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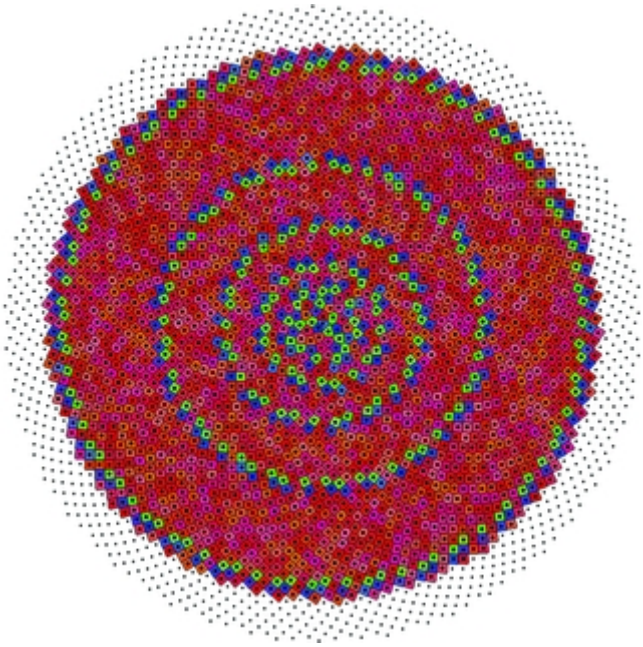
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2012 Nobel Prize in Chemistry announced 36

IUCR JOURNALS NEWS

Phyllotaxis: a non-conventional crystalline solution to packing efficiency in situations with radial symmetry

Acta Cryst. (2012). A68, 470-483 (http://doi.org/h9w)



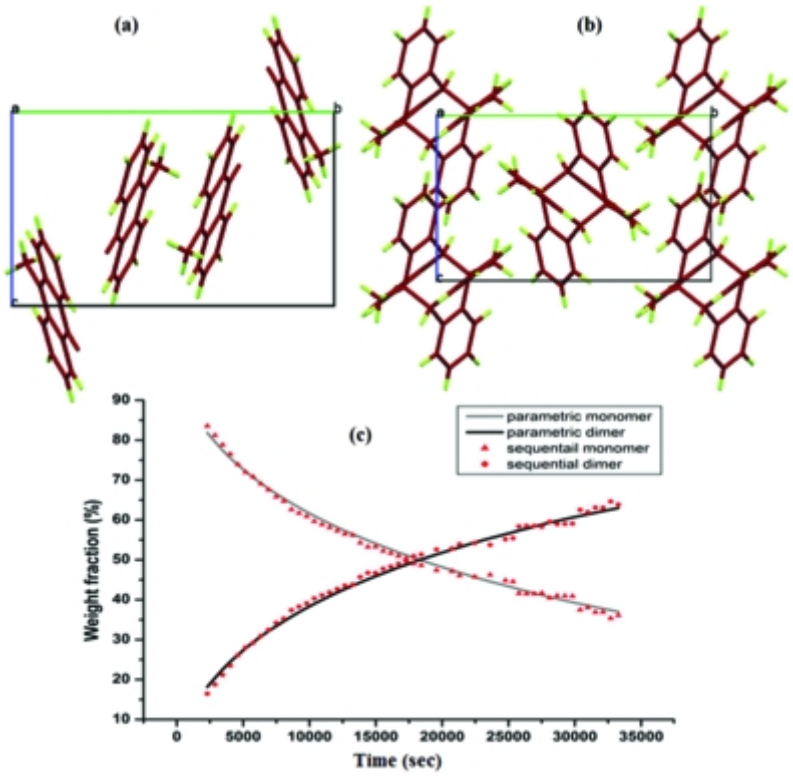
A Voronoi decomposition model.
Topological constraint of circular growth imposes an inflation-deflation invariance taking the place of the classical symmetries of crystallography. It appears in phyllotaxis, the arrangement of florets in composite flowers. Points placed regularly on a generative spiral constitute a spiral lattice, and phyllotaxis is the tiling by the Voronoi cells of the spiral lattice. The florets generated on a Fermat spiral have equal size, but are not all hexagonal. There are annular grains of hexagonal florets (red) separated by grain boundaries [quasiperiodic circular arrays of dislocations (green-blue)].

J.-F. Sadoc, N. Rivier and J. Charvolin

IUCR JOURNALS NEWS

A time-resolved powder diffraction study of in situ photodimerization kinetics of 9-methylanthracene using a CCD area detector and parametric Rietveld refinement

Acta Cryst. (2012). B68, 424-430 (http://doi.org/h9x)



Crystal structures of (*a*) 9-MA monomer and (*b*) dimer phases. (*c*) Comparison of the weight fraction progress with time for the monomer and dimer phases in sequential and parametric Rietveld refinements.

A time-resolved X-ray powder diffraction study of 9-methylanthracene (9-MA) during [4π + 4π] photodimerization was performed *in situ*, which is a typical example of solid-state photoreactions. The study overcomes the drawbacks of photoreaction in single crystals by the application of powder diffraction reaching higher completion (63.8%) of dimer fraction (Figure), and by taking advantage of full quantitative parametric Rietveld refinement of both monomer and dimer phases. The suggested reaction kinetics using the Johnson-Mehl-Avrami-Kolmogorov (JMAK) model is a heterogeneous decreasing nucleation and one-dimensional growth.

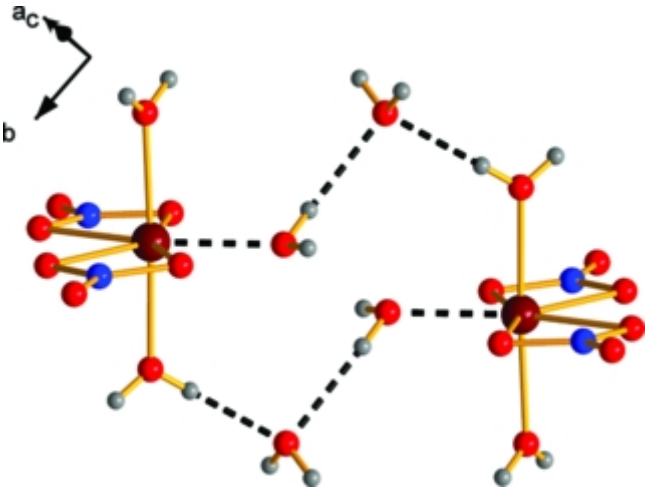
A. F. Mabied, M. Müller, R. E. Dinnebier, S. Nozawa, M. Hoshino, A. Tomita, T. Sato and S. Adachi

IUCR JOURNALS NEWS

New iron(III) nitrate hydrates: Fe(NO3)3·xH2O with x = 4, 5 and 6

New iron(III) nitrate hydrates: $Fe(NO_3)_3 \cdot xH_2O$ with x = 4, 5 and 6

Acta Cryst. (2012). C68, i29-i33 (http://doi.org/h9z)



Two pentagonal–bipyramidal $[Fe(NO_3)_2(H_2O)_3]^+$ units in $Fe(NO_3)_3 \cdot 4H_2O$.

Crystals of lower hydrates of iron(III) nitrate were grown from melts or solutions in concentrated nitric acid. While iron(III) is coordinated by six oxygen atoms in the hexahydrate and the pentahydrate, the coordination number of iron(III) in $Fe(NO_3)_3 \cdot 4H_2O$ is enhanced to seven. $Fe(NO_3)_3 \cdot 4H_2O$ represents the first simple iron(III) salt with pentagonal-bipyramidal coordination geometry. In our research we are interested in the study of the phase formation in inorganic salt-water systems. We have started systematic investigations and further results will be published soon.

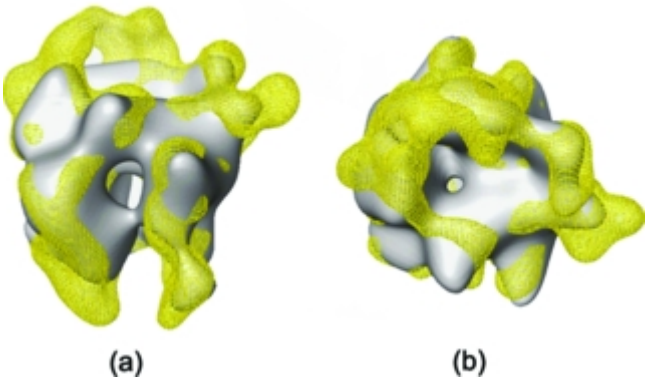
H. Schmidt, A. Asztalos, F. Bok and W. Voigt

IUCR JOURNALS NEWS

Low-resolution structure determination of Na+-translocating NADH: ubiquinone oxidoreductase from Vibrio cholerae by ab initio phasing and electron microscopy

Low-resolution structure determination of Na^+-translocating NADH: ubiquinone oxidoreductase from *Vibrio cholerae* by *ab initio* phasing and electron microscopy

Acta Cryst. **(2012). D68, 724-731 (http://doi.org/h92)**



Overlay of the 16 Å crystal structure (yellow) and the EM reconstruction (grey). (*a*) Side view, (*b*) top view of the Na^+-NQR complex.

A 16 Å resolution envelope of the membrane protein Na^+-NQR was determined by connectivity-based *ab initio* phasing. The found envelope was used as a reference in three-dimensional reconstruction of the Na^+-NQR from negative-stain EM images. The two methods displayed similar dimensions and features of the particle. Despite the resolution limitations, the method could provide important structural information in many X-ray crystallographic projects where the molecule of interest is a membrane protein or membrane protein complex yielding crystals of low diffractive power.

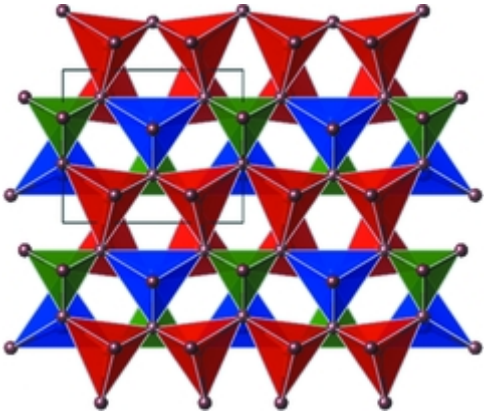
V. Y. Lunin, N. L. Lunina, M. S. Casutt, K. Knoops, C. Schaffitzel, J. Steuber, G. Fritz and M. W. Baumstark

IUCR JOURNALS NEWS

Redetermination of the low-temperature polymorph of Li2MnSiO4 from single-crystal X-ray data

Redetermination of the low-temperature polymorph of Li_2MnSiO_4 from single-crystal X-ray data

Acta Cryst. (2012). E68, i68-i69 (http://doi.org/h93)



Structure model of Li_2MnSiO_4 determined by the present study with projection view along [001]. Polyhedra are indicated by red color for LiO_4, blue color for MnO_4, and green color for SiO_4.

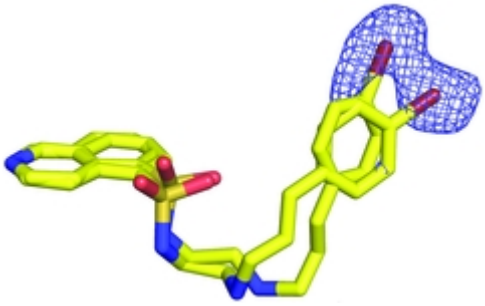
Dilithium manganese(II) orthosilicate, Li_2MnSiO_4, is currently investigated as an alternative cathode material in lithium ion batteries. The redetermination of the crystal structure of the low-temperature polymorph based on single-crystal X-ray data revealed a perfectly site-ordered model for the Li and Mn sites, consistent with recent solid-state NMR studies. The structural set-up can be derived from a distorted hexagonal close-packed arrangement of O atoms with half of the tetrahedral voids occupied by the three types of cations.

M. Sato, T. Ishigaki, K. Uematsu, K. Toda and H. Okawa

IUCR JOURNALS NEWS

Anomalous dispersion analysis of inhibitor flexibility: a case study of the kinase inhibitor H-89

Acta Cryst. (2012). F68, 873-877 (http://doi.org/h94)



Anomalous difference density map (4 σ) from the bromine signal shows two binding positions for the atom, with consequences for the modelling of a linker segment.

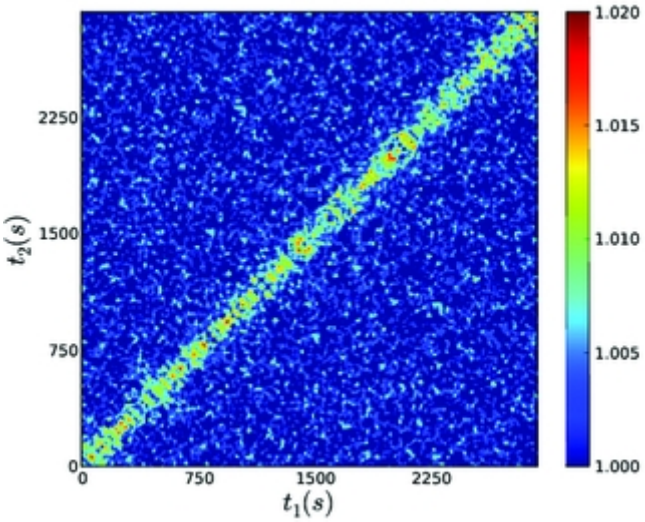
The anomalous dispersion signal from bromine was used to identify two binding geometries for the inhibitor H-89 bound to protein kinase A (PKA). Inhibitors often bind to proteins flexibly, with a range of binding geometries, but limited data resolution (or automated structure solution) may hinder their explicit inclusion into a structural model. Instead, flexibility is implicitly modelled with high temperature factors, implying more broadly unstructured binding throughout the volume in question. The serendipitous presence of an anomalous scatterer in the inhibitor enables more accurate modelling.

A. Pflug, K. A. Johnson and R. A. Engh

IUCR JOURNALS NEWS

A novel event correlation scheme for X-ray photon correlation spectroscopy

J. Appl. Cryst. (2012). 45, 807-813 (http://doi.org/h95)



Two-time correlation function of an organic molecular glass, DC705.

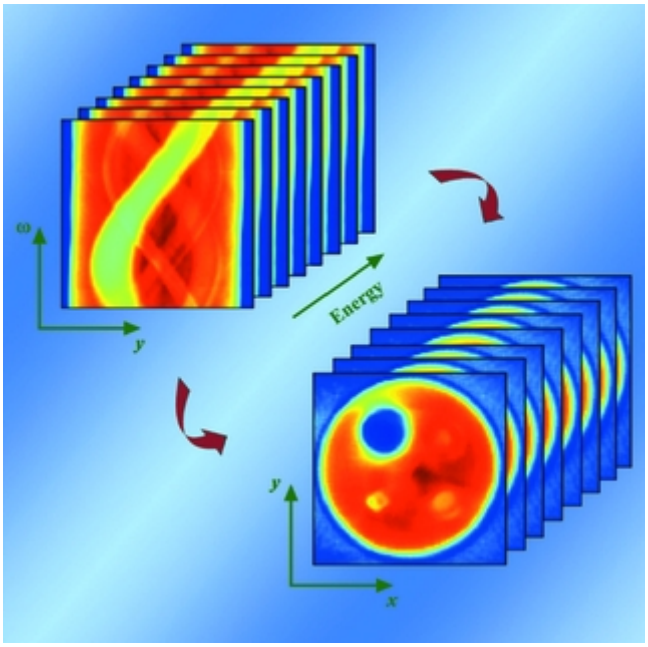
Experimental access to slow dynamics at atomic and molecular length scales is challenging but important for the understanding of structural relaxations in disordered systems, *e.g.* glasses and supercooled liquids. X-ray photon correlation spectroscopy was used to measure structural relaxations at the molecular scale in organic glasses. A novel method applicable to weak signals is described, allowing fast calculations of time correlations by an event correlation scheme. This method may be the only possible path forward in analyzing huge data sets acquired at X-ray free-electron lasers.

Y. Chushkin, C. Caronna and A. Madsen

IUCR JOURNALS NEWS

A new approach to synchrotron energy-dispersive X-ray diffraction computed tomography

J. Synchrotron Rad. (2012). 19, 471-477 (http://doi.org/h96)



Reconstructed two-dimensional slices from sinograms.

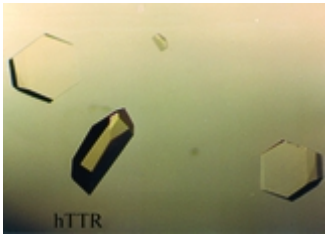
A new data-collection strategy for performing energy-dispersive X-ray diffraction computed tomography has been devised which overcomes previous limitations of such methods, in particular spatial resolution. The method is best suited to studying large bulk objects, e.g. for engineering and materials science applications, because it does not suffer from diffraction broadening effects. Using a computed tomography approach, diffraction signals can be imaged inside bulk objects and used to identify specific materials.

O. Lazzari, C. K. Egan, S. D. M. Jacques, T. Sochi, M. Di Michiel, R. J. Cernik and P. Barnes

MISCELLANY

What’s YOUR favorite crystal??

Transthyretin



Thyroxine is the primary thyroid hormone synthesized in the thyroid gland and is critical to healthy survival in mammalian species. Transthyretin is one of three major proteins that transport thyroid hormones in the body. The preparation of large, perfect single crystals of transthyretin made it possible to determine its three-dimensional structure and learn how the hormone is taken up by the protein for transport. The structural data showed how the competitive binding of pharmaceutical agents used in the treatment of non-thyroid diseases altered their efficacy in the treatment of those diseases and often led to thyroid disease where there had been none. Structures of transthyretin mutants found in cases of familial polyneuropathy also led to the design of novel treatments. Structural data are still not available for three other proteins essential to thyroid hormone action, thyroxine-binding globulin, iodothyronine deiodinase, and thyroglobulin. Beautiful single crystals of these three proteins could provide greater insight into the causes and potential treatment of thyroid disorders that effect tens of thousands of people.

V. Cody and J. Luft, Hauptman Woodward Medical Research Inst., USA

Let us know what your favorite crystal is. Send the image with a short discription to iucrnewsletter@gmail.com.

MEETING REPORT

ECM-27

Bergen, Norway, August 2012
http://ecm27.ecanews.org/



ECA President Andreas Root with Hartmut Fuess, Perutz Award winner, Pavel V. Afonine, Bertrout Award winner, and outgoing ECA president Santiago Garcia-Granda.



New ECA council: (front) Sec. Georgina Rosair (UK), V. P. Alessia Bacchi (Italy), Pres. Andreas Root (S. Africa), Past Pres. Santiago Garcia-Grande, (back) Olga Yakubovich (Moscow), Joke Hadermann (Belgium) and Christian Lehman (Germany).

Over 600 crystallographers from 46 countries, including 114 students and 65 exhibitors, attended the 2012 European Crystallography Meeting in remarkably picturesque Bergen, Norway. Over the course of three and a half days, 16 plenary lectures and 44 microsymposia covered the latest advances in all aspects of X-ray crystallography including instrumentation, methods and applications. Plenary lecturers included the most recent winner of the prestigious Aminoff Prize, Mark Spackman (see article here) and former Aminoff awardee, Michael Rossmann. Faced with the difficult choice of which of the six simultaneous sessions to attend each day, this review covers only a small sample of the excellent science reported. Summaries of other sessions would be welcomed by the editors.

The opening session featured a masterful lecture by D. Schwarzenbach (Switzerland) entitled 'The Laue Centennial. The Birth of X-ray Diffraction'. He described how, following the discovery of X-rays by Roentgen, von Laue surmised that crystals would diffract X-rays and that the diffracted pattern would reflect the underlying structure within the crystal, as had been suggested earlier by morphological studies. In 1912, together with Friedrich and Knipping, von Laue demonstrated that his predictions had been accurate and, in the following year, the Braggs reported the structure of table salt. Schwartzenbach covered one hundred years of crystallographic highlights in a most entertaining fashion.



'Dynamics in Crystals' speakers and chairs: (front) A. Kuzmanic, L. Kroon-Batenberg, A. Madsen, (back) N. Pannu, F. Fabbiani and B. Zakharov.

In a session entitled 'Dynamics in crystals – experimental techniques and software', L. Kroon-Batenburg (Netherlands) illustrated how, a century after the discovery of X-ray diffraction, data collected with synchrotron radiation provides a wealth of knowledge about molecules that would have been beyond the imagination of the early pioneers: atomic resolution macromolecular structures; images of subtle crystal fractures; patterns of anisotropic and diffuse scattering related to dynamic and static disorder; incommensurate structures; and the effects of temperature and pressure on structure.

A. Madsen (Denmark) described how differences in the solid-state entropies of polymorphic compounds can be obtained from analysis of anisotropic displacement parameters, information of practical importance to materials and pharmaceutical research.



'Design, Structure and Function of Multicomponent Crystals' speakers and chairs: (front) U. Griesser, G. Coquerel, P. Bombicz, (back) F. Topić, A. Lemmerer, A. Crispini and L. Fabian.

In a session on 'Design, structure and function of multicomponent crystals', F. Topić (Finland) discussed the molecular architecture of chains, channels and walls comprised of urea, thiourea and tetraalkyl

ammonium salts, and how they aggregate to produce an array of new types of channel and cage inclusion compounds. A. Lemmerer (S. Africa) described covalent assistance to supramolecular assembly and his battles with referees about the use of the term 'blocking agents' to describe his methods of crystal engineering that involve replacement of hydrogen bonding donors with inert-hydrocarbons. Other talks in the session included co-crystallizing pharmaceutical agents to increase solubility (U. Griesser, Austria), trouble with the nomenclature of salt co-crystals with exotic stoichiometries (G. Coquerel, France) and Zn^{II} complexes with luminescent properties useful in photonics (A. Crispini, Italy).



'How To' speakers and chairs: J. Helliwell, S. Garcia-Granda, S. Coles, E. Boldyreva, L. Roces and H. Powell.

An innovative session entitled 'How To' addressed a range of important issues, including funding opportunities in the European community (S. Garcia-Granda, Spain), and strategies that produce better lectures (H. Powell, UK) and scientific articles (J. Helliwell, UK, who tapped in to his Yorkshire roots). In this session, A. Bacchi (Italy) described how to survive in academia and had valuable advice for all young crystallographers, especially women. When Bacchi received her PhD and considered applying for an advertised professorship her advisor told her not to bother because the post was earmarked for a man. Twenty years later statistics on women in senior positions in the sciences have improved to some extent but they have yet to achieve parity. Bacchi did point out that women have done better in crystallography than other areas of science. Her advice to young crystallographers was: teach at every level, be passionate about your work, serve the community, network, and be courageous, original and selfless.

E. Boldyreva (Russia) discussed the future of crystallography and teaching. She expressed concern over the fact that most courses in crystallography have disappeared from university curricula. She offered interesting examples of inductive teaching models in which observation generates theories and deductive models in which theory guides experiment.



'Intermolecular Interactions at Ambient and Extreme Conditions' speakers and chairs: (front) O. Grineva, A. Olejniczak, V. Vasylyeva, (back) E. Boldyreva, A. Maloney, J. J. Lipkowski and P. Gilli.

A session on 'Intermolecular interactions at ambient and extreme conditions' revealed how a broad range of studies at non-ambient temperatures and pressures have led to new ways of growing crystals and new information on material properties. A. Olejniczak (Poland) studied 10 polymorphs of a ferroelectric relaxor. These relaxors possess dielectric constants of over a thousand and are extremely effective at storing electricity in capacitors. Olejniczak's experiments produced hydrated solvates unattainable at ambient conditions and revealed that the high dielectric constants of the materials disappeared at the highest temperature and pressures. Her talk included phase diagrams that were accompanied by beautiful pictures of crystals and structures.

In her plenary lecture on time-resolved crystallographic process in molecular systems, S. Techert (Germany) illustrated the inter-conversion of a low-energy monomer and high-energy dimer of a compound of potential relevance to the development of optoelectronics. The cyclical process of irradiation inducing formation of a stable dimer and heat causing the dimer to revert to the monomer was persuasively illustrated with a stunning movie. She also illustrated the change in the diffraction pattern associated with the transition.



'Bioinformatics Informs MX' speakers and chairs: (front) L. Fabian, A. Bacchi, N. Bathori, (back) L. Nassimbeni, J. Ridout, R. Centor and U. Englert.

In 'Bioinformatics Informs MX (materials X-ray crystallography)', A. Bacchi (Italy) described the relative stabilities of α-, β- and γ-forms of tetraphenyl butadiene (TPB). The molecule has C_2 point symmetry in the commercially available α-form and C_i symmetry in the β- and γ-forms. Bacchi explored the energy landscape of the three forms of TPB in isolation and in crystals by a variety of measures, discovering new properties including a fourth crystal form having two molecules in the asymmetric unit, one with each of the point symmetries, C_2 and C_i. The results were illustrated with a movie of a whimsical stick figure dancing across the hills and valleys of an energy landscape. N. Bathori (S. Africa) discussed the profit motive behind the preparation of pure enantiomorphs and contrasted efforts to use inclusion compounds to effect enanantiomorphic separation with the Dutch Resolution Method. In the Dutch Resolution Method (Vries, T. *et al.*, 1988, *Angew Chem. Int. Ed.*, **37**, 2349) a combination of two or three homochiral resolving agents with structures related closely enough to co-crystalllize are used to improve enantiomeric isolation. J. Ridout (UK) crystallized isomers of liquid fluorotoluenes at low temperature and high pressure and studied the properties of the resultant polymorphs to gain insight into the factors controlling crystallization. He reported that packing efficiencies were greater for the high-pressure forms than for the low-temperature forms. R. Centore (Italy) gave a lively presentation of single-crystal to single-crystal transitions including a movie of an exploding crystal.



'Hot Topics and Structures in Molecular Chemistry' speakers and chairs: (front) F. Fabbiani, G. Dan Pantos, D. Stalke, (back) T. Linden, M. Petrukhina and L. Erra.

In 'Hot topics in molecular chemistry' F. Fabbioni revealed how high pressure induced greater order in guest molecules (including water) in cyclodextrins. Also described were fullerene ion pair complexes within supramolecular nanotubes of naphthalene diamides (G. Pantos, UK), a hexasilabenzeneone structure with an intriguing silicone cluster (D. Stalke, Germany) and cyclic peptoid derivatives of potential pharmaceutical potential (L. Erra, France). M. Petrukhina (US) resolved a long-standing mystery by crystallizing the smallest fullerene fragment, $C_{20}H_{10}^{+4}$, as a lithium salt in which five lithium ions are sandwiched between two convex fullerenes (that curve away from the ions).

William Duax

MEETING REPORT

Argentinian Crystallography Association Meeting

San Carlos de Bariloche, Argentina
November 2011



Participants of the 7th Meeting of the AACr.

The 7th Meeting of the Argentinian Crystallography Association (AACr) had approximately 100 participants from different provinces of Argentina in attendance, giving the meeting a truly national relevance. Other countries represented included: Brazil, Uruguay, Venezuela, Spain and France. The meeting included four plenary talks (Gabriel Cuello, Oscar Piro, Griselda Polla and Juan Manuel García Ruiz), one special talk given at the Inst. Balseiro Colloquium (Juan Rodríguez-Carvajal), 10 oral presentations, 90 posters and a panel discussion on large facilities for crystallography research. In addition, a special session was held in memory of Andrés Goeta, an outstanding Argentinian crystallographer working at Durham U. (UK), who passed away in July of 2011.

A satellite event, the 3rd School of Crystallography, focused on X-ray and neutron diffraction in polycrystalline materials, held November 7-18, was partially supported by the IUCr. It was attended by 41 students from Argentinia, Brazil, Uruguay and Colombia. This School was divided into two modules. The first module, led by Juan Rodríguez-Carvajal and Gabriel Cuello, consisted of a compact version of the well-established 'FULLPROF School' held annually at the Inst. Laue Langevin in Grenoble. The second module, led by Raúl Bolmaro, Javier Santisteban, Miguel Vicente-Álvarez, Aldo Craievich and Eduardo Granado, focused on scientific and technological applications in polycrystals, such as internal stresses and strains, texture and size effects, and synchrotron radiation techniques. The afternoons were dedicated to demonstrations and practical sessions.

The ordinary AACr Annual Assembly was held during the meeting, where new officers of the association were elected and it was confirmed that the 8th Meeting will be held in Santa Fe from October 31-November 2, 2012. The 4th School of Crystallography will focus on fundamentals and applications of X-ray powder diffraction, and will include a workshop on synchrotron light techniques for materials characterization. The 9th Meeting will be held in 2013 at Córdoba and crystallographers of other Latin American countries will be invited to organize this event as the First Latin American Congress on Crystallography.

Diego G. Lamas and Gabriela Aurelio
Taken from ACA RefleXions, Summer 2012

MEETING REPORT

Centennial of X-ray Diffraction

Rome, Italy, May, 2012
www.cristallografia.org



Speakers and organisers of the meeting.

The centennial of X-ray diffraction was celebrated in Italy in the Palazzo Corsini, the headquarters of the Accademia dei Lincei (founded in 1603). The conference was organized by the Accademia dei Lincei and Accademia delle Scienze di Torino, and supported by the Associazione Italiana di Cristallografia (AIC), European Molecular Biology Organization (EMBO), University Roma Tre and the European Crystallographic Association (ECA).

Speakers included two Nobel laureates and a recipient of the 2011 Ewald prize. Talks covered most aspects of X-ray diffraction, historical issues and cutting-edge research. The speakers and topics included: G. Allegra (Milan), 'The structures of crystalline polymers'; G. Artioli (Padua), 'Science and cultural heritage'; A. Bacchi (Parma), 'Design of an active pharmaceuticals'; M. Bolognesi (Milan), '100 years of X-ray diffraction, 50 years of structural biology'; T. Boffa Ballaran (Bayreuth), 'Diffraction at extreme conditions: a window into the Earth's interior'; M. Cammarata (Rennes), 'Laser pump and X-ray probe: insights in the dynamic nature of matter'; G. Chapuis (Lausanne), 'Aperiodic structures'; F. Frontera (Ferrara), 'Laue lenses for gamma-ray astronomy'; C. Giacovazzo (Bari), 'Phasing in crystallography'; R. Huber (Martinsried), 'Architecture of proteins, the building blocks of life'; S. Merlino (Pisa), 'Mineral crystal chemistry'; N. Robotti (Genoa), 'The discovery of X-ray diffraction'; P. J. Steinhardt (Princeton), 'Quasicrystals: a brief history of the impossible'; B. Vallone (Rome), 'Time-resolved crystallography for protein structure'; D. Viterbo (Alessandria), 'X-ray crystallography in Italy'; J. Ernst Walker (Cambridge), 'Biological machines with rotary motors' (EMBO Lecture). A special issue of *Rendiconti Lincei - Scienze Fisiche e Naturali* based on the talks will be available at www.springer.com/environment/journal/12210.



Attendees at the lectures in the Palazzo Corsini.

Up to 150 scientists and graduate students contributed to lively discussions and found time to enjoy the recently renovated Renaissance gardens of Villa Farnesina opposite the Palazzo Corsini and to admire the

frescos of Raffaello, B. Peruzzi, S. del Piombo and Sodoma. A delicious dinner was offered to the speakers by Accademia delle Scienze di Torino.

The committee (M. Brunori, G. Ferraris, A. Mottana (chair), R. Oberti, R. Righini, P. Rossi, G. Setti, A. Zecchina) organized a superb and comprehensive review of the past, current and potential future accomplishments of X-ray diffraction. The meeting was an excellent introduction to Italian initiatives to be held during the forthcoming International Year of Crystallography.

Roberta Oberti

MISCELLANY

Alex Wlodawer meets Ban Ki-moon



Alex Wlodawer (left) and UN Secretary-General, Ban Ki-moon (right), at the United Nations in New York. (Photo credit: UN Photo/J. C. McIlwaine).

On August 26, 2012, Alex Wlodawer (Macromolecular Crystallography Laboratory, NCI, Frederick, MD, USA) participated in a reunion of a youth group that had previously visited the United States 50 years ago. They came then as participants in Operation VISTA, commemorating the 100th anniversary of the establishment of the US Red Cross. Now and then, they visited both the White House and the United Nations. Although the get-together this year was of a high profile, it had an informal and friendly atmosphere and allowed the participants to establish personal contacts with the UN Secretary General, Ban Ki-moon, who was also a VISTA participant. It is rewarding to see our colleague so well connected, especially in view of the UN resolution that has established the International Year of Crystallography, IYCr2014.

Mariusz Jaskolski

MEETING REPORT

ICTP Advanced School

Trieste, Italy, April 2012



Participants at the ICTP Advanced School in Trieste, Italy.

The ICTP Advanced School, 'From genes to atomic structures: an introduction to synchrotron-based structural biology', was organied by S. Onesti, G. Paolucci and J. Niemela, and sponsored by ICTP, IUCr, IUBMB, Elettra and Douglas Instruments. Lecturers included H. Amenitsch, D. Lamba, A. Leslie, S. Onesti, A. Perrakis, B. Rupp, Z. Sayers, P. Shaw-Stewart, R. Steiner, J. Sussman, T. Unger and M. Yousef.

The application of synchrotron radiation to structural biology has had a significant impact on molecular and cellular biology, medicine and biotechnology. SESAME, the new synchrotron facility being built in Jordan, will be an important scientific centre for Middle Eastern countries. A MAD beamline is among the scheduled SESAME phase I beamlines and is expected to be operational when the machine is commissioned.

As a joint initiative between the International Centre for Theoretical Physics (ICTP), SESAME and the Italian synchrotron facility Elettra, an advanced school on structural biology was held in Trieste, with the aim of exposing the participants to the methodologies used to solve macromolecular structures using synchrotron radiation single-crystal X-ray diffraction techniques. Although teachers and participants came from all over the world, 4 out of 12 lecturers, and 14 out of 31 students, came from countries that are SESAME members. The program featured lectures and practical sessions, including crystallization, data collection, data processing and structure solution. The students included researchers actively working in protein crystallography and less experienced scientists looking for an overview of the state-of-the art. The combination worked well, providing an opportunity for people who are new to the field to network with experienced peers. Similar events are planned for the future, hoping to foster the formation of new structural biology laboratories in the Middle East.

Silvia Onesti

MEETING REPORT

Canadian Powder Diffraction Workshop

Saskatoon, Canada, May 2012



T. rex, the oldest attendee.



Attendees at the Canadian Powder Diffraction Workshop.



Practical session at the Canadian Powder Diffraction Workshop.

The 9th Canadian Powder diffraction workshop was held in the Dept of Geology, the U. of Saskatchewan in Saskatoon. Over 50% of the 30 attendees were from Saskatchewan and further west. There was an evening barbecue and a tour of the Canadian Light Source (CLS) synchrotron.

It was the first time *GSAS-II* had been unveiled publicly, and students were given the opportunity of training on this and the established *GSAS*/*EXPGUI* suite. To enhance the training experience, all attendees worked on their own laptops. There were morning lectures and afternoon practicals,with

hands-on experience in operating *PDFGUI*, *GSAS* and *GSAS-II*. Bob Von Dreele (ANL), Joel Reid (CLS), Ian Swainson (NRC and CCNI), Pamela Whitfield (NRC), Angus Wilkinson (Georgia Tech), and Thomas Proffen (ORNL) covered neutron and synchrotron diffraction; crystallography fundamentals; powder diffraction basics; sample preparation and phase identification; Rietveld fundamentals; *GSAS*, PDF, total scattering, and *PDFGUI*. The workshop was sponsored by the Canadian Centre for Nuclear Innovation and supported by the U. of Saskatchewan, CLS, the National Research Council, and the Canadian Institute for Neutron Scattering.

Ian Swainson

MEETING REPORT

International School of Crystallography

45th Course – Present and Future Methods for Biomolecular Crystallography

Erice, Italy, May 2012



The event was held in Erice, Italy, at the Ettore Majorana Foundation and Centre for Scientific Culture. The course included a total of 141 participants from 31 countries. The main objective of the Course was to equip the next generation of scientists with a deep understanding of the tools they need to solve challenging structural projects. The students were largely from universities (PhD students, post docs and young researchers), with researchers from chemical and pharmaceutical companies. Poster preview sessions and several other general events organized during the day and in the evenings provided several opportunities for students and teachers to mingle and have many constructive discussions, which resulted in the determination of at least three new structures during the school.

The lecturers were chosen from world leaders in the field of structural biology, and all made great efforts to present cutting-edge science at a level accessible to participants with limited experience. Most presented two lectures, one focused on methodology and the other illustrating the structural insights that can be obtained using their methods; many lecturers also presented a demo or tutorial.



Participants at the International School of Crystallography 45th Course in Erice, Italy.

A total of 56 lectures were scheduled, including 7 chosen from the submitted poster abstracts. In addition, there were 4 software demos and 11 different tutorials (each repeated twice). The participants presented a total of 90 posters in two poster sessions, each of which was preceded by short oral presentations. The course concentrated on single-crystal X-ray diffraction, covering all aspects of structure determination, from protein production (Stephen Kent, Todd Yeates) to crystal preparation (Martin Caffrey) and data collection and analysis (Sean McSweeney, Kay Diederichs, Elspeth Garman, Tatiana Petrova and Dominika Borek), to structure solution (Randy Read, Isabel Uson, Zsbyszek Dauter, Tim Gruene, Felix Frolow, Clemens Vornhein and Vladimir Lunin) and validation (Jane Richardson and Zbyszek Otwinowsky). Different approaches for solving the structures were also presented by Tom Terwilliger, Tassos Perrakis, Paul Emsley, Pavel Afonine, Garib Murshodov and Axel Brunger. In addition, the horizons were broadened with a number of complementary approaches, including X-ray free electron lasers, neutron diffraction and small-angle X-ray scattering (Nobuo Niimura, Petra Fromme, Pierre Thibault, Frank DiMaio, Tatiana Latycheskaia and Dmitri Svergun). Jaime Prilusky showed how the

structure obtained can be presented to the world through the Protopedia website, and challenged the participants to prepare their own Proteopedia pages during the course.

A number of speakers presented the structural results of their research: complement proteins (Piet Gros), Z-DNA at 0.55Å resolution (Zbyszek Dauter), enzymes mutated in lysosomal storage diseases (Randy Read), viral membrane fusion proteins (Felix Rey), monoamine oxidase inhibitors (Andrea Mattevi), proteins involved in Ca-triggered vesicle fusion (Axel Brunger), retropepsin (Mariusz Jaskolski), autotaxin (Tassos Perrakis) and the eukaryotic ribosome (Sergey Melnikov).

As always, the school had participants from all over the world, this year with a particularly large contingent of young scientists from eastern European and South American countries, where the field has recently begun to develop. The international composition of the school, as well as the friendly and informal atmosphere of Erice, played an important role in facilitating communication between students and world-renowned professors, which will foster further scientific collaborations.



Poster prize winners at the International School of Crystallography 45th Course in Erice, Italy.
Several prizes were awarded during the course. The prize for best poster presentation was given to Denise Cavalcante Hissa (Federal U. of Ceara, Graz, Austria), with a special mention to Andrea Pica (U. of Naples 'Federico II', Italy); the winners for the best Protopedia page were Wee Lee Chan (U. of Cambridge, UK) and Tomas Klumper (Masaryk U., Czech Republic); the Lodovico Prize was awarded to Abhay Kotecha (U. of Oxford, UK) and a special mention was awarded to Marcus Fislage (Vrije U. Brussel, Belgium).

After the school, a large number of participants gave feedback by filling in a detailed questionnaire. They were unanimous in agreeing that a similar meeting should be held in the future, with the vast majority (99%) believing it should be held within the next 4 years. The majority considered the course to have been very successful in most of its objectives (score 91/100). There was some very helpful feedback that will be used to improve the future courses

Annalisa Guerri

MEETING REPORT

Workshop on Errors, Pitfalls and Problems in Single-Crystal Structure Analysis

Kiel, Germany, July 2012



Participants at the 10th Kiel Workshop.

Single-crystal X-ray diffraction is a routine method used by an increasing number of young scientists who have limited formal training. Unfortunately, sometimes problems occur that lead to incorrect structure determinations, some of which get published. Even if a structure seems to be successfully determined, errors might have occurred which are difficult to detect. These problems were addressed at the 10th Kiel Workshop. The workshop was organized by Christian Näther (Inst. of Inorganic Chemistry, Kiel) and Michael Bolte (Inst. of Inorganic Chemistry, Goethe-U., Frankfurt) as a shared activity of the German Crystallographic Assn (DGK) and the German Chemical Society (GDCh). This course was given in German and was intended for people who already had some practical experience with structure determination.

The workshops addressed problems in five areas: determination of the crystal system, the Laue symmetry and space group; structure solution; structure refinement; twinning; treatment of disordered hydrogen atoms and assessment of the quality of a structure determination. For each topic, an introductory lecture was held and the participants had to tackle structural problems with well-prepared data sets using standard software as described in the workshop manual. This included refinement: in an incorrect space group, in too small and too large unit cells, of sub- and super-structures, of twinned crystals, and using incorrect chemical elements. The organizers believe that people can only resolve problems if they are confronted with them. All solutions were discussed with the whole group.

Assessment by the participants afterwards was unequivocally positive. Students apply half a year before the course begins, even if it is not announced. We have learned that some old structures have been solved with the knowledge acquired in the course.

Christian Näther and Michael Bolte

MEETING REPORT

Slovenian-Croatian Meeting

Pokljuka, The Julian Alps, June 2012
http://abra.fkkt.uni-lj.si/fn01leban/slkr21/



Plenary lecturers (from left): F. Perdih, Z. Popović, L. McCusker, and K. Koch.

The 21st Slovenian-Croatian Crystallographic Meeting was held at Triglav National Park in the highest mountains in Slovenia in June 2012. There were four plenary lectures, describing different aspects of crystallography: L. McCusker (ETH Zurich, Switzerland), 'Powder diffraction, electron microscopy and microdiffraction - meeting the challenge of zeolite structure analysis'; K. R. Koch (Stellenbosch, South Africa), 'Deceptively simple, rich platinum(II/IV) and rhodium(III) chemistry viewed through new eyes: what secrets can the ^{195}Pt/^{103}Rh nuclei reveal about their molecular disguise in the solution and solid-state'; Z. Popović (Zagreb, Croatia), 'Correlation between supramolecular interactions and structural characteristics of Ag^{I} complexes'; and Franc Perdih (Ljubljana, Slovenia), 'Structural aspects of organotitanium fluorides'.

There were 38 oral contributions concerning macromolecules, organic, organometallic, pharmaceutical and inorganic compounds, crystal architecture, crystal engineering, metallurgy, solid solutions, powder diffraction broadening, small-angle scattering, synergy of diffraction, microscopy, structure and properties, and nanocrystallography. The meeting featured a visit to a lake and castle and a presentation about the Julian Alps. There were 60 active participants from 9 countries including many young scientists.



Visit of participants to Bled Castle.

We thank the sponsors, the Slovenian Research Agency and the Faculty of Chemistry and Chem. Technology, U. of Ljubljana, for making this meeting registration free. Additional details and a photo gallery are available at http://abra.fkkt.uni-lj.si/fn01leban/slkr21/.

The 22nd Cro-Slo Cryst Meeting (CSCM22) will be held June 12-16, 2013, in Biograd, in the center of the Croatian Adriatic coast.

Ivan Leban

AWARDS AND PRIZES

2013 Aminoff Prize



Carlo Gatti



Mark Spackman

The Royal Swedish Academy of Sciences (RSAS) has awarded the Gregori Aminoff Prize in Crystallography 2013 to Carlo Gatti (Inst. of Molecular Sciences and Technology, Italian National Research Council (CNR-ISTM), Milan, Italy) and Mark Spackman (U. of Western Australia, Crawley, Australia), 'for developing experimental and theoretical methods to study electron density in crystals, and using them to determine molecular and crystalline properties'. SEK 100,000 to be shared equally between the Laureates.

Both Carlo Gatti and Mark Spackman have independently developed concepts for interpreting electron-density distributions related to quantum chemistry theory, using multipole analysis of high-quality X-ray diffraction data. This approach has, in particular, significantly demonstrated and quantified the role of hydrogen bonding in molecular systems. 'Charge density topology' is important for classification of the type and strength of chemical bonding in solid compounds and molecules. The Prize will be awarded at the Royal Swedish Academy of Sciences' Annual Meeting on April 5, 2013.

One key concept developed by Carlo Gatti is the *source function* (Bader & Gatti, 1998), which permits visualization of chemical bonds and other fundamental chemical properties using only information from observed electron density and its derivatives. The function equates values of observed density at any point within the crystal to a sum of atomic contributions. Mark Spackman devised and implemented a new scheme for partitioning crystal space into molecular and atomic volumes limited by *Hirshfeld surfaces*, which reflect the nature and strength of interatomic and intermolecular interactions in quantitative terms. An exploratory paper (Spackman & Byrom, 1997), focusing on electron distributions derived from X-ray diffraction data on urea, clearly demonstrated the significance of Hirshfeld surface analysis.

IUCR ACTIVITIES

New Editor-in-Chief

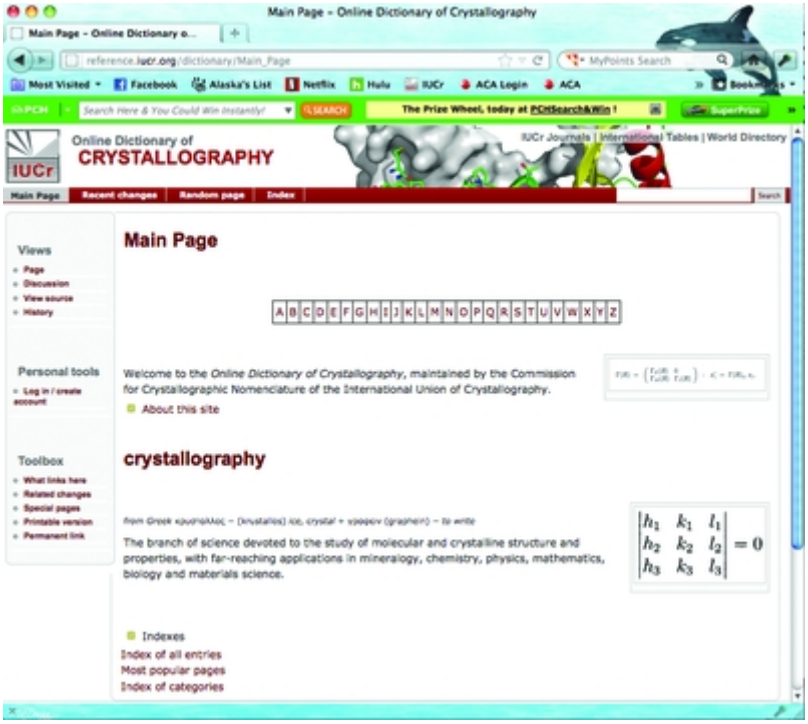


Samar Hasnain

The Executive Committee is pleased to announce that Samar Hasnain (Max Perutz Professor of Molecular Biophysics, U. of Liverpool, UK) has been appointed Editor-in-Chief of IUCr journals. Hasnain takes up this role at a time of great change in the journal publishing field and will take forward plans resulting from the general review of the journals that has recently been undertaken. The Executive Committee takes this opportunity to thank Gernot Kostorz for his dedicated high-quality work for the past seven years. His willingness to work with the new Editor-in-Chief to ensure a smooth transition is appreciated. Gernot will continue as a Co-editor for Journal of Applied Crystallography.

IUCR ACTIVITIES

Expanding the Online Dictionary



The IUCr Online Dictionary of Crystallography (ODC) is a very popular resource with currently over 250 definitions of key concepts and terms in crystallography. The system is based on the Wiki principle, allowing community authoring and editing of the content, but with some restraints on the selection of authors. Currently there are close to 50 registered authors, who have been selected or accepted by the administrators of the ODC. In order to increase the attractiveness of the ODC, and to improve the quality of the definitions and the number of entries, the board of editors have studied various proposals.

IUCR ACTIVITIES

Call for nominations



Jon Gjønnes

The Gjønnes Medal in Electron Crystallography recognizes an outstanding contribution to the field of electron crystallography. The award is accompanied by a certificate and funding to present an invited Keynote Lecture at the triennial International Congress of Crystallography.The award is named in honor of its first recipient, Jon Gjønnes (U. of Oslo), who received the award at the XXI IUCr Congress in Osaka, in August 2008.

Nomination is open to scientists and engineers in all areas of electron crystallography.The next Medal will be awarded at the Montreal Congress in August 2014. Further details of the award and the nomination procedure can be found at www.iucr.org/news/notices/announcements/chesternotice_2012_03.The deadline for receipt of nominations is 30 April 2013.

MISCELLANY

Monumental molecules



Virtual sculpture of the DNA component of the tetranucleosome complex. Schalch, T. *et al.*, *Nature* (2005) **436**, 138-141. Setting: Longwood Gardens, near Philadelphia, PA, USA. cf. http://molecular-sculpture.com/WebSampler/Sampler.html



Edgar Meyer in his garden.

Throughout the ages crystals have been admired for their beauty and order. The Laue experiment 100 years ago let us peer deeply into an ordered universe and elucidate structures from salts to macromolecular complexes. Crystallography has elevated our understanding of our world and of ourselves.

But what does the world understand of atomic and molecular structures? Pictures in books and rarely on television suggest collections of atoms or iconic images like the double helix – they are necessary but not sufficient. And what about tomorrow? How many of these images have sustaining and aesthetic value, worth passing on to the next generation?

Recent editions of the ACA *RefleXions* and several European crystallographic newsletters have addressed current efforts to depict molecular structures as sculptures and animated images. In 1972 Rubin and Richardson used Byron’s Bender to shape muffler pipe to depict the secondary structure of rubridoxin at Duke. I began making precisely scaled wooden sculptures just over 10 years ago. Other examples can be found by searching Google for 'images for molecular sculpture'.

Rapid prototyping has become a facile way of creating desktop models of molecules. Some university or industrial shops have installed such devices; leaders in the field have been the Scripps Inst. (http://models.scripps.edu/) and 3D Molecular Designs (www.3dmoleculardesigns.com/).

Several software packages make it possible to start with atomic coordinates and produce a hand-held model with in-house rapid prototyping equipment.

While atomic models have been known since 1866, they are rarely found in the world around us – or even in the lab next door. There are monuments to generals and poets, athletes and animals, there are graceful sculptures and amorphous abstractions. Where are the sculptures of molecules? Should not such sculptures be part of a park or public space, part of our heritage, monuments to magnificent molecules, passed down to future generations?

In 2005 the Smithsonian commissioned scaled bronze sculptures (http://molecular-sculpture.com/Castings/Polio-bronze/SI-bronzes/SI-bronzes.html) of the polio virus capsid and the capsid:receptor complex (Hogle lab). In no time, the patina was worn to bronze from visitors feeling the symmetry of the surfaces. Sculptures are meant to be seen, felt, enjoyed. Metal structures weather the four seasons. Children can play on them – they thus will be our legacy to future scientists and the world of art.

But molecular sculptures are static, a snapshot view of a dynamic process. Why not create an animated video, a 'Laterna Magika', that shows how the sculpted structure plays a major role in one or more acts of the drama of life? Multilingual soundtracks could describe to the world some of the joy we know when we absorb the beauty of a new structure.

OK, you really would like to see a sculpture of your most significant structure out in front of your lab building. But how? By seeking industrial or foundation support? Or, many institutions have a provision associated with renovation or new construction to allocate 1-2% of the cost for decorative arts. It would require including colleagues in other fields to support the idea – but imagine the publicity – a bronze that would break the barriers of contemporary art by actually depicting a scientifically relevant image – the public would be amazed, scientists would be astounded, and children would be delighted to be able to play on a nitrogen or carbon atom.

So, to tell the world about the monumental success of our discipline, it will require individual scientists to take the initiative and 'sell' the idea. Future generations will thank you as they think back to this, our 'golden age' of crystallography.

Edgar Meyer

NOTICE

2012 Nobel Prize in Chemistry announced



As the final proofs for this issue were being checked it was announced that the 2012 Nobel prize in chemistry has been awarded to Robert Lefkowitz and crystallographer Brian Kobilka for studies of G-protein coupled receptors. A news feature in *Nature* in Aug 2011 (Vol. 476, pp. 387-390) describes the years Kobilka devoted to preparing single crystals essential to the structure determination.