouTube. Two award and two historical videos are now available on the Portal: D. Watkins's presentation in honor of the 2010 Fankuchen Award and R. Hamlin's celebration talk for the Charles Supper Award in 2012, and lectures given by S. Byram and D. Caspar at the 2012 ACA annual meeting in Boston, entitled, respectively, 'Evolution of Small Molecule Instrumentation in North America' and 'Origins of Structural Biology and Trials and Errors in its History: An Idiosyncratic View'.

AWARDS AND PRIZES

IUCr Ewald Prize to Janner and Janssen

From RefleXions Spring 2014





T. W. J. M. (Ted) Janssen.



Aloysio Janner.

Aloysio Janner and T. W. J. M. (Ted) Janssen, Emeriti Professors at U. of Nijmegen, The Netherlands, have been awarded the tenth Ewald Prize, 'for the development of superspace crystallography and its application to the analysis of aperiodic crystals'. The award will be presented on August 5, 2014, at the opening ceremony of the IUCr congress in Montreal, Canada.

Aperiodic crystals are well ordered materials that lack translational lattice periodicity. One of the most famous examples of an aperiodic crystal is calaverite, a gold telluride mineral discovered in the gold mines of California. At the beginning of the 1900's, mineralogists had noticed that the morphology of calaverite's crystal faces did not follow the accepted empirical rule of crystal growth (Haüy's law of rational indices). The diffraction patterns of calaverite also departed from those of a perfect crystal, then defined as an ordered and periodic arrangement of atoms in space. De Wolff linked these spots to the absence of lattice periodicity in Na_2CO_3 crystals. He described these crystals as 'incommensurately modulated structures' - they are superimpositions of basic periodic structures, with a symmetry that can be described by a three-dimensional space group. Janner and Janssen, who were investigating the relationship between symmetry and physical properties in condensed matter, began collaboration with de Wolff. Together they conceived and developed the 'super space' theory, publishing the first complete list of (3+1)-dimensional super space groups in 1981. De Wolff, Janner and Janssen shared the 1998 Gregori Aminoff Prize awarded by the Royal Swedish Academy of Sciences.

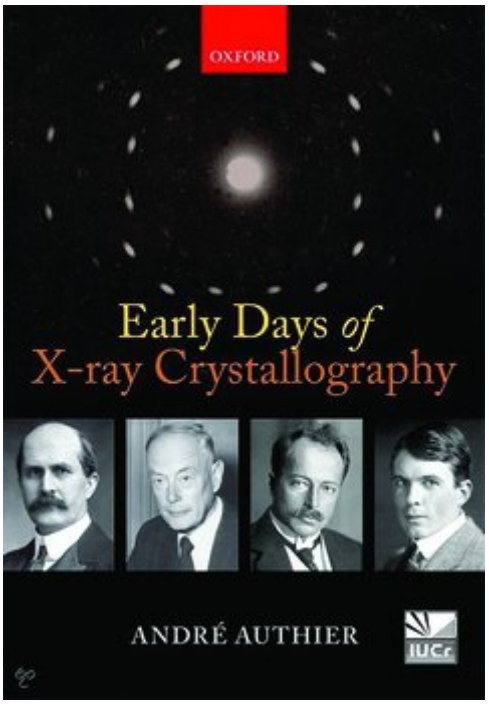
Janner and Janssen have dedicated more than thirty years to expanding the theoretical treatment of aperiodic crystals. They laid the groundwork for the development of methods to solve and refine the

structure of aperiodic crystals, with applications from condensed matter physics to structural biology. Their superspace formalism also applies to the analysis of quasicrystals, a specific class of aperiodic crystals, described in 1982 by Schechtman who won the 2011 Nobel Prize in Chemistry for the discovery. The award of the Ewald Prize to Janner and Janssen highlights the tremendous impact that their work has had on the development of crystallography.

BOOK REVIEW

Review of Authier's 'Early Days of X-ray Crystallography'

ISBN 978-0-19-965984-5



Over many years of teaching first year chemistry I found myself with increasing frequency introducing a subject with the question, 'How do we know that?' This marvelously eclectic book provides an almost encyclopedic source of how we know what we know about the structures and properties of crystals, and Andre Authier tells it in an intellectually and scientifically rigorous and constantly entertaining way. Whoever said that history - or this history of science - is boring and dry would be converted by this account.



Joel Bernstein.

Virtually every introduction to crystallography or the history of crystallography recounts the extraordinary number of Nobel prizes awarded to crystallographers and the variety of research endeavors to which they applied crystallographic techniques. But the history of crystallography can be traced, as Authier does, to the Greeks. However, in an historical trump Authier begins the book in 1912. As in many classic movies he sets the stage by opening Chapter 1 with a description of the 'defining moment' - the April 1912 discovery of the diffraction of X-rays by crystals. And in the tradition of those cinematographic magicians (artisans) he then paints the picture of the state of crystallography on the eve of the discovery, and a brief account of the subsequent impact in such a wide variety of fields. The rich early history is not neglected, but rather artfully detailed when we come full circle to the final two chapters (11 and 12) appropriately titled, 'Unravelling the mystery of crystals - the forerunners' and 'The birth and rise of the space-lattice concept'.

Authier's Preface points out the exigencies or writing about the history of science - the advantage, or disadvantage, of hindsight - and the difficulty of placing oneself at the time, place and general level of knowledge and understanding of those who made the discoveries and developments that now fit so well into the overall scheme of things.

The diffraction of X-rays by crystals is the interaction of light (electromagnetic radiation) with lattices, so the stage is then set to embark on the detailed scientific and historical developments that led (inexorably?) to the 1912 discovery.

Chapter 2 is devoted to the development of the concept of the lattice, and naturally Chapter 3, appropriately titled 'The dual nature of light', is concerned with the nature of light, ending very appropriately with Einstein's explanation of the photoelectric effect as being due to the particle nature of electromagnetic radiation.

As an advocate of the role of serendipity in science I was intrigued by Authier's description of Roentgen's discovery of X-rays:

'It is sometimes written that the discovery of X-rays was made fortuitously. It was not. What was fortuitous about it was the way Roentgen noticed the faint glimmer on the barium platinocyanide screen; he would have found X-rays eventually in any case.'

Biographical sketches for major players and footnotes for many others, personal accounts, title pages from original papers, and notebook entries, make the whole story come alive. And Authier enhances that personal approach and intimacy, for instance by often referring to Sir Lawrence Bragg as 'Willie'.

Roentgen mailed the first X-ray photos to 90(!) leading physicists on New Year's Day 1896. The detail of the description of how rapidly the word spread even in those days leaves one breathless with excitement. The chapter concludes with many other accounts of Roentgen's predecessors who apparently had produced X-rays, but lacking his experience, curiosity and passion failed to recognize the discovery.

In Chapter 5, Thomson's 'discovery' of the electron is put into proper perspective, in addition to providing a vivid account of the continuing confusion, competition and controversy, as well as the intellectual discourse among the contemporary physicists about the nature and behavior of light, waves and particles.

Chapter 6 returns to Munich and the discovery of the diffraction of X-rays by crystals, again detailing the human aspect (*e.g.* a picture of the Hofgarden in Munich 1912). The description of one of my heroes, P. Groth - whose monumental five volume compilation *Chemische Kristallographie* was obsolete by the time publication was completed in 1919 - creates a vivid picture of the physical, cultural and intellectual atmosphere in Munich in 1912 at the dawn of crystallography. In response to Ewald's request, Groth could call upon his encyclopedic knowledge of crystals to suggest testing Ewald's theory of refraction and reflection on $CaSO_4$.

Authier definitely has a talent for distilling the most poignant biographical details to tell his story. In Chapter 6 one almost feels like he is following the players from locale to locale as the story of the discovery unfolds. Valuable documented timelines provide a concise record of what happened when, again so future chroniclers are saved the drudgery of these compilations. He also provides convincing evidence that major discoveries are not made in an intellectual vacuum but almost always made when and where there is a critical mass of human and physical resources, as related in the critical review of the Forman-Ewald controversy on this issue (Section 6.12). He sums it up beautifully:

Finally, concerning the 'clan of crystallographers', it is certainly true that there is a tightly bound community of crystallographers. What keeps them together is not the occasions to celebrate a 'myth of origins', and neither is it a common technique. The inner structure of a material, ordered or not, its imperfections, at the nanoscopic, microscopic or macroscopic scales, are directly related with its

physical, chemical, mineralogical or biological properties. The common goal of unraveling these structures or their defects by a large variety of techniques, and understanding their relations to the properties of materials, is what keeps the crystallographers together.

And this book will strengthen the commitment and spirit of that community. It should be compulsory reading for anyone who ever deals with the interactions of X-rays and solid matter.

Chapter 7 is an account of the events of 1913, including Bragg's solution of the crystal structure of NaCl and diamond, and conveys the rush of activity and very significant achievements, many of which confirmed earlier theories (*i.e.* the tetrahedral carbon atom) or the ionic nature of rock salt. As Bragg later described it,

'It was like discovering an alluvial gold field with nuggets lying around waiting to be picked up' (Bragg 1943).

And Authier takes the reader on an exciting, oft breathtaking, tour of that alluvial field. His command of the science allows him to present the essence of the developments and put them into appropriate historical perspective. He presents not just the accomplishments, but the interpersonal dynamics of the crucial catalytic meetings of the day. In one remarkable year the following developments (among others!) took place: the first experiments in reflection geometry, the equivalence of the Bragg and Laue derivations, X-ray ionization spectrometer, the first structure determinations by the Braggs, Moseley's high-frequency spectra of the elements (which finalized the order for the periodic table), Debye's development of the temperature factor, the rotating crystal method and Friedel's rule. The chapter ends with the awarding of the Nobel Prizes to von Laue in 1914 and the Braggs in 1915, with an accounting of the complications and delays due to the outbreak of World War I in August of 1914.

Chapter 8 recounts the parallel development of experimental techniques (*e.g.* Debye-Scherrer, rotating crystal, Weissenberg method), crystallographic theory and the determination of increasingly complex crystal structures, with special attention to 'landmark structures' (*e.g.* hexamethylene tetramine, graphite, diamond, hexachlorobenzene).

Chapter 9 covers the optical properties of X-rays from Ewald in 1917 through Compton to Borrman (anomalous dispersion) in 1941. Chapter 10 is titled 'Early Applications of X-ray Crystallography', summarizing important contributions and emphasizing the almost ubiquitous - and often crucial - role crystallography has played in every branch of science. It includes a fascinating discussion of the development of definitions and accepted values of atomic and ionic radii, as well as poignant examples from chemistry (inorganic and organic), metallurgy, crystal imperfections and metal physics, mineralogy, materials science (crystal engineering), structure-property relations, biological sciences and X-ray spectroscopy.

Chapter 11 returns to the early history with more revelations - back to the beginning: 'Unraveling the mystery of crystals - the forerunners'. It will be of special interest to non-crystallographers, or those crystallographers who wish to educate the public about the beauty and fascination of our science, going back to the Greeks through to Rome de l'Isle's 1783 determination of the constancy of interfacial angles.

Since I received the book it has provided many hours of delightful reading, browsing and reminiscing, and has already served me well as a sourcebook for writing and lecturing. It documents a rich history and tradition of which all crystallographers should be proud, and it should enjoy a cherished place on the bookshelf of anyone with an interest in science, history and the human role in creating the two.

Joel Bernstein
Other reviews of Authier's book can be found in the Spring 2014 issue of RefleXions, written by Joe Ferrera, and in Acta Cryst., written by John Helliwell.

EDITORIAL

Editorial



This issue of the *IUCr Newsletter* includes reports on the opening celebration of the International Year of Crystallography at UNESCO headquarters in Paris, and the first meeting of Crystallographers of Central and South America.

The IYCr 2014 provides an opportunity to explain to the world how crystallography has improved so many aspects of our lives and why so many crystallographers have been honored with Nobel Prizes. Science Fairs and museums in many nations are welcoming exhibits of crystallographers' accomplishments; crystal growth competitions are being held for students of all ages in dozens of countries; many countries are issuing commemorative stamps; crystallographers in India and the PDB staff have produced commemorative calendars for 2014; and commemorative glassware etched with crystal structures is being produced.

Nature and *Science* have each published special issues. The articles in these issues present the history of crystallography from the perspective of the authors. While well written and highly informative they are not without bias. It is ironic that the special issue of *Nature* includes an article entitled 'Crystallography needs a Governing Body'. Although *Science* is a US publication, the articles in the special issue neglected the important contributions of many US crystallographers, including those who have won Nobel Prizes.

The IUCr. The International Union of Crystallography is one of the oldest and most active scientific 'governing bodies'. While there may be fewer than 20,000 crystallographers in the world, there are millions of users of crystallographic results. The exceptional foresight and care with which crystallographers have compiled and stored their data and results of their studies on minerals, materials, drugs, hormones and proteins in major data bases, and the efforts they have made to be sure that these data were accurate, reliable, uniformly recorded and accessible to individuals throughout the world at little or no cost, is noteworthy. The IUCr has played a major role in establishing protocols and formats for data deposition and supported their distribution. For over 20 years the IUCr has supported the production of this newsletter as a means of enhancing communication and cooperation of the international community of crystallographers.

Latin American Regional Affiliation of the IUCr. The first meeting of crystallographers in Central and South America was held in Cordoba, Argentina, in October of 2013, in conjunction with the annual meeting of the Argentina Crystallographic Association. The meeting was held to discuss the formation of a Latin American Regional Affiliate of the IUCr. Representatives from most Latin American countries attended and discussed the details of how a regional affiliate might be formed and governed. The proposal will be submitted at the IUCr Congress in Montreal in 2014. The founding of a Latin American Regional Affiliate of the IUCr may well be the most significant accomplishment of the IYCr 2014.

William Duax

SPECIAL REPORT

Start planning your travel to Montréal today!

Montreal, Quebec, August 5-12, 2014
www.iucr2014.org

Imagine days filled with intellectual stimulation and nights filled with great food and entertainment. Old friends, new colleagues and family surround you, all equally inspired by new ideas and places to explore. You sit back, sigh contentedly and simply enjoy the moment...



To make this dream a reality, you just have to have to join us in Montréal. IUCr 2014 will deliver.

The Program for this exciting congress has come together very nicely. Our Call for Abstracts resulted in over 2000 abstracts being submitted from 76 different countries. The top five submitters were the United States, Japan, the United Kingdom, Germany and Canada, with France, India and Russia taking the next three spots. Over 400 students applied for travel funding, which we believe is a good indication that there will be a high level of youthful enthusiasm at the congress.

The Plenary speakers will cover a vast array of crystallographic topics. John Miao will discuss Coherent Diffraction Imaging and Atomic Resolution Electron Tomography. Dave Bish will explore the First X-ray Powder Diffraction Measurements on Mars. Juan Manuel Garcia-Ruiz will talk about the Route to Biomimetic Self-assembled Nanostructured Materials, and Dan Shechtman will of course cover Quasicrystals.

Each day of the Congress you will have your choice of Keynote Lectures, with our leading crystallographers covering the most exciting topics in crystallography, including the latest advances in macromolecular and chemical sciences, materials characterization, theoretical foundations, techniques and international facilities. You can also get updates on your favorite software packages from the authors themselves at the always popular Software Fayre.

It isn't too late to submit an abstract for consideration as a poster presentation, with a process for Late Submissions now in place. Furthermore, Keynote and Invited Speakers have been given the opportunity to submit an abstract for poster presentation in addition to their abstract for oral presentation.

Several IUCr Workshops have been organized covering Aperiodic Crystals, XAFS, Crystal Structure Prediction using the *USPEX* Code, XFEL Sources, *SHELX* Small Molecule and Macromolecular Applications, and Advanced Structure Refinement Techniques, Disorder Modeling and CIF Preparation using *OLEX2*. More subjects will be covered by industry-sponsored workshops and Lunch-and-Learns that will be held throughout the week. For information on these and on the Satellite Meetings that are being held before and after the congress in Canadian cities other than Montréal, please see our website.



IYCr festivities will be highlighted in several forms. A series of off-site public lectures is being planned to coincide with the congress. Onsite, delegates can learn about international IYCr activities at the IYCr microsymposium taking place on August 11, at the IYCr display that will run throughout the Congress, on the same level as registration, as well as enjoy a selection of photos from the 'Crystallography in Everyday Life' competition. Finally, a fully public display of materials from *Voyage dans le Cristal* (*Journey into the Crystal*) will be featured at the Palais des congres.

Several upcoming program deadlines are good to keep in mind. Authors who have submitted an abstract for consideration will have been notified if they have been accepted for oral or poster presentation. All authors, including Keynote and Invited Speakers, should be registered by May 1st, 2014, to confirm acceptance of the place in the program they have been offered. May 1st is also the last day to submit an abstract for poster consideration at the rate of $25 CAD, after which the rate increases to $50 CAD for Late, Late Abstracts.





Now that we've excited the scientific side of your mind, we want to entice you further with the softer side of your trip by reminding you of the arrangements we've made for accommodation, tours and entertainment. Montréal is known as a safe city both day and night, proud of its bustling nightlife which includes countless gourmet restaurants, clubs and cafés for you to enjoy with friend and family. Jazz and modern circuses highlight the entertainment scene, both of which you can sample through the IUCr 2014 program itself. Our Opening Ceremony will feature performances by Cirque Éloise and tickets are available online through our registration page to attend an optional Jazz Night.

All the hotels listed on our accommodation page are within a short walking distance from the Congress venue, the Palais des congrès, and many of them can be accessed *via* the underground city if rain threatens to spoil an otherwise pleasant stroll. The Palais is located directly in the heart of Montréal's tourist district, with the Old Port, Place des Arts and the city's China Town surrounding it. A variety of carefully selected tours and excursions are listed through our social program page to keep you and your family entertained either before or after the congress, as well as during your free time throughout the congress itself. Hotels and tours fill up quickly in Montréal's warm summer months, so we recommend that you book early while selection is at its peak.

If you have questions about the program, social activities or any other aspect of your trip to Montréal for IUCr 2014, please don't hesitate to contact us at IUCR14@nrc-cnrc.gc.ca. We're here to help!

IUCR JOURNALS NEWS

You've published your article; now who's going to read it?



During 2014 the IUCr will start work in partnership with a company called Kudos to help its journal authors maximize the impact of their publications.

IUCr authors will use the Kudos service to improve the visibility and impact of their research work *via* email and social media. As well as helping authors through these various opportunities, the Kudos service will also measure the effects of these activities on abstract views, downloads and Altmetric scores.

During 2013 Kudos ran a pilot scheme with a number of other publishers where it saw an average of 19% higher daily downloads of articles shared in this way.

'I have found Kudos really useful', says IUCr journal author Philip Gale, Professor of Supramolecular Chemistry and Head of the School of Chemistry at the University of Southampton, UK. 'It not only helps me improve the visibility of my papers, by highlighting them to my social network, but also provides a way of widening the audience for the work by linking a lay summary of the work to the paper.'

After publication of an article within an IUCr journal, authors will receive a personalized email from the IUCr in-house editorial team, sent by Kudos, requesting them to log on to the Kudos platform. On the platform, authors will be led through various steps that prompt them to explain their article, add context *via* links to other content such as images and data, and share their article *via* social networks and email.

The Kudos platform will enable authors to see the effect of their actions on Altmetrics and from usage data.

To find out more about Kudos and our plans, please contact me at ja@iucr.org.

Jonathan Agbenyega, IUCr Business Development Manager