INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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Original article text and available illustrations

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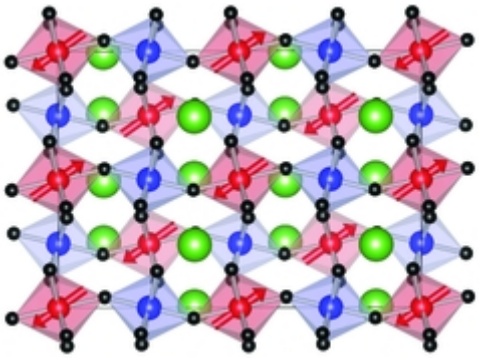
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IUCR JOURNALS NEWS

Tabulation of irreducible representations of the crystallographic space groups and their superspace extensions

Acta Cryst. (2013). A69, 388–395 (http://doi.org/mt6)



This $A_2BB'O_6$ double-perovskite example (an idealization of La_2CoRuO_6) simultaneously exhibits a variety of order parameters, all of which can be projected using IRs of the parent cubic symmetry $Pm{-}3m$. Here, the IRs M_3^+ and R_4^+ generate ferrorotational and antiferrorotational octahedral rotations, respectively; R_1^+ generates the B–B' site ordering; $m\Lambda_3$ generates the antiferromagnetic structure; and Γ_3^+ and Γ_5^+ generate the strains.

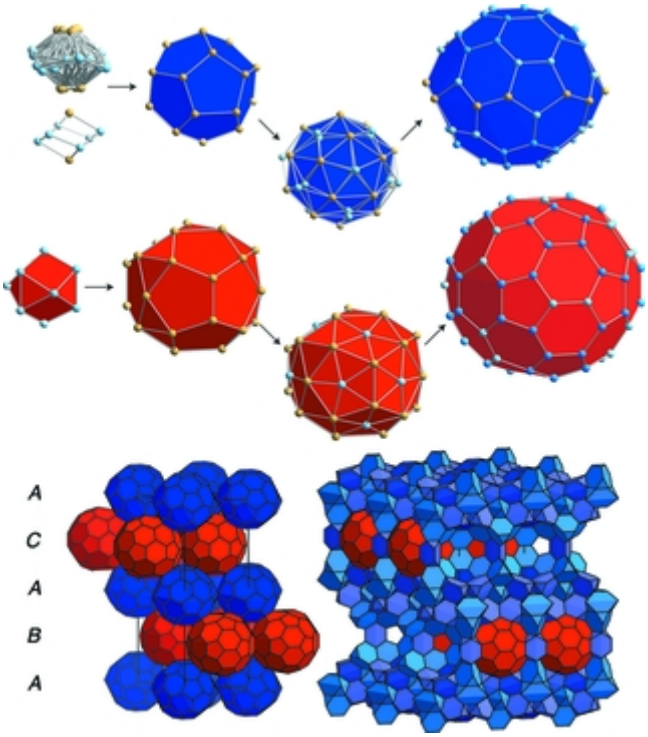
The irreducible representations (IRs) of the parent symmetry of a system provide a symmetry-motivated parameter set for describing any periodic or aperiodic system distortion. We present complete-group IRs for all crystallographic space groups and their extensions to (3+d)-dimensional superspace, including all special and non-special **k** vectors, commensurate and incommensurate. A new matrix form makes their exhaustive tabulation possible for the first time. They can now be incorporated into diverse software packages and applied to the solution and refinement of low-symmetry structures that arise in phase transitions.

H. T. Stokes, B. J. Campbell and R. Cordes

IUCR JOURNALS NEWS

A new complex intermetallic phase in the system Al–Cu–Ta with familiar clusters and packing principles

Acta Cryst. (2013). B69, 238–248 (http://doi.org/mt7)



Cluster description of the new intermetallic phase, highlighting the packing of recurring building blocks.

Why do complex structures form in intermetallic compounds? In order to determine critical structure-forming factors, common building principles have to be discovered for known and newly discovered structures. The article presents a new complex intermetallic phase in the Al–Cu–Ta system, comprising already three cubic giant-unit-cell structures. The structure is described by different approaches and its disorder motifs are discussed. The prerequisite for understanding structure–property relationships is the full comprehension of crystallographic structures, while the consequence should be no less than the tailoring of novel functional materials.

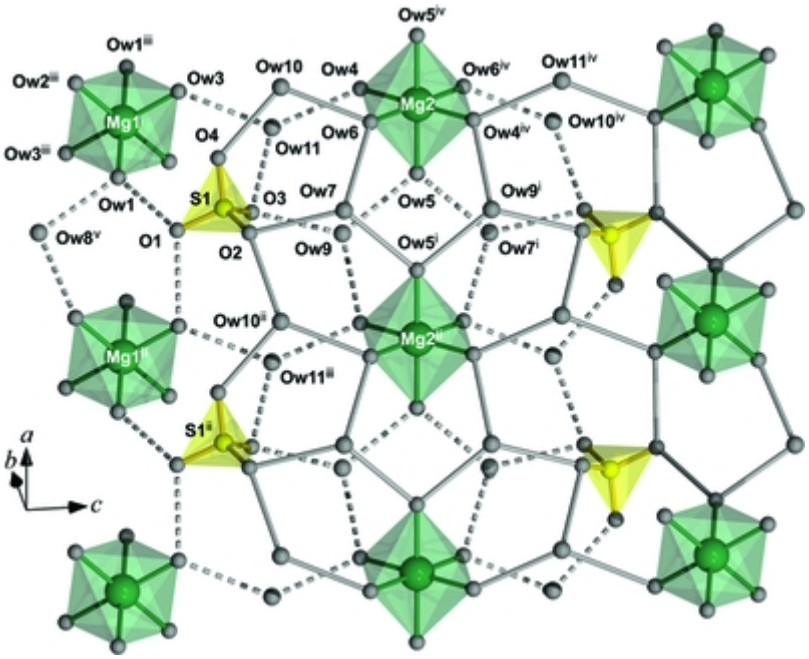
J. Dshemuchadse, S. Bigler, A. Simonov, T. Weber and W. Steurer

IUCR JOURNALS NEWS

MgSO4·11H2O and MgCrO4·11H2O based on time-of-flight neutron single-crystal Laue data

$MgSO_4·11H_2O$ and $MgCrO_4·11H_2O$ based on time-of-flight neutron single-crystal Laue data

Acta Cryst. (2013). C69, 324–329 (http://doi.org/mt8)



Meridianiite consists of $Mg(H_2O)_6$ octahedra and SO_4 tetrahedra 'immersed' in a hydrogen-bonded framework of water molecules. Exchanging these units for others of differing dimensions imposes an internal strain, the propagation of which through the structure we report in this paper.

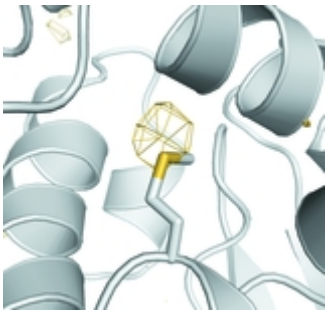
Studies of ionic substitution in inorganic frameworks have been done in the past with materials in which the coordination polyhedra are linked either by corners or edges. There have been few studies of 'matrix isolated' polyhedra, such as those that occur in meridianiite ($MgSO_4•11H_2O$); we have sought analogues containing other ionic substituents in order to better understand factors affecting the framework's properties. We present single-crystal neutron Laue data from the first of these new analogues, $MgCrO_4•11H_2O$, which serves to advance our knowledge of these structures.

A. D. Fortes, I. G. Wood and M. J. Gutmann

IUCR JOURNALS NEWS

Anomalous signal from S atoms in protein crystallographic data from an X-ray free-electron laser

Acta Cryst. **(2013). D69, 838-842 (http://doi.org/mt9)**



Serial femtosecond crystallography (SFX) using free-electron lasers (FELs) allows protein structures to be solved from nano- to micrometer-sized crystals using femtosecond pulses. However, SFX data collection and processing are challenging, and so far all protein structures determined using FEL data were phased by molecular replacement. Experiments at the SACLA FEL in Japan show that the quality of SFX data can be high enough to detect the weak anomalous signal of endogenous sulfur in a protein, opening the way to *de novo* phasing from FEL data.

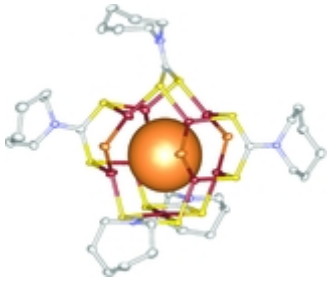
T. R. M. Barends et al.

IUCR JOURNALS NEWS

Tris(μ4-azepane-1-carbodithioato)bis(μ3-azepane-1-carbodithioato)-μ9-bromido-tetra-μ2-bromido-octacopper(I)copper(II)

Tris(μ_4-azepane-1-carbodithioato)bis(μ_3-azepane-1-carbodithioato)-μ_9-bromido-tetra-μ_2-bromido-octacopper(I)copper(II)

Acta Cryst. **(2013). E69, m275-m276 (http://doi.org/mvb)**



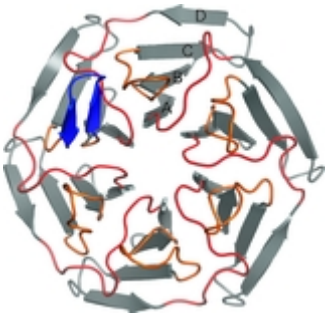
There is much interest in the design and synthesis of this kind of compound; in particular, the establishment of a rational synthetic method for mixed-valence metal clusters is important in developing the chemistry of functional materials, because these complexes have potential applications as new opto-electronic materials based on carrier-transport properties, valence fluctuations and intervalence charge-transfer transitions. In this paper, a new mixed-valence nonanuclear Cu(I)/Cu(II) cluster, $[Cu^{I}_{8}Cu^{II}Br_5(Hm\text{-}dtc)_5]$ ($Hm\text{-}dtc^-$ = azepane-1-carbodithioic acid) with a dithiocarbamate derivative, has been synthesized and structurally characterized.

T. Okubo, H. Anma, M. Maekawa and T. Kuroda-Sowa

IUCR JOURNALS NEWS

Crystal-contact engineering to obtain a crystal form of the Kelch domain of human Keap1 suitable for ligand-soaking experiments

Acta Cryst. **(2013). F69, 592-596 (http://doi.org/mvc)**



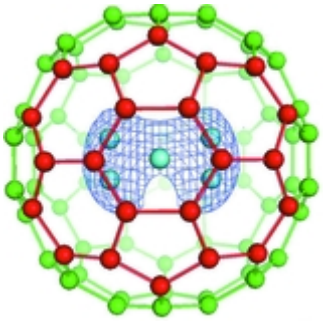
Keap1 is a substrate adaptor protein for a Cul3-dependent ubiquitin ligase complex and plays an important role in the cellular response to oxidative stress. It binds Nrf2 with its Kelch domain. The article describes the generation of a new crystal form of Keap1 which is suitable for ligand-soaking experiments. This makes possible the rapid generation of structures of Keap1 in complex with ligands, thus enabling rational design of Keap1-binding compounds.

S. Hörer, D. Reinert, K. Ostmann, Y. Hoevels and H. Nar

IUCR JOURNALS NEWS

Element-selective charge density visualization of endohedral metallofullerenes using synchrotron X-ray multi-wavelength anomalous powder diffraction data

J. Appl. Cryst. **(2013). 46, 649-655 (http://doi.org/mvd)**



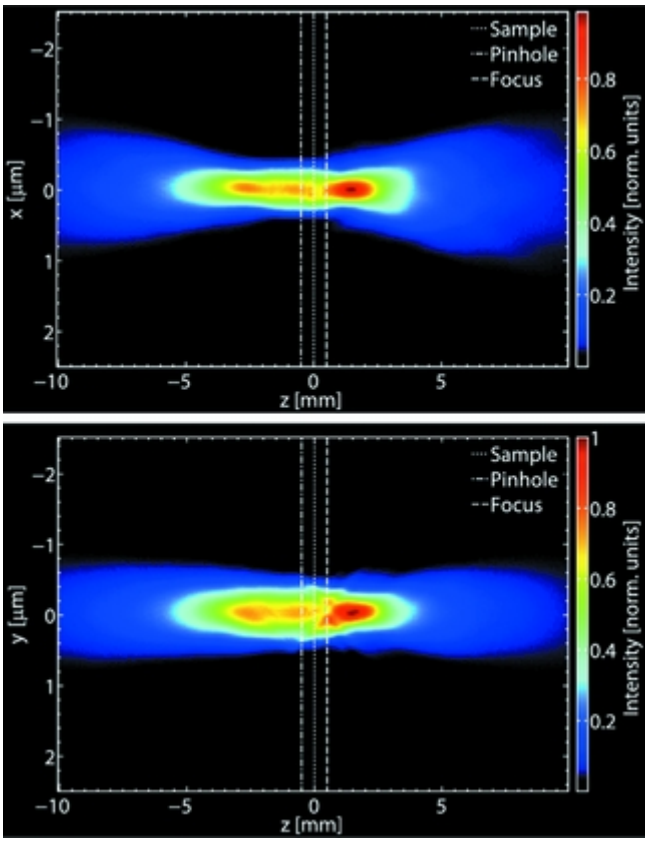
The accurate determination of specific atom sites in a crystal structure during crystallographic analysis is an area of immense importance. In this study, we have developed a method for the determination of an element-selective structure from multi-wavelength anomalous powder diffraction (MAPD) via the combination of Rietveld and MEM charge density analysis. The capabilities and usefulness of the present method are demonstrated by the structural analysis of endohedral metallofullerene, $Y@C_{82}$, 1:1 co-crystallized with toluene, which shows some complicated disorder involving the yttrium atom.

S. Maki, E. Nishibori, D. Kawaguchi, M. Sakata, M. Takata, T. Inoue and H. Shinohara

IUCR JOURNALS NEWS

Versatility of a hard X-ray Kirkpatrick-Baez focus characterized by ptychography

J. Synchrotron Rad. (2013). 20, 490-497 (http://doi.org/mvf)



In the past decade Kirkpatrick-Baez (KB) mirrors have become an increasingly popular tool for efficient focusing of high-power third-generation synchrotron beams. Taking the dedicated nano-imaging setup GINIX (Göttingen Instrument for Nano-Imaging with X-rays) at the P10 beamline of the PETRA III synchrotron in Hamburg, Germany, as an example, the versatility of such a focusing device has been explored. By full characterization of the complex focal wave field using ptychography it is shown how a spatial filter near the focal plane can be used to obtain a nearly Gaussian focus with a smooth far-field intensity distribution. The focal size is shown to be precisely adjustable by variation of the entrance aperture.

K. Giewekemeyer, R. N. Wilke, M. Osterhoff, M. Bartels, S. Kalbfleisch and T. Salditt

IYCR 2014

What does the International Year of Crystallography mean for you?



Michele Zema

This issue of the *IUCr Newsletter* is the first to host a special section dedicated to the International Year of Crystallography (IYCr2014). This section will accompany us in the next issues and throughout 2014. It will be the place for all crystallographers to keep informed about and get involved in the activities arranged to celebrate IYCr2014. There are a few months to go before IYCr2014 officially starts with the Opening Ceremony on January 20-21, 2014 at the UNESCO Building in Paris (see here). These are months that many of us are dedicating to the planning of a variety of initiatives, such as exhibitions, workshops, conferences, special publications, activities for school children and the design of postage stamps. It is now time that all these events are connected in a network through the iycr2014.org website to gain the highest visibility.

The iycr2014.org website needs the contribution of all active crystallographers to grow: you can now find an easy procedure for uploading information about the event you are organizing on the IYCr2014 Calendar or List of events. These can then be browsed by date, place or category. Each country participating in IYCr2014 celebrations has its own space on the iycr2014.org website (see Directory of contacts or Events by country). The national and regional coordinators are now working to set up these pages. National working teams are being formed specifically for IYCr2014 activities, and I would like to stress here the importance that all communities related to crystallography are represented. Who is 'eligible' to celebrate IYCr2014? Just think of scientific societies for mineralogy, synchrotron light, structural biology and chemistry, physics and so on. In many countries, these are very active and include many crystallographers: that’s why in my letter to the coordinators of regional and national associations I asked them to invite representatives to join the working teams and act as go-betweens with their societies.



Countries that adhere to the IUCr are shown in red.

Furthermore, one of the aims of IYCr2014 is certainly to provide access to crystallographic knowledge and technology to many more people in the world, and that is the reason why most of the activities the IUCr is conducting — in a friendly and active collaboration with UNESCO — will involve countries in the developing regions. As pointed out by the IUCr President in his Letter, many countries, in particular in

Africa and Latin America, do not adhere to the IUCr (see map). Hopefully, IYCr2014 will allow our community to grow and welcome more people and new countries under the umbrella of the IUCr.

Starting with the next issue of the *IUCr Newsletter*, a column will be launched titled 'What does the International Year of Crystallography mean for you?' Everybody is invited to give her/his thoughts about this. Please send your contribution to iycr2014@iucr.org. All contributions will be collected on the iycr2014.org web site and a few selected letters will be regularly published in the *IUCr Newsletter* in this IYCr2014 section. When I first thought about IYCr2014, three words came to my mind: celebrate, disseminate and innovate. If IYCr2014 was only a (well-deserved) celebration of the past century from the birth of X-ray crystallography, then it would have generated only scarce interest. We should instead join our efforts to make 2014 mark the *beginning* of a new century, with new challenges and frontiers to be explored, and exploit the opportunity of IYCr2014 for the popularization and dissemination of crystallography.

I look forward to receiving your ideas, suggestions and comments, and wish us all a successful IYCr2014.

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

IYCR 2014

IYCr2014 Opening Ceremony



Photo © UNESCO/Michel Ravassard.

The Opening Ceremony of IYCr2014 will take place in Room 1 at the UNESCO Headquarters, place de Fontenoy, Paris, France, on January 20–21, 2014. Situated in the 'Accordion' building, Room 1 is the Organization’s biggest space and hosts the biennial UNESCO General Conference. For more details of the IYCr2014 Opening Ceremony, see www.iycr2014.org/events/other/iycr2014-opening-ceremony.

IYCR 2014

Q: What crystal do you think was the most important ever and why?

Here are some possible answers without including the word 'ever'



Crystal structure of activated beta-2 adrenergic receptor in complex with Gs. Søren G. F. Rasmussen *et al.*, *Nature* (2011), **477**, 549–555. PDB entry 3SN6.

This year the most important crystal structure that has been solved is that of the ligand-free G-protein-coupled receptor (GPCR), which will help design more effective drugs. So this could be appointed as the 'most important' candidate for the year 2013.

Last year, the structures were established of several GPCRs bound to their ligands, including the structure of a GPCR bound to the G protein it activates in cells which was considered of sufficient significance to merit the Nobel Prize in Chemistry. Given the importance of the discovery, these crystals could be considered the most important crystals in 2012.

We had an incredible number of fundamental crystal structures studied and solved in the last 100 years of crystallography. Many of them had a tremendous impact at the time: Nobel prizes were awarded. But it is very difficult to find answers for the question above if we include the word 'ever'.

If the question is to be answered personally, the most important crystals ever were borazaro-phenanthrene crystals, whose phase transitions I observed in a polarizing microscope in the Crystallography Lab of the CNEA in Bs. Aires in the late 60s. They captured my imagination and helped me decide my future career as a crystallographer.

If the question is to be answered from the point of view of Science and Social Welfare, the most important ever are salt and sugar crystals: UNICEF reports that half of the children in developing countries that die of dehydration could be saved with a home-made recipe of diluted salt and sugar water solution: those items sometimes are not available in their homes.



A study by researchers from the School of Earth and Environment at the U. of Leeds and the Lab de Estudios Cristalográficos CSIC-U. of Granada found that gypsum starts off as tiny crystals of a mineral called bassanite. Most of us know this as Plaster of Paris as we use it in building, art-work, casts and fireproofing. Currently bassanite plaster is manufactured at a rate of 100 million tons per year by dehydrating quarried gypsum at 150°C. For the full article, visit www.leeds.ac.uk/news/article/3113/how_to_plaster_the_world_cheaply. (Photo credit: Javier Trueba/Madrid Scientific Films)
If we focus the answer on the wonders of Nature, the most important ever would be the giant crystals of selenite discovered in the caves of México, Chile, Perú and Spain.

And this is just in a general context: for us crystallographers, really obsessed people, the crystal we are studying is the most important ever. This is the spirit and drive that has led several generations of crystallographers to obtain remarkable achievements during the last century.

Iris Torriani

IYCR 2014

Shapes that run the world

From ACA *RefleXions*, Spring 2013



Photo from Molecular Graphics Laboratory at The Scripps Research Institute.

With the celebration of the International Year of Crystallography, the time is ripe to create models to let the world experience the beauty of molecular complexity and help the public to see the shapes of life-saving drugs and molecular machinery. Many laboratories and department machine shops are acquiring 3D printers at a typical cost of $30–$50k but you can build your own from a $2k kit. As an alternative to having your own printer, several groups provide 3D printing services on an at-cost basis for academic sites using user-supplied descriptor files, for example the Scripps Inst. (http://models.scripps.edu/) and 3D Molecular Designs (http://www.3dmoleculardesigns.com).

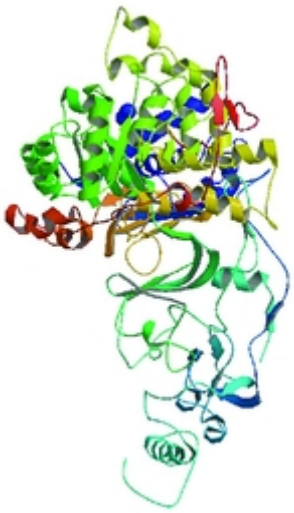
George Phillips used PyMOL to generate a descriptor file of the unit cell of one of his structures which was printed with a Z-corp printer in the departmental shop at the U. of Wisconsin; more examples are at www.molecular-sculpture.com/PDBweb/GP-Rice. A commercial service can be found at http://www.shapeways.com/create.

Istvan Botos alerted me to a service offered by Staples in Germany: send them a .obj, .stl or .wrl file (and some Euros) and they will print your model for you. What could be easier? Even though it is a challenge to choose descriptive parameters such that the beauty of the molecule is properly expressed, it is well worth the effort and helps fulfill our obligation to demonstrate to the world that crystallography is also an art form.

Edgar Meyer

IYCR 2014

Favorite crystal



Asymmetric unit of 1E9Z - crystal structure of *Helicobacter pylori* urease.
I nominate urease. It demonstrated that proteins actually HAD a structure, instead of being some amorphous glop...

From Wikipedia:



James B. Sumner
At Cornell, James B. Sumner began his research into isolating enzymes in pure form, a feat which had never been achieved before. The enzyme he worked with was urease. Sumner's work was unsuccessful for many years and many of his colleagues were doubtful, believing that what he was trying to achieve was impossible, but in 1926 he demonstrated that urease could be isolated and crystallized (http://en.wikipedia.org/wiki/Crystal). He was also able to show by chemical tests that his pure urease was a protein. This was the first experimental proof that an enzyme is a protein, a controversial question at the time.

His successful research brought him to full professorship at Cornell in 1929. From 1924 on his laboratory was located on the second floor of the new dairy science building, Stocking Hall (today home to Food Science), at Cornell, where he did his Nobel prize-winning research. In 1937 he succeeded in isolating and crystallizing a second enzyme, catalase. By this time, John Howard Northrop of the Rockefeller Inst. had obtained other crystalline enzymes by similar methods, starting with pepsin in 1929. It had become clear that Sumner had devised a general crystallization method for enzymes, and also that all enzymes are proteins.

George N. Phillips Jr

IYCR 2014

MCC celebrates IYCr2014



JuanMa García Ruiz introduces the students to symmetry at the first lecture of the 2012 MCC.

Every year, Module 1 of the Master in Crystallography and Crystallization (MCC), directed by JuanMa García Ruiz (U. of Granada, Spain), ends with a 'Crystallography and Society' workshop in Santander, Spain, on a variety of topics geared to the popularization of crystallography and crystallization and to promote awareness of the impact of crystallography in our daily lives. This year, the two-day workshop on July 8–9 is devoted to the different activities that are being planned and developed for IYCr2014. Master and PhD students in the different fields where crystallography is relevant, as well as journalists and journalism students, will hear talks given by representatives from the key organizations involved in IYCr2014: IUCr, ACA, AsCA, ECA and UNESCO. For more information, see http://lafactoria.lec.csic.es/mcc/index.php/program-a-courses/module-3-specialized-courses/cryst-society.

IYCR 2014

Sponsors wanted

If anyone is interested in sponsoring IYCr2014, please contact iycr2014@iucr.org for details of sponsorship packages.

IYCR 2014

Range of IYCr2014 logos available

If you are planning an event associated with IYCr2014, please go to www.iycr2014.org/about/logo to read the logo usage guidelines and download the appropriate logo.

IYCR 2014

Get ready to be intrigued



As part of the celebration of IYCr2014, the e-book *Magnetic Group Tables – 1-, 2- and 3-Dimensional Magnetic Subperiodic Groups and Magnetic Space Groups* by Daniel B. Litvin is available to download free of charge. In PDF format, this publication tabulates the structure, symbols and properties of magnetic groups, illustrated by beautiful colour diagrams. For more information, see www.iycr2014.org/events/publications/magnetic-group-tables.

FEATURE ARTICLE

The Worldwide Protein Data Bank: safeguarding an indispensable archive

July 1, 2013, marks the 10-year anniversary of the founding of the Worldwide Protein Data Bank (wwPDB; wwpdb.org), the international collaboration that manages the PDB archive [1].

From modest beginnings



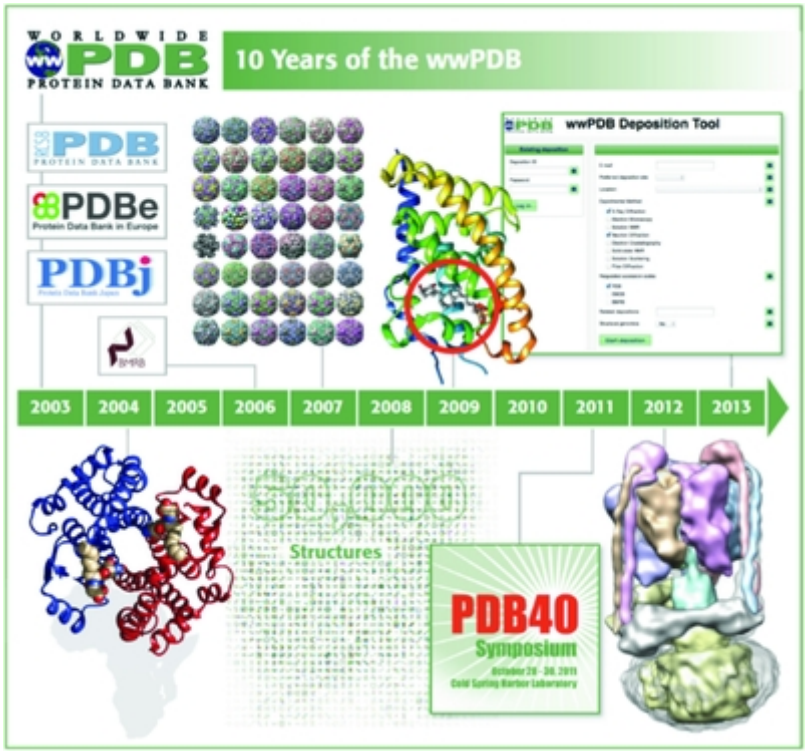
Subtilisin, one of the first structures deposited to the PDB archive. 1sbt, R. A. Alden, J. J. Birktoft, J. Kraut, J. D. Robertus, C. S. Wright. (1971) Atomic coordinates for subtilisin BPN′ (or Novo). *Biochem. Biophys. Res. Commun.* 45, 337-344.

Starting from just 7 protein crystal structures in 1971, the PDB archive has grown rapidly over the past 42 years. Last year alone, 9,972 new structures were deposited, more than in the first 25 years of the PDB combined. Today, the archive contains over 90,000 structures and at its current rate of growth will reach the 100,000 structure mark in 2014, the International Year of Crystallography.

On July 1, 2003, the way in which the PDB archive was managed was transformed by the founding of the Worldwide Protein Data Bank organization. From its inception, the PDB has been an international archive and the establishment of the wwPDB ensured that these valuable data will continue to be stored, managed and kept freely available for the benefit of scientists worldwide.

The wwPDB organization nowadays consists of four partners: the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB; http://rcsb.org) and BioMagResBank (BMRB; http://bmrb.wisc.edu) in the USA, the Protein Data Bank in Europe (PDBe; http://pdbe.org) and the Protein Data Bank Japan (PDBj; http://pdbj.org).

wwPDB milestones through the years



Selected highlights from the first 10 years of the wwPDB. 2003: The wwPDB is established. 2004: First PDB entry from Africa released (1ydk[2]). 2006: BMRB joins the wwPDB. 2007: First archive-wide remediation includes improved representation of virus assemblies. 2008: The PDB archive passes the 50,000 entry mark. 2009: Second release of remediated data includes improved representation of binding sites of ligands and metal ions (shown: 1rjk[6]). 2011: Historic symposium commemorating 40 years of the archive held at Cold Spring Harbor Laboratory; the PDB is the oldest surviving electronic archive of biomolecular data. 2012: PDB data and EMDB maps become part of the same ftp tree, simplifying distribution of these two important structural archives (shown: EMD-5476[7]). 2013: Testing of the next-generation wwPDB system for deposition and annotation begins.

2003 wwPDB established.

2004 First X-ray crystal structure from Africa is released in the PDB (1ydk[2]).

2005 PDB data available in PDBML/XML format.

2006 BMRB joins the wwPDB.

2007 First archive-wide remediation includes updated sequence information and primary citations, improved representation of virus assemblies, and standardized chemistry and nomenclature for monomers and ligands.

2008 50,000 entries in the PDB archive. Experimental data are mandatory for deposition. X-ray Validation Task Force (VTF) is convened[3].

2009 Second release of remediated data includes details about the chemistry of polymers and the ligands bound to it, biological assemblies, and binding sites of ligands and metal ions. NMR VTF is convened. Deposition of chemical shifts mandatory for NMR structures.

2010 Provision of wwPDB validation reports becomes a requirement for manuscript submission, starting with the IUCr journals. 3DEM VTF is convened[4].

2011 PDB40 symposium commemorating 4 decades of the archive held at Cold Spring Harbor Laboratory; the PDB is now the oldest electronic archive of biomolecular data. At a wwPDB workshop, the

major developers of X-ray structure-determination software agree to adopt PDBx/mmCIF as the principal format for structure deposition.

2012 PDB data and EMDB maps become part of the same ftp tree, simplifying distribution of these two important structural archives. SAS Task Force is convened[5].

2013 Testing of the next-generation wwPDB system for deposition and annotation begins. 10,000th NMR structure is released. PDBx/mmCIF is announced as the future standard format for deposition and distribution of PDB data. Updated wwPDB Charter goes into effect on July 1, starting the second decade of the wwPDB.

wwPDB activities

The wwPDB partner sites each act as deposition, processing and distribution centres for PDB data. They work together and in consultation with the wider community to define deposition and annotation policies, file formats and validation standards for structural data. This close collaboration between the member organizations is vital to guarantee that the global community of PDB users is provided with reliable and consistent data.

While working jointly on all aspects of data representation and processing, each partner site also offers independent tools and services that help make the wealth of data about biomacromolecular structure and function easily accessible to the user community.



Members of the PDB, past and present, in attendance at the PDB40 symposium. www.wwpdb.org/PDB40.html (Photo by Constance Brukin)
wwPDB activities are overseen by an international advisory committee comprising experts in X-ray crystallography, 3DEM, NMR and bioinformatics.

Future Challenges

The increasing volume, diversity and complexity of biological data being deposited in the PDB, and the emergence of hybrid techniques to obtain structural insights into biologically relevant molecules, complexes and molecular machines, all present major challenges for the management and presentation of structural data.

To address these challenges, the wwPDB partners are jointly developing a software system that will allow deposition, validation and annotation of complex and diverse macromolecular structures along with the underlying experimental data using a single interface. This new system will go into full production at all the wwPDB deposition sites early in 2014 and will then be able to handle depositions of structures of any size, determined using diffraction, NMR and/or EM methods.

Validation will be an integral part of the new deposition and annotation system. Assessment of coordinates, experimental data and associated metadata at the time of deposition is vital for improving

the quality of the archive. In addition, it will help users with no or limited structural biology background to select the most appropriate structural models for their purposes.

Whatever new challenges the next 10 years will bring, the wwPDB will remain committed to maintaining high standards of quality, integrity and consistency of the macromolecular structure archive, and to make it freely available to an increasingly large, diverse and demanding global community of users.

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MEETING REPORT

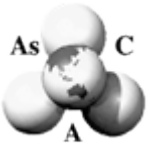
AsCA 2012/Crystal 28

Basic and applied crystallography, alive and well down under

Adelaide, Australia, December 2012
http://asca12.iucr.org/





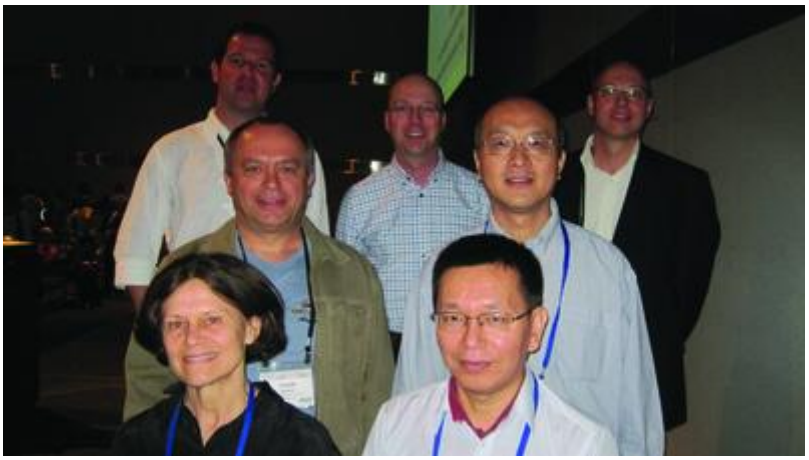




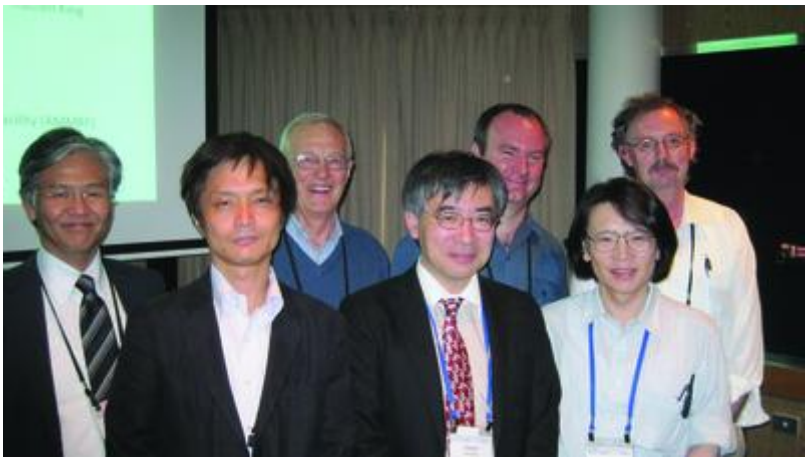
Attendees leaving the closing session.

The reports at the 2012 joint meeting of the Asian Crystallographic Association (AsCA) and Society of Crystallographers in Australia and New Zealand (SCANZ) provided structural data on the hottest and fastest moving areas of biological and materials science as well as technical advances that promise to keep crystallographic research at the cutting edge of science for years to come. Throughout the meeting three simultaneous sessions were held on broad topics that could be characterized as macromolecular, materials and technology. In each of these areas there were topics that had emerged in the last ten years to dominate much of the field: nanoscale, self assembly, in situ, high throughput, and dynamics. The opening ceremony featured a presentation on SAD Analysis of Macromolecular Structure by Wayne Hendrickson.

The first day of the meeting began with a plenary lecture by Henry Chapman (CFEL DESY) on protein nano-crystallography using X-ray laser pulses. The technique involves a remarkable new way to prepare and deliver samples, and to gather, record and analyze data. The development of this powerful new technique has required the creativity, ingenuity and cooperation of dozens of talented scientists. The electron laser has a million times more photons in a single burst than traditional radiation and the new technique makes it possible to reap the benefits of the increased power before the radiation destroys the sample. This was followed by parallel sessions on biological structures, metallo-organics and diffraction physics.



Speakers in session MS1, Hot structures in biology.



Speakers in session MS3, Diffraction physics and applications of crystallography.

Hot structures in biology included histone chaparones (R. Xu, Chinese Academy of Science), a respiratory complex (L. Sazanov, MRC), clathrin-meadiated endocytosis (D. Owen, U. Cambridge), nuclear receptors (E. Xu, Van Andel Research Inst.) and a signal recognition receptor complex (S. F. Ataide, U. Sydney). **Metallo-organic structures** covered polymeric networks (J. J. Vital, U. Singapore) and coordination compounds (D. Turner, Monash U.), porous molecular solids (C. Doonan, U. Adelaide), metal-adenine complexes (Y. Patil, Indian Inst. of Science), anion binding cages (J. Clegg, U. Queensland) and cyano anions as molecular building blocks (S. Batten, Monash U.). Topics in **diffraction physics** included dynamical diffraction from a curved crystal resonator (S.-L. Chang, NSRRC), electrostatic potential visualization via synchrotron radiation (M. Takata, Spring-8), a nanofabricated holographic grating (M. Uchida, Saitama Inst. Tech.), electronic field effect on atomic and electronic structure (A. Johnson, U. Western Australia), a new neutron diffractometer at J-PARC (T. Ishigaki, Ibaraki U.), and the battle of signal versus noise (J. Holton, U. California).



Speakers in session MS6, Synchrotron and neutron sources, instrumentation and application. Front: Kazuhisa Kakurai, Kia Wallwork, Shin Ae Kim, Masao Yonemura. Back: Garry McInytre (Co-Chair), Pawel Grochulski, Claude Lecomte.

The afternoon had simultaneous sessions on **membrane proteins**, **non-ambient and *in situ* studies**, and **synchrotron and neutron instrumentation and applications**. Ten years ago the determination of the structures of integral membrane proteins was considered unachievable. Now entire sessions are devoted to them. The **membrane protein** session covered genomics approaches (W. Hendrickson, Columbia U.), crystallization with antibody fragments (T. Murata, Chiba U.), electron crystallographic investigations (A. Mitra, U. Auckland), overlapping binding sites of water and lipids (M. Maher, La Trobe U.), and H+-translocating pyrophosphatase (Y.J. Sun, Tsing Hua U.). **Non-ambient studies** included high-pressure studies of minerals (A. Sano, Japan Atomic Energy), 1-D magnetic materials (J.-J. Lee, NSRC) and transformations in highly compressible crystals (S. Duyker, ANSTO). Hydrogen storage materials (E. Gray, Griffith U.) and steel corrosion (B. Ingham, Industrial Research Ltd.) were the focus of ***in situ* studies**. The **instrumentation** session had talks on a powder neutron diffractometer (M. Yonemura, KEK), polarized neutrons (K. Kakuri, Japan Atomic Energy), a neutron image-plate detector (S. A. Kim, Korea Atomic Energy Research Inst.), developments at Canadian (P. Grochulski, Canadian Light Source) and Australian (K. Wallwork, Australian Synchrotron Co. Ltd) synchrotron sites, and spin-dependant electron-density analysis using X-ray and polarized neutron data.



Speakers in MS8, Energy-related materials. Front: Myung Hyun Paik Suh (Co-chair), Jacqueline Cole, Denissa Murphy, Hongcai Zhou. Back: Chris Ling, Vanessa Peterson, Davide Viterbo, Stefan Adams.

The keynote lectures on the second day concerned a killer cell receptor (J. Vivian, Monash U.) and solid-solution studies using atomic probe microscopy (S. Ringer, U. Sydney). The morning's simultaneous sessions were on **drug discovery**, **energy-related materials** and **molecular dynamics in solid-state crystals**. The **drug-discovery** session covered inhibitors of kinases (S. Jacob, Novartis), phosphodiesterases (J. Pandit, Pfizer), BHRF1 (S. Caria, Le Trobe U.) and c-JNK (D. P. Karothu, Indian Inst. of Science), and the mechanism of action of an antibody to BACE1. Pandit discussed specific inhibitors for two phosphodiesterases (from a total of 60 in the central nervous system) that are associated with psychosis. BACE1 inhibitors may reverse, delay or prevent Alzheimer's disease. Topics on **energy-related materials** included metal-organic frameworks (H. Zhou, Texas A&M), lithium ion conductors (S. Adams, National U. Singapore), incommensurate modulated structures (C. Ling, U. Sydney), solar cooling applications (D. Viterbo, U. Piemonte Orientale) and dye-sensitized solar cells (J. Cole, U. Cambridge). The session on **dynamic aspects of crystallography** included studies of picosecond lattice and charge dynamics (Y. Moritomo, U. Tsukuba), dynamic disorder and fuel cells (J. Gale, Curtin U.), phonon softening (A. Baron, Spring-8), and phase transitions in pharmaceuticals (H. Uekusa, Tokyo Inst. of Technology) and lanthanide pyrochlore-florites (P. Blanchard, U. Sydney). Concurrent sessions in the afternoon concerned **macromolecular assemblies**, **chemical crystallography**, and **structural proteomics and genomics**. The session on **macromolecular assemblies** included talks on three types of viruses, insect pox virus (F. Coulibaly, Monash U.), hemorrhagic fever virus (Z. Lou, Tsinghua U.) and orf virus (K.

Krause, U. Otago), as well as DNA-protein complexes (X.-D. Su, Peking U.) and domain swapping in a survival protein (Y. K. Mathiharan, Indian Inst. of Science). **Chemical crystallography** addressed mesoporous inorganic frameworks (S.-L. Wang, Tsing Hua U.), *in situ* control of photochromism (A. Sekine, Tokyo Inst. of Technology), the structure correlation principle applied to Diels-Alder reactions (J. White, U. Melborne), accurate chemical characterization (A. Edwards, ANSTO) and crystal packing predictions (G. Gainsford, Industrial Research Ltd.). **Proteomic/genomics** talks concerned mobile gene elements (B. Mabbut, Macquarie U.), autophagic molecules (H. K. Song, Korea U.), protein-protein interfaces (P. Chakrabarti, Bose Inst.), protein crystallogenesis (J. Newman, CSIRO) and *de novo* models for *ab initio* phasing (K. Zhang, RIKEN).



Speakers in Session MS7, Enzymes.



Speakers in Session MS14, Small-Angle Scattering. Front: Angela Criswell, Charlotte Conn (Co-chair), Kevin Jack. Back: Patrick Kluth, Anthony Duff, Andrew Whitten.

The keynote lectures on the third day concerned optoelectronic applications of *in situ* photo-crystallography (J. Cole, U. Cambridge), and polar nanoregions and diffuse scattering in ferroelectrics (R. Welberry, Australian Nat. U.). The last morning featured simultaneous sessions on **enzymes**, **small-angle scattering** (SAXS), and **crystal growth and engineering**. **Enzymes** studied included phosphagen kinases (S. Ye, Chinese Academy of Science), full-length human plasminogen (J. Whisstock, Monash U.), CO photolysis in haem oxygenase (M. Sugishima, Kurume U. School of Medicine), ferredoxin-dependant glutamate synthase (K. Shinmura, Osaka U.), and something we can all raise our glass to, auxin amido synthetase in Cabernet Sauvignon (T. Peat, CSIRO). Topics explored by **SAXS** included high-energy ion tracks (P. Kluth, Austrian National U.), self-assembled polymers (K. Jack, Ctr for Microscopy and Microanalysis), membrane fusion (A. Whitten, U. Queensland), full-length human ezrin (A. Duff, ANSTO) and the structure of starch (E. Gilbert, ANSTO). A. Criswell (Rigaku) described high-throughput biological SAXS in the **home laboratory**. Techniques to improve **crystallization** included metal-mediated synthetic symmetrization (A. Soriaga, UCLA), solvothermal synthesis of metal-organic frameworks (I. Williams, HKUST) and protein sequence engineering (Z. S. Derwenda, U. Virginia). The merits of evaluating crystal forms using the Cambridge Structural Database (P. Wood, CSD) and of using

X-ray transparent plates for high-throughput protein crystallization (R. Thorne, Cornell U.) were also described.



Front row: Darren Goossens (winner of the Mathieson Medal of SCANZ), Lois Mathieson, Gautam Desiraju, Patience Thompson and Peter Colman (winner of the Bragg medal of the Society). Back: Award winners (identifications unknown).

The meeting closed with talks by the new editor in chief of *Acta Cryst.*, S. Hasnain, on a new era of crystallographic-based science, and a final plenary by X.-M. Chen (Sun Yat Sen U.) on metal azolate frameworks for crystal engineering of functional materials.

William Duax











These and over two hundred other photos taken at the 2012 meeting of AsCA, the SCANZ 28 and the Bragg Centennial Symposium are on the IUCr website (www.iucr.org). There is a complete set of photos of the people at individual tables at the AsCA banquet. We regret that we are able to provide only partial captions for some of these pictures and cannot identify all participants. If you attended either meeting it is very likely that a photo of you is on the website. The website has been designed by the talented staff in Chester to make it possible for you to help us identify all those pictured. Your assistance would be greatly appreciated.

OBITUARY

Tribute to Steve Wilkins

Taken from AsCA e-newsletter (May 2013)



Steve Wilkins, a prominent Australian crystallographer who contributed much to AsCA by successfully organizing the Bragg Centennial Symposium in Adelaide on December 6, 2013, passed away in Melbourne on March 25, 2013. He will be remembered by many of us as a dedicated scientist and a likeable person. An obituary is being written by Andrew Stevenson and Jose Varghese to be published in *Acta Cryst*. Please visit the following tribute web-pages for more details (www.synchrotron.org.au/index.php/news/news/steve-wilkins and www.csiroalumni.org.au/blogpost/952177/Tributes-to-Steve-Wilkins).

IUCR ACTIVITIES

Minutes of the AsCA Council Meeting

Adelaide, Australia, December 2012

19 delegates from 8 countries, a number of invited guests and interested meeting participants attended the meeting. ASCa President S. W. Suh opened the meeting and introduced the guests.



1st row: Pinak Chakrabarti (AsCA Vice President), Se Won Suh (AsCA President), Alice Vrielink (AsCA Secretary/Treasurer). 2nd row: Hwo-Shuenn Sheu, Takashi Kamiyama, Jennifer Martin, Altaf Hussain, Duong Ngoc Huyen, Samat Talipove, Ian Williams. 3rd row: Atsuhi Nakagawa (Japan), Jagadese Vital (Singapore).

IUCr President G. R. Desiraju presented an overview of the current activities of the IUCr. He commented on the growth of the community within AsCA and the high quality of talks and, particularly, the larger number of students in attendance. He described the International Year of Crystallography (IYCr) 2014 as an opportunity to highlight our science throughout Asia, including at the high-school level. UNESCO is willing to support a traveling exhibition of crystallographic equipment that will go to smaller Asian countries (Indonesia, Philippines, Vietnam and Bangladesh) to educate and inspire young people. Desiraju suggested that the larger countries (Australia, China and India) could play an important role in promoting crystallography in the region. He urged them to send their manuscripts to IUCr Journals and to help in gathering funds or in-kind contributions to support IYCr2014. He has asked that all National committees formulate plans for IYCr and communicate their plans to the IUCr. The IUCr encourages activities such as the publication of textbooks about crystallography in various languages to teach our science to the next generation of crystallographers. The IUCr has appointed a project manager to promote IYCr activities. All communications about regional activities should be sent to the project manager.

S. Talipov (Uzbekistan) gave a presentation detailing crystallography activities in his country.

IUCr Newsletter editor, W. L. Duax, urged attendees to send articles describing crystallographic activities and achievements in AsCA countries and especially plans for IYCr activities to him for publication in the *Newsletter* of IUCr. The *Newsletter* is sent electronically to all crystallographers in the IUCr database. Printed copies are also sent to libraries. If individuals would like to have copies sent to their local library they should send the name and address of the library to Duax. If you would like to have hard copies to distribute at meetings that you host or attend, notify the *Newsletter* office. Duax has asked everyone to identify a crystal that made a significant difference to the world (or just to them) and to write a

paragraph explaining their choice. If published the author will receive two glasses with the structure of their 'Most Important Crystal' etched on the surface.

Samar Hasnain, the newly appointed Editor in Chief of the IUCr journals, spoke about his vision for the IUCr Journals. His presentation is entitled 'Responding to a new era of crystallographic-based science and changes in its global distribution'.

His aims for the future development of the IUCr journals are:

- To make IUCr journals the natural home for many of the high-quality scientific publications that are currently published elsewhere;
- To encourage chemists, biologists, physicists, material scientists, mineralogists, computational scientists and archaeologists to report the best of their crystallographic results in the IUCr journals;
- Publishing original research articles review articles (topical, trends, opinions, etc) in all areas of the IUCr commissions; and
- A new Management Board for the IUCr Journals held its first meeting in October. Membership to the Board consists of the Editor in Chief of the IUCr Journals, the Executive Managing Editor, IUCr President, IUCr General Secretary and Treasurer and a Main Editor of each IUCr journal.

Meeting report: Ray Withers reported that AsCA2012/Crystal28 was running smoothly with three concurrent sessions, over 425 attendees and the prospect of a modest sum balance. R. Withers also reported on the Bragg Symposium. The expectation is that there will be ~350 delegates including school children. The city of Adelaide would unveil a bust of Lawrence Bragg on Friday, December 7th.

MEETING REPORT

Scientific conferences do not have to be boring!

Poznan, Poland, May 2013

On May 22, 2013, the Center for Biocrystallographic Research at the Inst. of Bioorganic Chemistry, Polish Academy of Sciences in Poznan, Poland, organized a conference on 'Structural Biology of Plants and Microbes', where the international PhD students supported by the Foundation for Polish Science presented the results of their research. In addition, there was a general poster session and lectures by invited speakers, including Zbyszek Dauter (ANL, Chicago, USA) who tried to 'apply common sense to PDB structures', Alex Wlodawer (NCI, Frederick, USA), who spoke about anti-cancer plant proteins, and Matthias Bochtler (IIMCB, Warsaw, Poland), who dissected the consequences of DNA methylation.

Among the students' presentations there were real crystallographic gems, for example a crystal structure with 28 independent protein molecules (Joanna Sliwiak), an example of enzyme optimization using structures from extremophiles as the tuning fork (Piotr Malecki), structural genomics of silkworm hemolymph with a bag of surprises (Agnieszka Pietrzyk), or structural biology of symbiotic nitrogen fixation from the point of view of phytohormone signaling (Milosz Ruszkowski) and symbiont enzymology (Tomasz Manszewski). There were attractive prizes for the best student talk (Milosz Ruszkowski) and poster (Patrycja Plewka and Stanislaw Wosicki).



The CrystallogRAPPERS' band. Left to right: Tomek Manszewski, Asia Sliwiak, The Professor, Piciu Malecki, Milas Ruszkowski.

All this could sound like a dry recounting of the agenda of yet another conference but there was a difference. The scientific program was elegantly blended with a number of attractive events. During an intermission, there was a concert by the Institute's choir performing a collection of classical and adapted choral music. Just after the scientific talks, there was a short 'Lecture on crystallography in the form of rap'. This serious/hilarious lecture was recited to bursts of laughter from the audience by a band of students together with their professor.

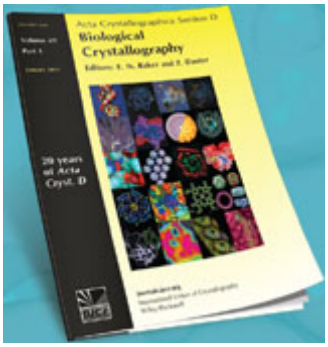
After the lecture, Dr Wlodawer (NCI Mentor of Merit) presented his thoughts about mentoring in science. The talk was followed by a short general discussion, with the conclusions that there is no one, 'the best', way of student mentoring, that the ability to listen to each other builds a successful mentee-mentor relation, and that proper selection of mentees is also important.

As an aperitif before the conference dinner, Joanna Sliwiak opened a bottle of champagne to celebrate her structure with 28 protein molecules in the asymmetric unit. Instead of the usual toasts, the dinner featured a long recital of crystallographic limericks composed by two (in)famous 'poets', Dr Zbyszek Dauter and Prof. Mariusz Jaskolski. At its height, the recital threatened to become a fierce duel. Fortunately no blood was shed, and the last poem, recited jointly, ended with a jolly and encouraging 'Long Live Crystallography!'. It was a memorable conference, indeed.

Mariusz Jaskolski

IUCR ACTIVITIES

Acta Cryst. D impact factor rises to 14.1



Acta Crystallographica Section D: Biological Crystallography again leads the Crystallography rankings in the latest Journal Citation Reports with its highest ever impact factor of 14.1, the third successive increase.

In addition to taking the number one spot in Crystallography, the journal is also No. 1 in Biophysics, No. 2 in Biochemical Research Methods and No. 7 in Biochemistry and Molecular Biology.

The journal would like to thank all the readers, authors, editors and referees who have contributed towards its success.

journals.iucr.org/d

MEETING REPORT

Mathematical Crystallography at Applied Mathematics Conference

Philadelphia, PA, USA, June 2013

www.crystallography.fr/mathcryst/



Eleven speakers (and one moderator) spoke at the three Mathematical Crystallography minisymposia. Top: Frank Morgan, Ma. Louise de la Penas, Egon Schulte and Bernd Souvignier. Middle: Massimo Nespolo, Uwe Grimm, Peter Zeiner and Marjorie Senechal. Bottom: Greg McColm, Henrik van Lengerich, Jean-Guillaume Eon and Mike Zaworotko.

Eleven speakers described recent research in mathematical crystallography at a Society for Industrial and Applied Mathematics (SIAM) conference on Mathematical Aspects of Materials Science in Philadelphia in June, 2013. The presentations occurred in three minisymposia co-organized by the IUCr Commission on Mathematical and Theoretical Crystallography.

Henrik van Lengerich described some difficulties in the self-assembly of finite structures. Egon Schulte and Ma. Louise de las Penas generated families of finite and infinite graphs. Peter Zeiner looked at lattices with nice sets of basis vectors. Bernd Souvignier and Jean-Guillaume Eon examined periodic nets from an algebraic point of view, while Frank Morgan looked at periodic minimal surfaces. Massimo Nespolo discussed properties of crystal structures related via phase transitions or isotypism, while Uwe Grimm discussed recent advances in diffraction theory.

Marjorie Senechal and Mike Zaworotko presented several challenges for the crystallography community to address. These were: how self-assembly works, what polygonal and polyhedral shapes of molecular building blocks are most useful and why, how one might make crystals with bent linkers, folding

(including protein folding), the behavior and properties of infinite structures, generating designs of tri-nodal nets, to what extent are some nets special cases of others, the origins of diffuse (diffraction) scattering, making crystal design a routine activity, and building a common vocabulary for the community.

The conference was organized by the SIAM Activity Group on Mathematical Aspects of Materials Science (www.siam.org/activity/materials_science/). During an open-floor session, participants discussed prospects for more meetings and other activities to promote mathematical crystallography. Some outcomes of that discussion, and other prospects for the subject, are posted on the Crystal Mathematician blog at http://blogs.iucr.net/crystalmath/.

Greg McColm

REGIONAL NEWS

News from the ACA

ACA *RefleXions*, Spring 2013



Tom Koetzle



Tom Terwilliger



Eric Ortlund

The spring 2013 issue of the ACA newsletter featured the lectures of Warren Award winner Paul Fenter and Etter Early Career awardee Emmanuel Skordalakes, and a historical essay by Marjorie Senechal describing her life in Science and Mathematics. There is also a review of a new book by Senechal, 'I died for Beauty, Dorothy Wrinch and the "Culture of Science”', a balanced picture of the accomplishments of the first woman to receive a doctorate of science degree from Oxford U.

The 2013 ACA awardees Tom Koetzle (Bau Neutron Diffraction), Tom Terwilliger (Trueblood Computational Chemistry) and Eric Ortlund (Etter Early Career) will present lectures at the meeting in Hawaii. Richard Dickerson, Frankuchen Awardee, will be unable to attend the meeting; Alex McPherson will give a retrospective on Dickerson's work.

AWARDS AND PRIZES

Awards to Crystallographers

From ACA *RefleXions*, Spring 2013



Helen Berman

Helen Berman, a professor at Rutgers U. and co-founder of the Protein Data Bank (PDB), has won the 2013 DeLano Award for Computational Biosciences from the American Society for Biochemistry and Molecular Biology for her efforts to make structural data universally available. About 25 new macromolecular structures are submitted to the PDB each day, and more than 88,000 structures have been made available since it was established in 1971.



Jennifer Doudna

Jennifer A. Doudna is the inaugural recipient of the American Society for Biochemistry and Molecular Biology Mildred Cohn award in Biological Chemistry. In addition Doudna, professor of biochemistry, biophysics and structural biology at the U. of California, Berkeley, was one of two recipients of the 2013 Hans Neurath Award for her study of three-dimensional structures of noncoding RNA and the regulation of protein products by ribonucleoproteins.

REGIONAL NEWS

ACA Canadian Division

From ACA *RefleXions*, Spring 2013

Members of the Canadian National Committee for Crystallography are: Jim Britten, Chair, Pam Whitfield, Vice Chair, Joe Schrag, Secretary, Marie Fraser, Treasurer, Stan Cameron, Lee Groat, Lynne Howell, and *ex officio*, David Rose.

The officers of the ACA Canadian Div. are Gerald Audette, Chair, and Brian Patrick, Secretary. The Canadian Div. is co-sponsoring several scientific sessions at the Hawaii meeting: Structure; Enzymology; Computational Tips and Tricks; Cool Structure; and Research at Undergraduate Institutions. Because Canadians co-chair these sessions, abstracts directed to them stand an excellent chance of being selected for talks. In addition, the Delbaere-Pauling Poster Prize is awarded annually to the top trainee poster from a Canadian laboratory.

AWARDS AND PRIZES

Tenth Ewald Prize Call for Nominations

Tenth Ewald Prize
Call for Nominations



The IUCr is pleased to invite nominations for the Ewald Prize for outstanding contributions to the science of crystallography. The Prize is named after Paul P. Ewald, in recognition of his significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography. Prof. Ewald was the President of the Provisional International Crystallographic Committee from 1946 to 1948, the first Editor of the IUCr publication *Acta Crystallographica* from 1948 to 1959, and the President of the IUCr from 1960 to 1963.

The prize, consisting of a medal, a certificate and a financial award, is presented once every three years during the triennial International Congresses of Crystallography. The next prize will be presented at the Montreal Congress in August 2014.

Scientists who have made contributions of exceptional distinction to the science of crystallography are eligible for the Ewald Prize, irrespective of nationality, age or experience. The Selection Committee will give careful attention to the nominations of outstanding scientists who have not yet won a Nobel Prize. Either an exceptionally distinguished scientific career or a major scientific accomplishment may be recognised. Current members of the Selection Committee and the President of the IUCr are not eligible. No restrictions are placed on the time or the means of publication of the nominee's contributions. The Prize may be shared by more than one contributor, but not more than three, for the same scientific achievement.

Nominations for the Ewald Prize should be submitted electronically using the Ewald Prize Nomination Form to the Executive Secretary of the IUCr (execsec@iucr.org). The closing date for nominations is August 31 2013.

Further information and the Nomination form can be found at www.iucr.org/news/notices/announcements/chesternotice_2013_01.

IUCR ACTIVITIES

Bursary scheme for inter-regional travel of students and post-docs attending meetings of Regional Associates

The IUCr has established a bursary scheme for young scientists attending the annual meetings of the Regional Associates. This is additional to the young scientist support that the IUCr already provides and is aimed at facilitating the attendance of young scientists from the area covered by one Regional Associate at a meeting of a different Regional Associate. The aim is to broaden the knowledge of the awardees and enable them to establish contacts that will be of great help to them in their careers. For more information, visit www.iucr.org/iucr/sponsorship/regional.

REGIONAL NEWS

A peek into the life of the IUCr 2014 International Programme Committee

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



The International Programme Committee for the XXIII IUCr Congress in 2014 met in Montreal to develop the meeting programme. There was an opportunity to visit the Congress venue. Front row: Enrique Gutierrez-Puebla, Wieslawa Sikora, Massimo Nespolo, Jim Britten, João Rocha, Przemek Dera, Elliot Gilbert, Silvia Onesti. Second row: Beatrice Gillon, Ron Lifshitz, Paolo Radaelli, Artem Oganov, Koichi Kakimoto, Hanna Dabrowska, Samar Hasnain, Michele Bourgeois-Doyle. Third row: Albert Berghuis, Tom Terwilliger, Pinak Chakrabarti, Laurence Marks, Susan Bourne, Marvin Hackert. Back row: Martin Schmeing, Chris Chantler, Richard Garrett, Dave Billing, Pamela Whitfield, Daniel Vega, Robert Von Dreele.

Montreal, May 6, 8 o'clock on a beautiful morning. The weather has been gorgeous, above 20˚C temperatures, and the coming few days will be equally nice. Also, the Montreal Canadians, better known by hockey enthusiasts as the 'Habs', have made it to the NHL playoffs, making the city even more festive than usual. All in all it is the perfect day to walk outside, have a croissant and a café *au lait* for breakfast and enjoy life the Quebec way. However, for 30 crystallographers from around the world, representing Australia, Asia, Europe, Africa, North and South America, this is not the plan for today. These scientists are members of the International Programme Committee for the 2014 IUCr Congress in Montreal next August (now just a bit over a year away), and they are gathered on the 26th floor of a downtown building, facing three days of hard work preparing the Scientific Program for the Congress. The men and women of the IPC represent the various IUCr Commissions and each is eager to lobby for session topics that will attract and excite their members. For continuity, the chairs of the 2011 and 2017 program committees are full and active members. Also on the committee are the Editor-in-chief of the IUCr Journals, Samar Hasnain, and two members of the Executive Committee, Hanna Dabkowska and Marv Hackert (for a complete list of IPC members see http://iucr2014.org/side_organization/international_program_committee_e.shtml).

Montreal, May 8, 4 o'clock in the afternoon …… it is again a beautiful day. Unfortunately, the Montreal Canadians have not done well in the NHL playoffs, and are about to be eliminated, but Montrealers will recover, as the croissants and café *au lait* are still a great way to start the day. The 30 crystallographers

from around the world are tired but happy. They have toured the Palais des Congrès de Montréal and are satisfied that it is an excellent site for the meeting, with the talks on one floor and the exhibits, coffee and posters one escalator away.

We are happy to share the following highlights of the program:

There will be Nobel Laureates sharing stories as well as croissants with you in Montreal. There will be a session dedicated to the late Louis Delbaere, a former ACA President and IUCr Executive Committee member who led the Canadian bid to host the 2014 meeting in Montreal. The basic format for the keynote lectures and microsymposia has not changed, although there will now be eight parallel MS sessions (previously seven), and each MS will have three invited speakers and three speakers chosen from submitted abstracts. The bottom line is that there will be: more diversity of topics; more presentations; more speakers selected from abstracts; and thus ever more reasons to attend IUCr2014. The IPC spent a lot of time refining and merging session topics, as well as identifying topics of cross-discipline interest. Each delegate worked hard to ensure that the sessions were distributed in a manner that minimized overlap of related topics. In recognition of the International Year of Crystallography, some lectures will be open to the public.

Both the Local Organizing Committee and the International Programme Committee have great expectations for IUCr2014, and more importantly they are making every effort to make this a 'Must Attend' event. Having the Congress coincide with the International Year of Crystallography, by its very nature, makes this a once in a lifetime happening, and we sincerely hope that you will come to Montreal and share this occasion with us. To receive future announcements and other information about the congress, please register your 'expression of interest' at www.iucr2014.org.

Albert Berghuis and Jim Brittan

OBITUARY

Jerome Karle (1918-2013)



We are saddened to report the death, on June 6, 2013, of Jerome Karle. Jerome was a former President of the IUCr (1981-1984) and the American Crystallographic Association (1972), and a co-recipient, with Herbert Hauptman, of the 1985 Nobel Prize in Chemistry for his work on development of direct methods for the determination of crystal structures. Among the many additional honors he received for his work, he was elected to the US National Academy of Sciences in 1976 and the American Philosophical Society in 1990.

A full obituary will be published in a future issue.