INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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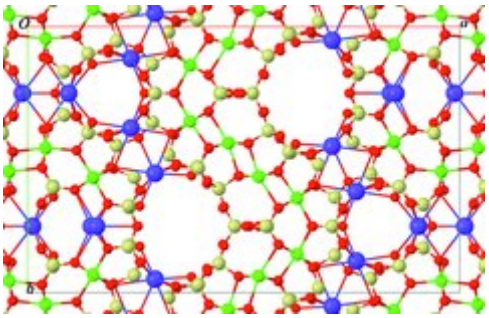
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IUCR JOURNALS NEWS

Application of δ recycling to electron automated diffraction tomography data from inorganic crystalline nanovolumes

Acta Cryst. (2013). A69, 396-407 (http://doi.org/nsj)



Model of the fibrous silicate Charoite90 obtained by δ recycling an incomplete set (80%) of electron ADT-PED intensities.

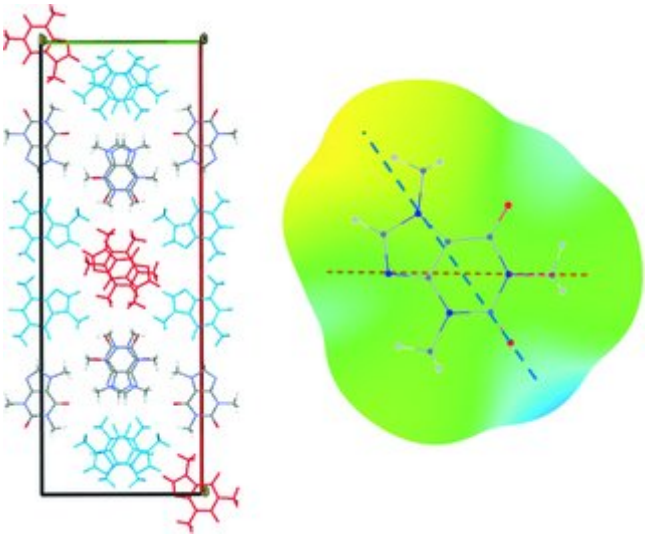
δ recycling is a simple phasing method based on properties of the Fourier transforms and was initially developed for single-crystal X-ray diffraction data. However, tests carried out on intensities of inorganic compounds acquired by combining automated diffraction tomography (ADT) and precession electron diffraction (PED) techniques also show its viability for electron diffraction data and demonstrate the quasi-kinematical character of intensities collected by tomographic methods from nanometric volumes. The tolerance to missing data and to deviations from kinematical behavior is analyzed, with particular attention to the Wilson-plot scaling procedure.

J. Rius, E. Mugnaioli, O. Vallcorba and U. Kolb

IUCR JOURNALS NEWS

Why don't we find more polymorphs?

Acta Cryst. (2013). B69, 313-328 (http://doi.org/nsk)



Few molecules have a uniquely favorable way of packing with themselves. The approximate symmetry in the intermolecular interactions of caffeine results in many almost equi-energetic structures, giving rise to complex disordered phases.

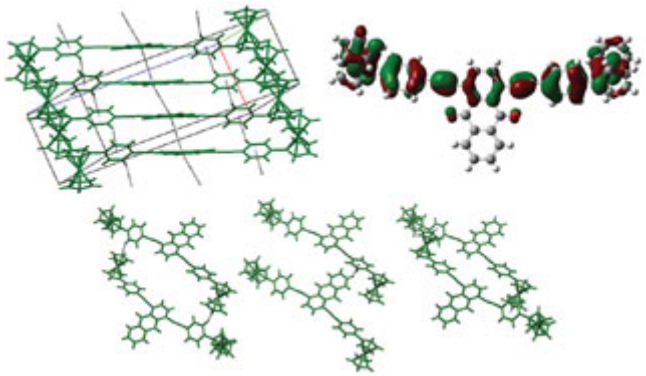
We have computationally generated thermodynamically plausible crystal structures for 200 organic molecular systems and compared these crystal energy landscapes with the results of experimental solid-form screening studies. There are usually far more structures within the energy range of possible polymorphism than known polymorphs. Seven possible explanations, ranging from the approximations in the calculation of crystal energies to experimental limitations in finding and structurally characterizing polymorphs, are given. This highlights the need to understand crystallization better before we can develop programs to predict polymorphs.

S. L. Price

IUCR JOURNALS NEWS

1,4-Bis[2-(4-ferrocenylphenyl)ethynyl]anthraquinone from synchrotron X-ray powder diffraction

Acta Cryst. (2013). C69, 696-703 (http://doi.org/nsm)



C—H···π interactions and HOMO of 1,4(FcPh)$_2$Aq.

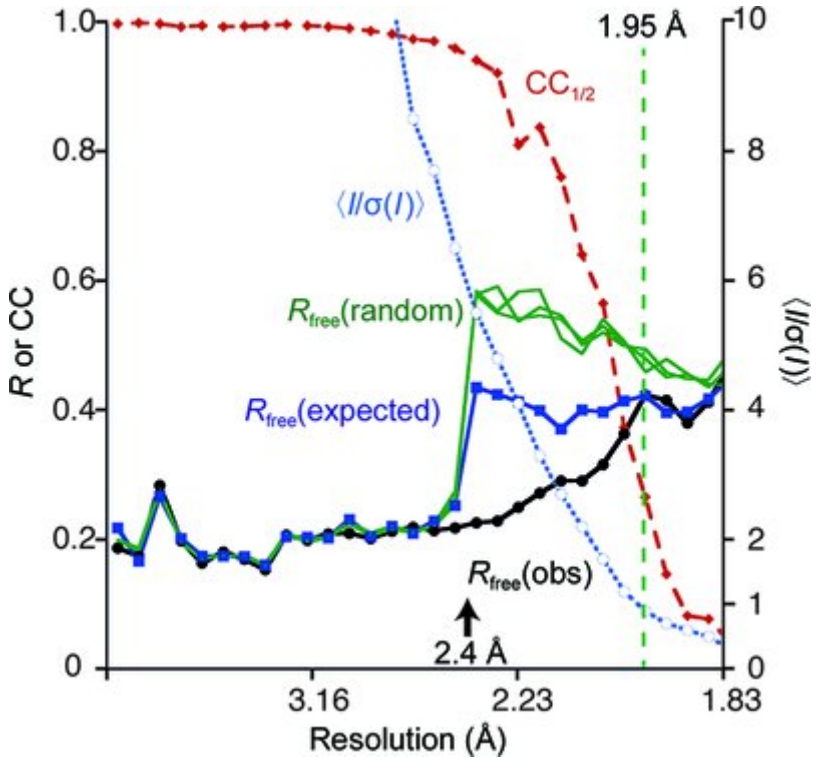
The crystal structure of 1,4-(FcPh)$_2$Aq [FcPh: 2-(4-ferrocenylphenyl)ethynyl; Aq: anthraquinone] was determined using synchrotron powder diffraction data. A direct-space method using a genetic algorithm was employed for solution. Charge densities by the maximum entropy method were employed for model improvement. The final models were obtained through Rietveld refinements. The planar Aq fragments are stacked alternately forming a one-dimensional column. The FcPh arms lie between the stacks and fill the remaining space, leaving no voids. C—H···π interactions between the Ph and Fc fragments mediate packing.

M. Sachiko, E. Nishibori, S. Aoyagi, M. Sakata, M. Takata, M. Kondo, M. Murata, R. Sakamoto and H. Nishihara

IUCR JOURNALS NEWS

Data merging statistics for assessing whether to omit measured intensities

Acta Cryst. (2013). D69, 1204-1214 (http://doi.org/nsn); 1215-1222 (http://doi.org/nsp)



Comparison of refinement statistics against real and simulated data (R_{free}) with data merging statistics ($\langle I/\sigma I\rangle$ and $CC_{1/2}$), plotted against resolution. For this example the observed data are better than simulated data out to 1.95 Å resolution, where $CC_{1/2}$ = 0.27 and $\langle I/\sigma I\rangle$ = 0.9.

These papers highlight again the half-dataset correlation coefficient $CC_{1/2}$ as a robust statistic for judging whether to include data to a higher resolution or from other crystals. They show that useful information extends beyond the cutoff point suggested by criteria based on R_{merge}, which is inappropriate for this purpose. Hard trimming of high-resolution data, omitting useful information, is unlikely to improve the final model, so premature data truncation is a mistake.

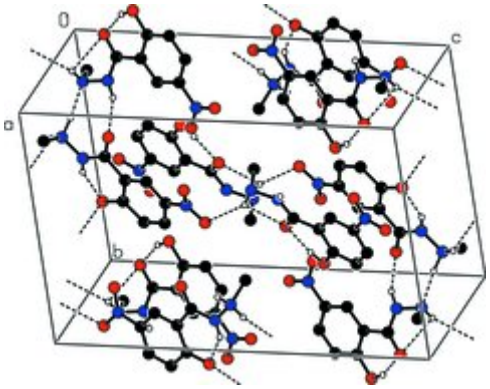
P. R. Evans and G. N. Murshudov; K. Diederichs and P. A. Karplus

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2-Hydroxy-N′-methyl-5-nitrobenzohydrazide

2-Hydroxy-*N*′-methyl-5-nitrobenzohydrazide

Acta Cryst. (2013). E69, o1305 (http://doi.org/nsq)



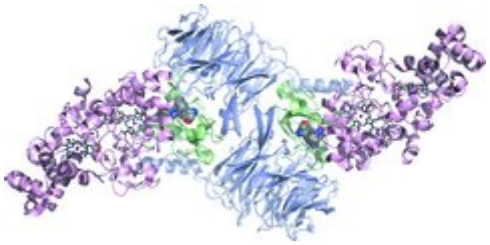
The crystal structure of 2-hydroxy-*N*′-methyl-5-nitrobenzohydrazide, $C_8H_9N_3O_4$, shows the highly unusual situation of one neutral and one zwitterionic molecule in its asymmetric unit. The zwitterion contains an intramolecular N—H···O hydrogen bond and the neutral molecule features both intramolecular N—H···O and O—H···O hydrogen bonds. In the crystal, the constituents are linked by N—H···O and N—H···N hydrogen bonds to generate a two-dimensional network.

M. Yang, C. Jin, X. Zhou and L. Jin

IUCR JOURNALS NEWS

Structures of MauG in complex with quinol and quinone MADH

Acta Cryst. (2013). F69, 738-743 (http://doi.org/nsr)



Complex between MauG (pink) and methylamine dehydrogenase (blue and green).

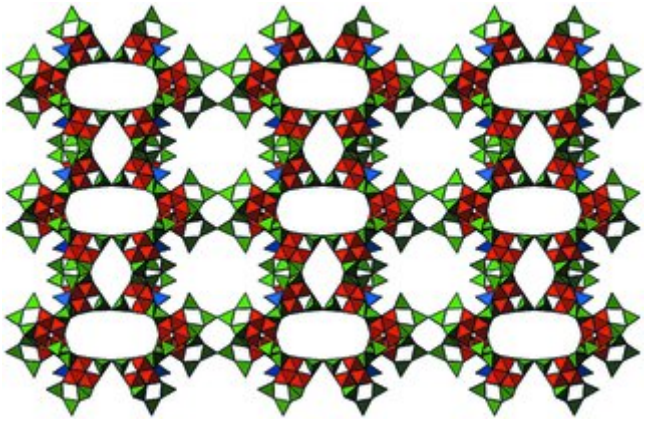
The bacterial enzyme methylamine dehydrogenase (MADH) contains a redox cofactor generated through the post-translational modification of two Trp residues. Biosynthesis of the tryptophan tryptophylquinone (TTQ) cofactor is completed by a di-heme enzyme, MauG. This article reports the structures of MauG in complex with MADH (the product) and quinol MADH (a catalytic intermediate). Although the overall structures were identical, the crystal forms were not. Changes in the redox state of the TTQ appear to alter flexibility at the interface with MauG, and ultimately crystal packing.

E. T. Yukl, L. M. R. Jensen, V. L. Davidson and C. M. Wilmot

IUCR JOURNALS NEWS

Solving complex open-framework structures from X-ray powder diffraction by direct-space methods using composite building units

J. Appl. Cryst. (2013). 46, 1094-1104 (http://doi.org/nss)



The open-framework structure of germanate SU-66 solved from X-ray powder diffraction using the software *FOX*. The framework was built by $Ge_{10}(O,OH)_{27}$ (Ge_{10}) clusters, each consisting of six GeO_4 tetrahedra (in green) and four GeO_6 octahedra (in red). Additional GeO_4 tetrahedra not belonging to any Ge_{10} clusters are in blue.

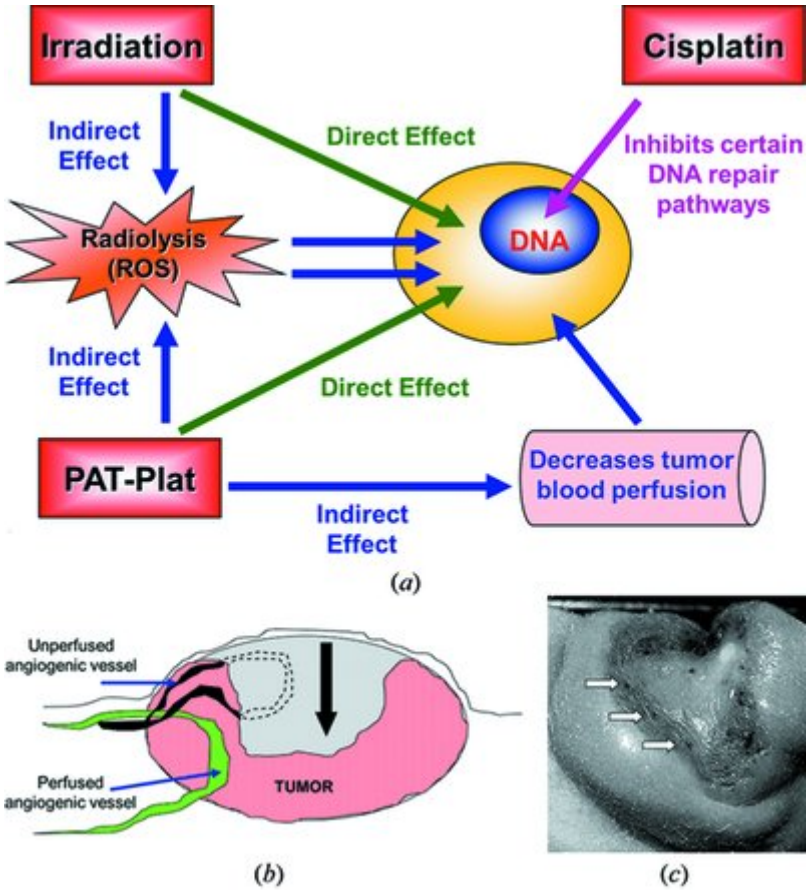
Solving structures of complex open-frameworks from powder diffraction is often challenging because of peak overlapping. We show that if the building units can be identified, open-framework structures can be solved *ab initio* from X-ray powder diffraction data using the parallel tempering algorithm implemented in the software *FOX*. Infrared spectroscopy was used for the first time to identify the building unit in a novel germanate denoted SU-66. The structure of SU-66, with 55 unique atoms in the asymmetric unit, was solved from in-house X-ray powder diffraction data.

A. K. Inge, H. Fahlquist, T. Willhammar, Y. Huang, L. B. McCusker and X. Zou

IUCR JOURNALS NEWS

Synergistic effect of cisplatin and synchrotron irradiation on F98 gliomas growing in nude mice

J. Synchrotron Rad. (2013). 20, 777-784 (http://doi.org/nst)



(*a*) General model of PAT-Plat effects. Irradiation leads to cellular damages such as DNA breaks directly or indirectly via the creation of reactive oxygen species. These damages are less repaired thanks to the inhibition of repair pathways by cisplatin. The PAT-Plat reduces further the tumor blood perfusion. (*b*) Schematic representation of the regression (gray area) observed on a F98 glioma one month after the treatment and (*c*) a macrophotograph; white arrows point to the dark spots of blood vessel coagulations. In the current study, we observed a synergistic effect of cisplatin and synchrotron irradiation on F98 gliomas growing in nude mice. Beside direct tumor cell-killing effects after photoactivation of cisplatin present in tumor cells, we observed an unexpected reduction of the tumor blood perfusion. At the time of photoactivation, cisplatin may also be present in proliferating vascular endothelial cells, creating a drastic inhibition of the tumor blood perfusion during growth. This inhibition of blood perfusion was not observed after synchrotron irradiation or cisplatin treatment alone.

C. Ricard, M. Fernandez, H. Requardt, D. Wion, J.-C. Vial, C. Segebarth and B. van der Sanden

IYCR 2014

IYCr2014: a programme for dissemination, training and cooperation



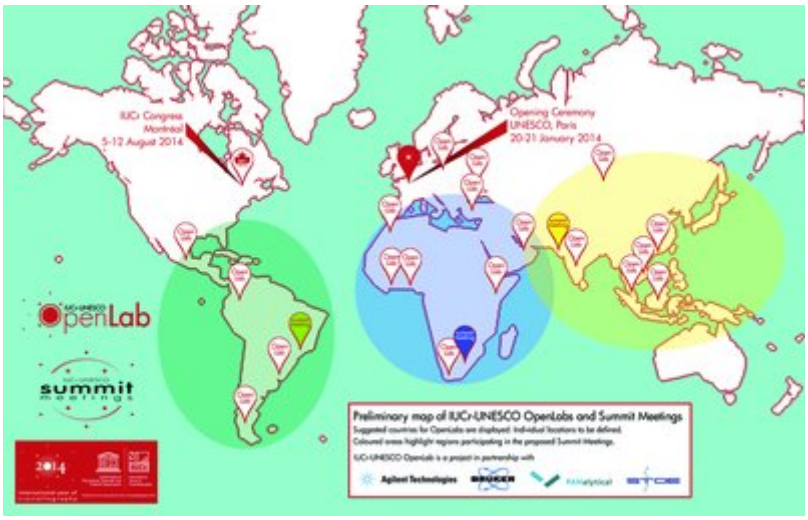
Michele Zema



Italian crystallographers show their support for IYCr2014 at ECM28 at Warwick Univ.

The International Year of Crystallography is approaching and there is growing enthusiasm in the crystallographic community. I could feel this energy at the ECM28 in Warwick, UK last August. Many colleagues called at the IUCr booth asking for information about the on-going programme, suggesting ideas, offering support, discovering activities planned throughout the world and, last but not least, looking for gadgets: T-shirts and lapel pins were very popular. The session on 'Crystallographic teaching and education' offered plenty of ideas and projects for IYCr2014. The number of activities aimed at celebrating IYCr2014 in all parts of the world is growing (see the official Calendar at www.iycr2014.org/events and follow IYCr2014 on Facebook).

The IUCr, in a close collaboration with the UNESCO International Basic Sciences Programme team directed by Maciej Nalecz, is developing an ambitious programme to disseminate the crystallographic culture in parts of the globe where it is still latent or absent and to foster new collaborations. Two main projects under development are the IUCr-UNESCO OpenLab and Summit meetings (hereafter, Summits). Both require involvement of local governments and institutions. The IUCr-UNESCO team is facilitating the implementation of as many of these activities as possible. A map showing the locations of the actions under consideration is shown below.



The IUCr-UNESCO OpenLab is intended to be a network of operational crystallographic laboratories based in Africa, Asia and South America. These laboratories will host workshops, tutorials and hands-on experiments for students and young professors from the hub country and neighbouring countries. The project is being developed in a partnership, which includes the IUCr, as responsible for the scientific and training activities; UNESCO, managing the diplomatic and educational outreach issues; and diffractometer manufacturers, supplying the instruments or making some existing laboratories available for the project. At the moment, Agilent Technologies, Bruker, PANalytical and STOE are the main company partners. The purpose of the IUCr-UNESCO OpenLab project is manifold: in threshold countries, the idea is to encourage the purchase of advanced instrumentation to increase the technological base and to spark interest in youngsters; in less privileged countries, the goal is to begin crystallographic activities and allow access to high-level training and education for young promising students.

The Summits, one for each IUCr region, will bring together scientists from countries in three widely separated parts of the world, using a common crystallographic theme. Campinas (Brazil), Bloemfontein (South Africa) and Karachi (Pakistan) are the locations proposed to host such events. These meetings will be attended by scientists in academia and industry, and by science administrators. They will focus on high-level science, highlight the difficulties and problems of conducting competitive scientific research, and promote cooperation between countries.

Like Us On facebook

Like IYCr2014 on Facebook at www.fb.com/iycr2014.org to keep informed about forthcoming activities. The Opening Ceremony (UNESCO, Paris, January 20-21, 2014) will stress the importance of crystallography for the advancement of science to the governments of all nations. The overall programme for IYCr2014 will be introduced, highlighting its main objectives of disseminating crystallography, providing educational possibilities to students from all parts of the world and fostering cooperation among countries.

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

IYCR 2014

National websites dedicated to IYCr2014

International Year of Crystallography 2014 - Japan Initiative - www.iycr2014.jp

The website of the IYCr 2014 Japan Initiative is now available, with information about events for IYCr2014 being organized in Japan, fund-raising, partnerships and collaborations, local coordinators, and some aspects of the history of crystallographic advances by Japanese scientists.

L'Année Internationale de la Cristallographie en France - www.aicr2014.fr

A website dedicated to Crystallography and the activities that will take place for the International Year of Crystallography 2014 in France is now active.

IYCR 2014

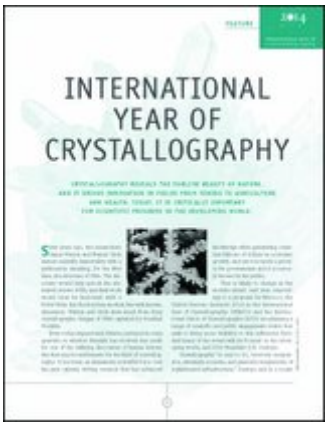
Doing science in the developing world – connecting with TWAS for 2014



IUCr/UNESCO/TWAS meeting, March 2013. Seated from left: Luc Van Meervelt (IUCr General Secretary and Treasurer), Claude Lecomte (IUCr Vice-President), Romain Murenzi (TWAS Executive Director). Standing from left: Juste Jean-Paul Ngome-Abiaga (UNESCO IBSP Assistant Programme Specialist), Michele Zema (IYCr2014 Project Manager).

The IUCr and UNESCO have set up a close and fruitful collaboration with TWAS, *The World Academy of Science for the advancement of science in developing countries*, for facilitating the implementation of IYCr2014 activities in Africa, Latin America and Asia. A delegation from the IUCr and UNESCO met the TWAS Executive Director Romain Murenzi on 27 March 2013 in Trieste, Italy (see photo). Romain Murenzi welcomed the focus on crystallography: 'Crystallography should be a prime field for focus and investment by policymakers and educators in developing nations,' he said. 'Nations that develop skill in this field create their own power – the power to address challenges in food production, clean water and health. That makes the International Year of Crystallography very important.' A number of initiatives are being planned by the IUCr and UNESCO in partnership with TWAS, starting with the participation of TWAS scientists in the IYCr2014 Opening Ceremony in Paris on January 20-21, 2014. Other actions will be communicated soon through the IYCr2014 and TWAS websites.





The 24th TWAS General Meeting (Buenos Aires, Argentina, October 1-4, 2013) hosted an invited lecture by G. R. Desiraju, President of the IUCr, titled 'Doing science in the developing world. The International Year of Crystallography as a facilitating event.'

An article about the International Year of Crystallography, written by Edward W. Lempinen, TWAS Public Information Officer, appeared in the latest issue of the *TWAS Newsletter*. It is available at http://twas.ictp.it/publications/nl/2013-volume-25/twas-newsletter-vol-25-no-1.

Michele Zema

IYCR 2014

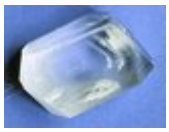
From crystal-growing competitions worldwide to a worldwide crystal-growing competition



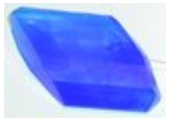
Borax, $Na_2B_4O_7.10H_2O$



Monopotassium phosphate (KDP), KH_2PO_4



Ammonium magnesium sulphate, $(NH_4)_2Mg(SO4)_2.6H_2O$



Copper(II) sulphate, $CuSO_4.5H_2O$



Potassium sodium tartrate, $KNaC_4H_4O_6.4H_2O$



Ammonium iron(II) sulphate, $(NH_4)_2Fe(SO_4)_2.6H2O$



Alum, $KAl(SO4)_2.12H_2O$

In many countries such as Australia, Belgium, Canada, England, France, Singapore and Spain, regional or national crystal growing competitions are organized, and the same is true in many schools on a more local basis. The local guidelines for these competitions can differ slightly, but in general pupils have to grow their own single crystals in the classroom in a fixed period. Instructions are available on the website

of the competition and in most cases a limited amount of starting material is provided to the schools. Each class is encouraged to send their best single crystals to the local coordinator who is always available to answer additional questions. Submitted crystals are judged on the weight and the quality of the crystal, with prizes for different age categories, best schools and best crystal quality. In Spain and Singapore, a scientific congress is organized where participants present posters and crystal models. Popular starting materials for growing single crystals include alum (aluminium potassium sulphate dodecahydrate), copper(II) sulphate pentahydrate, borax (sodium tetraborate decahydrate), ammonium iron(II) sulphate hexahydrate, potassium dihydrogen phosphate and ammonium magnesium sulphate hexahydrate.

With the celebrations of the IYCr2014 in mind, the lead partners IUCr and UNESCO are planning a worldwide crystal-growing competition in 2014 to illustrate that science – and especially crystallography – is fun! This practical competition will be accompanied by educational material to explain the importance and basic concepts of crystals and crystal growth. This worldwide competition will be organized at different levels. In countries that already hold competitions, it is logical that these challenges should continue during IYCr2014 using their specific guidelines. In addition, a competition for the best video report and/or essay will be organized on a worldwide basis. Of course it is also important to motivate crystallographers in countries where such competitions are not yet organized to set up one in the context of IYCr2014. Support will be given to future local organizers who wish to start a regional or national competition by providing mentoring, guides and a script. The UNESCO Associated Schools Project Network will help to implement the programme, in particular in those countries where a crystallographic community is lacking or lab facilities are poor. Starter kits and educational material, distributed through the UNESCO network, will hopefully create a multiplier effect in the coming years.

More information on the different levels of a worldwide crystal growing competition will soon be announced on a dedicated part of the IYCr2014 website. Keep an eye on it and be sure that your country also participates in this interesting challenge! If you have any questions, please send an email to iycr2014@iucr.org.

The photographs on the right-hand side illustrate the winning crystals from the Belgian Crystal Growing Competition, showing different possible starting materials.

Luc Van Meervelt

IYCR 2014

Website of Artificially Grown Crystals

As part of the celebrations of IYCr2014, the IUCr Commission on Crystal Growth and Characterization of Materials is launching a call for pictures of artificially grown crystals to create a gallery, which will be hosted by the iycr2014.org website.



Dysprosium scandate (contributed by Detlef Klimm, Leibniz Institute for Crystal Growth, Germany). Rare earth scandates are grown by the Czochralski method. The melting points are beyond 2000°C.
Nature provides us with beautiful and sometimes giant crystals. However, people worldwide put extraordinary effort into growing specific crystals, driven by a thirst for knowledge and beauty, and also to satisfy the needs of modern society for novel devices and applications. Thus, each artificially grown crystal is the result of a mixture of science, technology and inventiveness.

Every crystal grower in the world is invited to submit images of the crystals they have grown. This invitation is extended not only to scientists working in public institutions or private companies but also to nonprofessional crystal growers. Each image will be accompanied by information about the crystal, the method used to grow it and its main applications.

All images will be available for download and use for education or other purposes, with the sole obligation being to acknowledge the contributor. The website will also provide links to improve knowledge and feed curiosity. The call for pictures opens officially on the iycr2014.org website on October 15, 2013. Thus, we'll be waiting for your best crystal pictures.

Andrea Zappettini, Chair, IUCr Commission on Crystal Growth and Characterization of Materials

IYCR 2014

My favorite crystal

To celebrate IYCr2014, all readers of the *IUCr Newsletter* are being invited to identify a crystal of his/her personal signifiance.

The applicant should explain the reason for their choice of crystal in 500 words or less that can be understood by non-scientists of all ages. The first 50 people to identify a crystal will receive a glass that has the molecule of their crystal etched on its surface and ten words or less etched on the bottom of the glass identifiying the molecule and its significance.

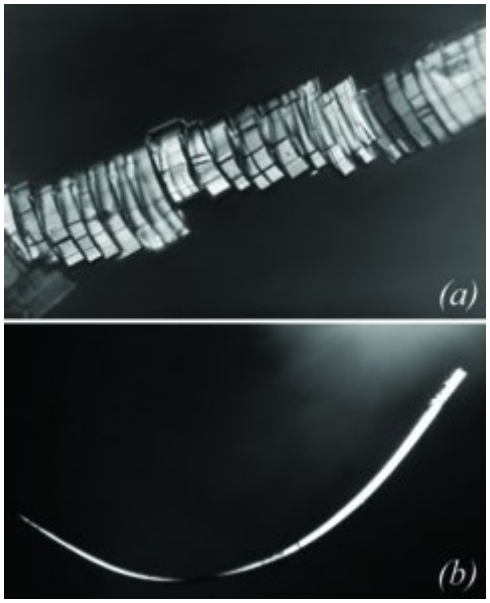
There are dozens of valid reasons to nominate a crystal structure: crystals that improved health and daily living, led to Nobel Prizes or just to your PhD, were used to test new technologies of crystallography, improved the economy and changed the world. Every member country of the IUCr and every state in the US could have a national or state crystal.

Serving drinks to your guest in glasses that have your favorite crystal etched on them is a great way to explain to people what you do and why there is an International Year of Crystallography. You can win one glass free or buy a half dozen with any structure you choose from the Abino Mills Glass Company of Buffalo (if interested, contact iucrnewsletter@gmail.com). The manufacturer has agreed to share a part of the profit from glass sales with the ACA to be used to support the attendance of students from outside the USA to attend future ACA Meetings.

Bill Duax

Member profile and favorite crystal





Crystals that bend reversibly and can be calibrated.



Elena Boldyreva with her students.

My favorite crystal is that of $[Co(NH_3)_5NO_2]Cl(NO_3)$. The compound has been known since the end of the 19th century and was mentioned in *Gmelin's Handbuch*. Iorgensen described photo-induced nitro–nitrito linkage isomerization in this compound and the reverse nitrito–nitro isomerization on storage or heating. Grenthe and Nordin followed the structural changes on thermal nitrito–nitro isomerization in the crystalline state by X-ray diffraction. Others studied the kinetics of the isomerization reaction and measured the quantum yield of photo-isomerization at different wavelengths.

This compound is related to the best memories of my scientific youth – my Diploma work at the Novosibirsk State U. in 1982, my PhD thesis at the Novosibirsk Inst. of Solid State Chemistry and Mechanochemistry in 1988, my first patent, my first invited talks at an international conference, my first Erice School in 1991, my research stays in foreign laboratories in the 1990s with fellowships from the Royal Society (Durham with Judith Howard), CNR (Milan with Angelo Gavezzotti and Angelo Sironi), DFG, and a Humboldt Fellowship (Marburg, with Friedrich Hensel, Hermann Uchtmann, and Hans Ahsbahs). The research ended with my Habilitation in Novosibirsk in 2000 and its results have been summarized in a number of reviews and book chapters.

Thirty years after my first experiments with Anatoly Sidel'nikov, I remember our excitement, when we observed the crystals 'disappearing from the microscope table' while we were trying to bring them into focus. Close examination revealed that the crystals had 'jumped' a very large distance away. Such observations of 'photosalient effects' became a subject of studies of many research groups, but at that time everyone took this as a curiosity, not more. We could grow long thin crystals of the same compound that would not split into smaller fragments or jump on irradiation, but bend elastically and reversibly. This was really great! We published these results in the Proceedings of the USSR Academy of Sciences [E. V. Boldyreva, A. A. Sidelnikov, A. P. Chupakhin *et al.*, *Doklady Physical Chemistry* (1984), **277**(4), 893–896], which at that time was as prestigious for USSR scientists as today's publications in *Science* or *Nature*. A practical outcome was to suggest a photometer, since the number of absorbed light quanta was proportional to the curvature of the crystals that could be easily and sensitively measured by deviation of light from a mirror glued to its end. Light-induced bending of crystals of other compounds was reported by the groups of Avakumov and Nevodchikov from Nizhnii Novgorod, and Ivanov and Urban of Novokuzneck, and we all got patents for different systems.

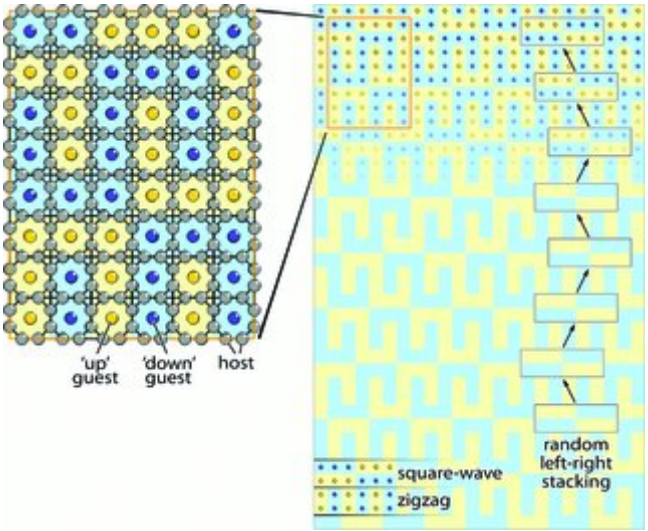
There followed a period of special attention to the role of strain and stress in the reactivity of solids, and research groups in many countries pursued these studies – McBride and Hollingsworth in the USA, Luty in Poland, Buchachenko in Russia, to name just a few. Our 'bending crystals' provided us with a superb tool to study the interrelation between strain and reactivity, not only at a qualitative but also at a quantitative level. We have measured the quantum yield in the crystals elastically bent by external load, and followed the anisotropic strain induced in the crystals by the reaction itself, both at macroscopic and microscopic levels. At that time, we could not even dream of the instruments that enabled the success of

modern photocrystallography thirty years later. Still, even with our modest experimental tools of the 1990s we succeeded to monitor the structural changes on irradiation, to solve and refine the structures of photo-products from powder diffraction data. We used this reaction as a model to develop the concepts of feedback and of flexible and active reaction cavities. I then decided to study this reaction under hydrostatic compression in a diamond anvil cell, and it is from these studies that my long-term interest in high-pressure research evolved. We started with high-pressure IR spectroscopy, proceeded with X-ray powder diffraction and eventually ended up with X-ray single-crystal diffraction. This was a really great time, when we had to start developing experimental methods and computational techniques (ranging from data processing to calculations of free space distribution, the shape and size of the reaction cavity, or Voronoi–Dirichlet polyhedra for molecular packing) 'from scratch', and could achieve the experimental precision that made it possible to follow reliably not only the changes in molecular packing but also the distortion of intermolecular hydrogen bonds and even of intramolecular bond lengths and the rotation of the nitro ligand.

All of this could justify my 'nostalgic' personal selection. But the story had a continuation – many years afterwards, as new instruments became available, linkage isomerization in general, and nitro–nitrito isomerization in particular, were revisited by other groups, and new exciting experiments were and are being performed ever since by Coppens *et al.*, Raithby *et al.* and other research groups worldwide. Photo- and thermo-mechanical effects of crystals became a 'hot topic' in view of their potential applications in supramolecular and biomimetic devices, and more examples of 'bending crystals' were reported. I myself have revisited it in a new collaboration with representatives from the younger generation [P. Naumov, S. C. Sahoo, B. A. Zakharov & E. V. Boldyreva, *Angew. Chem. Int. Ed. Engl.* (2013). **52**; doi: 10.1002/anie.201303757]. As 'my favorite crystal' and 'my favorite solid-state reaction' experience 'a second youth', I also feel younger again. It is so nice to see how much has developed from our days and nights of 'playing' in the lab, when doing research was our only concern, and we did not even know of such terms as 'grant application', 'rating' and 'impact factor'.

Elena Boldyreva

Huge high-pressure crystal structure



Barium at 19 GPa: representative unit (left) of 768 atoms, forming a 'host' framework (grey) and 'guest' chains with two different relative positions – 'up' (yellow) and 'down' (blue) – along channels in the host structure, in a sequence of two zigzag, two square-wave, two zigzag, etc. 'up'/'down' arrangements. There is a random single step to the left or right between the square-wave pairs on either side of each zigzag pair. [I. Loa, R. J. Nelmes, L. F. Lundegaard & M. I. McMahon. *Nature Materials* (2012), **11**, 627–632; doi: 10.1038/nmat3342.]

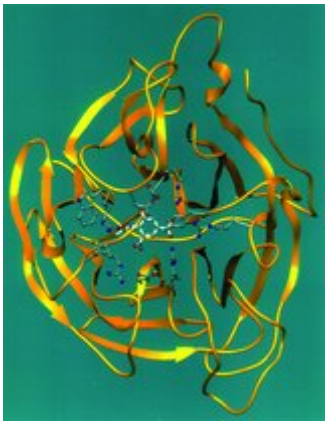
At the Seattle Congress in 1996, the IUCr Executive Committee decided to create a Commission for High Pressure. At that time, new powder diffraction techniques developed from 1990 had already borne a lot of fruit, and we were starting to look for ways to extend high-pressure single-crystal diffraction as well. In 1998, we obtained single-crystal data from barium at 12 GPa that revealed a very surprising incommensurate host–guest structure – a well known structural form in binary systems, but a very weird thing to find in an element. There was clearly an even weirder version at a higher pressure, but the structure was far too complex to solve without much more refined single-crystal methods. Now 15 years later, after developments made by my Edinburgh colleagues Malcolm McMahon and Lars Lundegaard, we have been able to determine a host–guest structure with a 768-atom representative unit – huge for a metallic element – with an intriguing S-shaped patterning of the guest-chain positioning and a disordered sequencing from one row of S-shaped arrays to the next. This very remarkable structure solution was achieved by my colleague, Ingo Loa. It will surely stand as the most puzzlingly intricate of elemental structures – unless there are more surprises yet to come! And, for me, nearly 25 years after starting out with the hope of extending the range of high-resolution crystallography at high pressure, it is astonishing that it has proved possible to get this far!

Richard Nelmes

Great Australian crystals



Halite (salt) crystals.

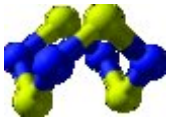


Segmented representation of the neuraminidase inhibitor compound sitting inside a cave-like contour of the neuraminidase enzyme surface.

Two extremely important single crystals connected with Australia are those of sodium chloride and neuraminidase. Sodium chloride, the first crystal for which the atomic structure was determined, was the Nobel Prize winning work of the Braggs (Australians working in the UK). The neuraminidase structure determined by Peter Colman and Jose Varghese in Australia led to the first major drug designed in Australia, Relenza, and was very influential in persuading the government to support structural biology and the construction of the Australian Synchrotron facility.

Mitchell Guss

Sulfur nitride or nitrogen sulfide?



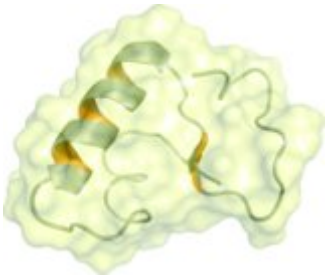
Ball-and-stick model of the tetrasulfur tetranitride molecule, S_4N_4, from the crystal structure.

My favorite crystal is sulfur nitride (S_4N_4). It took me 4 years to prepare a single crystal which revealed that in the structure four nitrogens are in a plane with two sulfurs above and two below that plane, as opposed to the proposal by Nobel Laureate Hassel who claimed from electron diffraction that it was nitrogen sulfide with four sulfurs in a plane and two nitrogens above and two nitrogens below. After a decade of acrimony involving the likes of F. Albert Cotton, it was agreed that my crystallographic work proved S_4N_4 to be sulfur nitride not nitrogen sulfide as claimed by Hassel.

The S_4N_4 structure is important as it led MacDiarmid *et al.* of the U of Pennsylvania to create new plastic electrical conductors and the award of the 2000 Nobel Prize in Chemistry.

Brahama D. Sharma

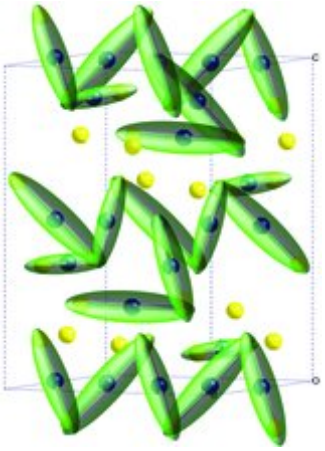
Crambin



Crystal structure of crambin from PDB 3nir.
I nominate as my favorite crystal for IYCr2014 the 46-residue protein crambin. The anomalous scattering method of solving protein structures was first developed with crambin (SAD phasing) in early 1980 (Hendrickson and Teeter). Crambin diffracts to the highest resolution of any protein crystal to date (0.38 Å; Chen, Ginell *et al.*, unpublished). In crambin, one-third of the protein residues adopt alternative conformations and waters link these alternates. This cooperative water side-chain interaction has been linked to protein function. Finally, rings of water in pentagons, hexagons and heptagons are seen at low temperature, with pentagon water rings present at room temperature.

Martha Teeter

The Verwey phase of magnetite, an all-time important crystal structure



Magnetite (Fe_3O_4) is the original substance from which our concept of a magnet and the words 'magnetic' and 'magnetism' derive. It occurs as a mineral and as nanoparticles in magnetotactic bacteria. Our ancestors extracted iron from magnetite and discovered magnetism leading to the development of the compass. Magnetite has many modern applications, from ferrite magnets and memories to nanoparticles for water remediation and MRI imaging.

The importance of electron transfer between different valence states (Fe^{2+} and Fe^{3+}) to the properties of magnetite was identified in the mid-twentieth century, and other important mixed-valent materials such as the high-temperature superconducting copper oxides were subsequently discovered. Fe^{2+}/Fe^{+3} electron transfer is central to redox reactions of iron complexes in solution, and to the role of iron in biology. In 1939, the Dutch scientist E. J. W. Verwey reported that electron transfer in magnetite diminishes sharply on cooling below −150°C, accompanied by a complex distortion of the crystal structure. He attributed this to the freezing of Fe^{2+} and Fe^{3+} states into a regular array, a phenomenon now known as 'charge ordering' that is important to many electronic materials. However, the low-temperature structure proved difficult to determine and became a contentious issue, leading to research over many decades to uncover the nature of the Verwey phase. The full single-crystal X-ray structure was published in 2012 and shows that Verwey's charge-ordering idea is correct to a good first approximation. However, some residual electron transfer still occurs within linear groups of three iron atoms known as 'trimerons'. The complex electronic order is shown as a network of trimerons superimposed on the Fe^{2+}/Fe^{3+} charge-ordered array in the image.

J. Paul Attfield

MEETING REPORT

46th Erice Course The Future of Dynamic Structural Science

46th Erice Course
The Future of Dynamic Structural Science

Erice, Italy, May 2013
www.crystalerice.org



Participants at the 46th Erice Course – The Future of Dynamic Structural Science.

The 46th Course of the International School of Crystallography, 'The Future of Dynamic Structural Science', was held in Erice (TP), Italy, from 30 May to 8 June, 2013, at the Ettore Majorana Centre and Foundation for Scientific Culture. 77 participants attended the course from universities and corporations in 23 countries. The aim of the course was to increase the knowledge of younger scientists in the crystallographic and spectroscopic techniques that are essential for them to work successfully in the field of dynamical structural science, thus bridging the traditional scientific disciplines of chemistry, biology, physics, mathematics and engineering. The course program consisted of a mixture of lectures, software demonstrations and hands-on workshops. In total 43 lectures were given by the teaching staff, which included overviews of various crystallographic and spectroscopic techniques, and cutting edge research results. The lectures clearly showed the strength and breadth of the subjects under discussion. Ten participants were selected, based on their submitted abstracts, to give a 25 minute oral presentation; the selection aimed to include a variety of topics within all the areas discussed during the course. The participants who presented the 42 contributed posters also gave a two minute overview of their poster. The majority of the lecturers emphasized the need for very accurate time-resolved spectroscopic data to understand the changes in molecular properties driven by variation in the sample environment. These data, together with careful kinetic measurements, can inform the specific experimental conditions required prior to undertaking high-resolution crystallography studies. As well as dynamical diffraction methods, a range of spectroscopic techniques were the subjects of several of our speakers, including time-resolved absorption and Raman spectroscopy, XAFS and fluorescence spectroscopy.

Student presentations, selected from the submitted abstracts, were given by 10 of the participants. *Jose Trincao* discussed the work of the dynamic structural science consortium in the UK; *Anton Targonsky* described a method for ultrasonic modification to explore crystal defects; *Matthew Robinson* discussed the table-top time-resolved electron diffraction equipment that had just been built in his home laboratory. *Davide Altamura* showed how it is possible to use grazing incidence SAXS to explore nanostructured materials; *Surajit Kayal* presented some of his Raman studies including the results of

Raman loss spectroscopy. *Jonathan Hanson* explored the simultaneous use of diffraction and IR spectroscopy to study catalytic reactions *in situ* and *Matteo Levantino* presented the results of time-resolved X-ray scattering into protein structural dynamics. *Hideyuki Miyatake* talked about the development of a dynamic light-scattering based protein crystallisation equipment and presented some early results. *Elenora Conterosito* discussed her work using fast *in-situ* powder X-ray diffraction examining layered double hydroxides and *Gyula Faigel* took us into the world of XFEL, showing models of how eventually it could be possible to study the dynamics of single molecules using intense, short X-ray pulses. Care was taken to include young scientists from eastern European and South American countries, to expand their horizons and provide them with new capabilities. The international composition of the school, and the informal atmosphere of Erice, played an important role in facilitating communication between students and world renowned professors, and may foster future scientific collaborations.



Participants receiving awards during the closing ceremony (from left to right): Hazel Sparkes, Alexander Theodossis, Matthew Robinson, Maike Joester, Joshua Hill, Franziska Pinker, Ahmed Farghaly, Judith Howard, Nikita Marchenkov, Annalisa Guerri, Paola Spadon and Eleonora Conterosito.

During the concluding ceremony several awards were presented. The best poster prizes were given to Maike Joester (Berlin, Germany) and Ahmed Farghaly (Cairo, Egypt). Special mentions for the posters were awarded to Franziska Pinker (Strasbourg, France), Joshua Hill (Oxford, UK) and Nikita Marchenkov (Moscow, Russian Federation). The Lodovico Prize (acknowledging the most active student inside and outside the lecture hall) was shared by Eleonora Conterosito (Alessandria, Italy), Alexander Theodossis (Melbourne, Australia) and Matthew Scott Robinson (Edinburgh, UK).

A questionnaire was sent to all participants. Their feedback indicates that a similar meeting should be held in 3-4 years and that the course has been successful in most of its objectives. Participants also gave suggestions that will help the organizers to improve future courses.

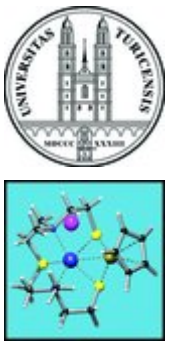
Annalisa Guerri

MEETING REPORT

Zürich School of Crystallography Bring Your Own Crystals

Zürich School of Crystallography Bring Your Own Crystals

Zürich, Switzerland, June 2013



The fifth Zürich School of Crystallography took place at the Inst. of Org. Chem. at U. Zürich (UZH), June 9-22, 2013. The 19 participants were instructed in the theory and practice of small-molecule single-crystal X-ray crystallography. Despite the intensity of the program, the enthusiasm of the participants remained high throughout. They appreciated the personal attention made possible by the 2:1 student:tutor ratio. The participants included 13 PhD and 1 MSc student, and a postdoc. The 8 women and 11 men, with ages ranging from 24 to 50, came from Canada, Finland, Ghana, Italy, India, Nigeria, Poland, Romania, Slovenia, Switzerland, Sweden, Thailand, Turkey, The Ukraine and Uzbekistan. The 10 tutors were from the Universities of Basel, Bern, Geneva, Zürich, the EPFL Lausanne, the ETH Zürich and the Inst. of Physics, Prague.







Alternating lectures and practical work allowed the participants to assimilate the theory and practical aspects together. The practical work included hands-on experience in groups of two at one of the five diffractometers available in the chemistry institutes at the UZH and ETH Zürich. The tutorial exercises and structure refinements were done in the computer classroom of the Inst. of Organic Chemistry. We gave the participants two test data sets to learn to use the software and recognise and resolve unexpected difficulties with structures. Each participant then solved the structure of the compound they had provided crystals of in the lead-up to the School. They were excited to solve the structure of a compound of interest to them. The samples provided a wide range of crystal types (organic, organometallic, coordination polymer, natural product and mineral) and some included challenges, such as twinning, disorder, solvent inclusion, and unusual or ambiguous space groups. All participants were able to complete their structures successfully.

Each participant gave a ten minute presentation on their structure. Those desiring credit points took a two-hour written exam. Others took the exam to test their knowledge. Each day concluded with a discussion of the experiences. We offered repetition lectures on topics nominated by participants who felt that they did not quite grasp a certain aspect the first time. Discussions with the tutors often continued over the evening meal. Social events included a mixer, barbeque and a half-day excursion to the Swiss Light Source and SINQ neutron spallation facility of the Paul Scherrer Institute.

The central goal of the School is to equip each participant to determine structures when they returned to their home laboratory. The practical sessions were designed to allow the participants to go behind button-pushing and understand the operations they performed and how to evaluate the accuracy and relevance of their results.

Every participant completed a questionnaire. They often suggested including more example structures, but we believe a balance of theory and practical work is important. Each participant received a certificate and a copy of 'Crystal Structure Refinement, A Crystallographer's Guide to *SHELXL*' by Peter Müller, donated by the IUCr and OUP. After two weeks together, many new friendships had been

established.The personal impressions of one of the participants are given further below. The next School will be held in June, 2015.

We are very grateful for the generosity of the sponsors: Institute of Org. Chem. UZH, Swiss Society of Crystallography, Cambridge Crystallographic Data Centre, European Crystallographic Association, IUCr, Verlag Helvetica Chimica Acta, Oxford U. Press, Agilent Technologies, Bruker AXS, Oxford Cryosystems and the X-ray Diffraction Services, CSEM, U. of Neuchâtel, and the Chemistry Platform of the Swiss Academy of Sciences.

Tony Linden and Hans-Beat Bürgi

Excerpts from the report of a participant

The school featured excellent lecturers/tutors assembled by Tony Linden (Editor: Acta Cryst. C; U. Zürich) and Hans-Beat Bürgi (Emeritus U. Bern/U. Zürich), which included H. Flack (Emeritus U. Geneva), J. Hauser, P. Macchi (both of U. Bern), G. Chapuis (Emeritus EPFL: Lausanne), O. Blacque (U. Zürich), M. Neuberger (U. Basel), L. Palatinus (Inst. Physics, Prague) and M. Wörle (ETH: Zürich). I’ve been involved with X-ray diffraction before, but had never solved a structure of my own, nor did I understand the meaning of much of the data commonly reported with X-ray diffraction data. We were able to see and tour Switzerland's Synchrotron facility and meet scientists there who are involved in X-ray, neutron and related diffraction experiments. It was wonderful to get to know students from very wide backgrounds and almost every corner of the world. The ZSC provided me with all the tools I need to solve crystal structures but also taught me what the common mistakes are and how to recognize them. I would highly recommend this course for anyone wanting to expand their knowledge of the subject or as a refresher course for those who might want more cutting-edge instruction in modern crystallography.

MEETING REPORT

Croatian - Slovenian Meeting

Biograd, Croatia, June 2013
www.hazu.hr/kristalografi/CroSlo/22biograd/index.htm

The 22nd Croatian-Slovenian Crystallographic Meeting (CSCM22) was held in Biograd, Croatia, in June 2013. Biograd, once a coronation town of Croatian kings, is a tourist and nautical resort on the Adriatic coast. The meeting was dedicated to Boris Kamenar.



During the session: deep silence.

Six plenary and 54 short oral contributions were presented. The plenary lecturers were: Andreas Roodt (keynote; President of the European Crystallographic Association; U. of the Free State, South Africa), 'Kinetics and other systematic probing of electron density at transition metal centres for application in chemical processes'; C. B. Aakeröy (Kansas State U., USA), 'From molecular sociology to functional materials'; A. Altomare (Inst. of Crystallography-CNR, Bari, Italy), 'The challenge of the *ab initio* crystal structure solution by powder diffraction data'; V. Bermanec (U. Zagreb, Croatia), 'The importance of collecting and investigation of mineral samples from ore deposits - example of Stari Trg (Trepča) mine'; M. Jeršek (Slovenian Museum of Natural History, Ljubljana), 'Inclusions in gemstones - origin, identification and valuation'; J. Popović (Ruđer Bošković Inst., Zagreb, Croatia), 'Nanocrystalline metal oxides: synthesis, structure and properties'.

Short oral contributions dealt with all types of applications of crystallography. A. Altomare organized a workshop on 'Crystal structure solution by powder diffraction – the EXPO software'. G. Jovanovski (Macedonian Academy of Sciences and Arts, Skopje), discussed his monograph 'Comprehensive study of minerals from the Republic of Macedonia'.



Meeting excursion to Kornati Archipelago: Ognjen Milat and Mariusz Jaskolski.

80 participants and 10 accompanying persons from 14 countries attended the meeting: Austria, Italy, Poland, Germany, Switzerland, UK, US, South Africa, Macedonia, Montenegro, Ukraine, Iran, Croatia and Slovenia. There was an excursion to the Kornati Archipelago of 365 islands. The meeting closed with a movie concerning Croatia's national heritage to celebrate the acceptance of Croatia in the European Union. The 23rd Slovenian – Croatian Meeting will be held in 2014 in Slovenia and the 29th European Crystallographic Meeting will be held in Rovinj, Croatia, in 2015.



Stanko Popović, Christer Aakeröy, Angela Altomare, Jasminka Popović, Andreas Roodt and Ivan Leban. After the meeting Christer Aakeroy commented, 'The strength of structural chemistry in Croatia and surrounding areas is very impressive, and the enthusiasm of the young generation bodes well for the future of this unique meeting.'

The meeting was organized jointly by the Croatian Crystallographic Assn (CCA) and the Slovenian Crystallographic Society (SCS), under the auspices of the Dept. of Mathematical, Physical and Chemical Sciences of the Croatian Academy of Sciences and Arts.

The Chairs of the meeting were Stanko Popović (CCA) and Ivan Leban (SCS), and the members of the Organizing Committee were: M. Bijelić, M. Cetina, M. Đaković, M. Luić, D. Matković-Čalogović, J. Popović, Ž. Skoko, Z. Štefanić, A. Tonejc, A. Višnjevac, M. Vrankić (CCA), A. Golobič, N. Lah, A. Meden (SCS).

There was no registration fee. Financial support came from the Ministry of Science, Education and Sport of the Rep. of Croatia; PLIVA Pharmaceutical Company, Croatia; Zagrebačka Banka, Croatia; Agilent Technologies, UK; Dectris, Switzerland; Rigaku, Croatia; Incoatec, Germany; Oxford Cryosystems, UK; Bruker, Germany; Mikro+Polo, Slovenia; Renacon-Panalytical, Croatia; Scan-Jeol, Slovenia; Incoatec, Germany; Hotel Ilirija, Biograd; and The Croatian National Tourist Board.

Stanko Popović and Ivan Leban

MEETING REPORT

American Crystallographic Association



Cheryl Stevens

The annual ACA meeting in Honolulu was both a scientific and social success, with 767 attendees. Crystallography informs many diverse areas of science; more and more our meetings have become venues for educating members in the theory and applications of crystallography in disciplines other than their own. The four-day meeting format made it challenging to fit in the 3 workshops, the 20 oral sessions (263 talks) and 3 evening poster sessions (291 presentations). However, despite the beautiful surroundings and the near perfect weather, all were well attended. A record 78 students were given travel grants to support their attendance. The first Bau Neutron Diffraction Award was presented to Tom Koetzle, the Frankuchen Award went to Richard Dickerson (as Dick was not able to attend, Alex McPherson presented a retrospective on Dickerson's work). The Trueblood Award went to Tom Terwilliger, and Eric Ortlund won the Etter Early Career Award. The strategic planning committee met in Hawaii and established action items to help us move forward. Each committee member had an assignment. Action items are related to organizational structure by-laws, marketing, education and expanding involvement of members. We are committed to continuing the process until we have developed a plan for the future ACA.

As we consider where we are going, I think it is important to remember where we have been and to remember the colleagues and friends we have lost recently; Jerome Karle (past ACA and IUCr president), Ray Davis (past ACA president), Charles Caughlan (local chair for the Bronzman ACA meeting back in 1964) and Dave Rognlie (known to crystallographers as the smiling face of Blake Industries). Each of these individuals contributed to our community and each will be missed.

Cheryl Stevens

MEETING REPORT

ACA Council Meeting Highlights, July 2013



Patrick Loll

President Cheryl Stevens announced that the program chairs for the 2014 annual meeting in Albuquerque, NM, will be Petrus Zwart and Christine Beavers. In an update on the new ACA journal, *Structure and Dynamics*, Judy Flippen-Anderson reported that an editorial board has been formed, and a temporary website set up. Policies are being set to encourage submissions from ACA members, notably a discounted publication fee for members.

Considerable discussion was devoted to the International Year of Crystallography 2014 (IYCr2014), and specifically to how the ACA could best support this initiative. Vice president Martha Teeter has assembled an International Year of Crystallography 2014 task force, which is considering a wide range of relevant topics, including schools outreach, media, web outreach, funding, and liaisons with politicians and other scientific organizations. Council decided that the ACA should commit some funds to activities related to IYCr2014 in North America, and agreed on a sum of $20k. This is approximately equal to the organization's dividend income for a year, which means this amount can be committed without dipping into reserves. Funds will be allocated *via* a call for proposals, which will be coordinated by the IYCr2014 task force.

The 2013 class of ACA fellows was approved, and the names were announced at the banquet during the Hawaii meeting. The 6 new fellows are: Sidney Abrahams, Wim Hol, Jim Ibers, Alex McPherson, Keith Moffat and Alex Wlodawer.

Past President George Phillips reported that many inconsistent and outdated items have accumulated in the ACA by-laws, owing to years of neglect. He has embarked on an effort to streamline and update this important document, but warned that this will be an ongoing and iterative process. Given the strategic process that was initiated earlier this year, this is an opportune time to address this problem.

Council has also decided to try a new policy of using videoconferencing for their spring and fall meetings, in order to save money. The first test of this approach will be at the Council meeting this fall.

Patrick Loll, ACA Secretary

FEATURE ARTICLE

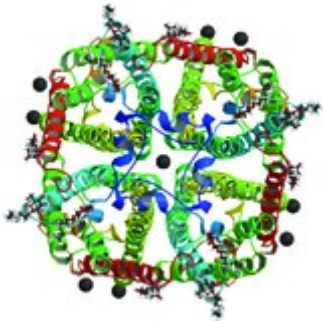
Structures that impact our daily lives

Since the last *IUCr Newsletter* was published, many structures illustrating aspects of the molecular machinery essential to life have been reported, including the size and shape of the nuclear pore complex, the details of mechanisms of ion transport through membrane channels, mechanism of cell division in bacteria, carbon utilization for survival, molecular details of angiogenesis, nucleosome organization vital to chromatin integrity, evolution of the respiratory chain and synthesis of enzymes.

Some specific recent crystallographic findings with impact on our daily lives include the following.

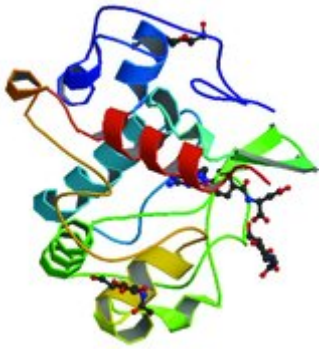
Macromolecular structure determination of the crystalline complex of phosphatidyl inosital phosphate bound to the surface of the vitamin E transfer protein reveals the nature of the binding, the importance of the binding to vitamin E function and why specific inherited mutations lead to familial vitamin E deficiency [N. Kono *et al.*, *Science* (2013), **340**, 1106, doi: 10.1126/science.1233508].

The structure of a toxic protein from the *Salmonella* strain responsible for typhoid fever has been found to be a complex of three well defined and separate domains in which two subunits are connected by a single disulfide link [J. Song *et al.*, *Nature* (2013), **499**, 350-352, doi: 10.1038/nature12377]. The structural insights could lead to the design of new antibiotics and vaccines to combat typhoid, which kills 200,000 people worldwide each year.



PDB ID 3zoj.
A high-resolution (0.8 Å) structure of an aquaporin [U. Kosinska *et al.*, *Science* (2013), **340**, 1346, doi: 10.1126/science.1234306] provides details about the exact pathway that water molecules follow through a channel of 6 transmembrane α-helices. The identity of the residue in the channel also explains why OH and H_2O^+ do not pass through the channel.

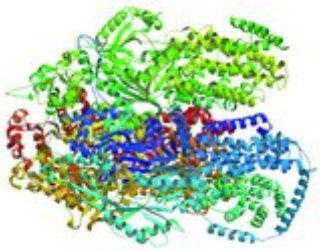
Structures of wild type and mutant forms of hemagglutinin from an H5N1 virus bound to avian or human receptor sialic acid analogs reveal a conformational transmission from birds to humans [W. Zhang *et al.*, *Science* (2013), **340**, 1463].



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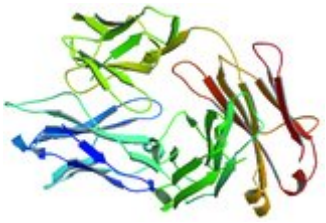
The structures of the folate receptor (a major target for cancer chemotherapy) with folic acid in the active site [K. Melcher, *Nature* (2013), **500**, 486-489, doi: 10.1038/nature12327] will foster design of better anticancer agents.

The structure of the first member of class B G-protein-coupled receptors, corticotrophin releasing factor receptor 1, revealed features useful for the development of new drugs to combat diseases of the brain and of metabolism [K. Hollenstein *et al.*, *Nature* (2013), **499**, 438].



PDB ID 3w9h.
Because E. flux transporters are responsible for drug resistance in Gram-negative bacteria, the recent determination of a complex of a selective inhibitor bound to one of these transporters [R. Nakashima *et al.*, *Nature* (2013), **500**, 102-106, doi: 10.1038/nature12300] reveals the site of binding and can be used to design potential and selective blockers of drug resistance.

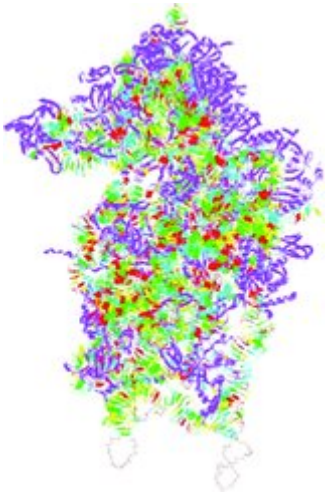
The cause of a debilitating side effect of a sulfonamide antibiotic that has been used for over 50 years was recently determined to result from binding of the antibiotic to an enzyme essential to the production of neurotransmitters. The crystal structure of the complex of sulfamerthazine to the enzyme (sepiaperin reductase) should lead to redesign of antibiotic derivatives with reduced neurotransmitter inhibition. [K. Johnsson, *Science* (2013), **340**, 987-991, doi: 10:1126/scoemce1232972.]



PDB ID 4jha.
Respiratory syncytial virus (RSV) infects nearly all children by 3 years of age and is a leading cause of infant mortality. The crystal structure of the complex of an antibody and the glycoprotein F of RSV reveals the mechanism of binding and will support design of improved vaccine antigens. [J. S. McLellan *et al.*, *Science* (2013), **340**, 1113-1117, doi: 10.1126/science.1234914.]

The structures of a corona virus responsible for severe pulmonary disease in humans and its complex with the cellular receptor [G. Lu *et al.*, *Nature* (2013), **500**, 227-231, doi: 10.1038/nature12328] reveal a common core in the structure of coronoviruses but high variation in the external binding motifs region responsible for virus-specific pathogenesis and insight into pathogen-targeted therapy.

Comparison of the crystal structures of wild type and mutant forms of an inhibitory receptor on macrophages complexed with CD47 (an antiphagocytic signal) provides molecular details of a synergistically increased phagocytosis *in vitro* and enhanced antitumor response *in vivo* that may be a universal method of augmenting the efficacy of therapeutic anticancer antibiotics. [K. Weiskopf *et al.*, *Science* (2013), **341**, 88-89, doi: 10.1126/science.1238856.]



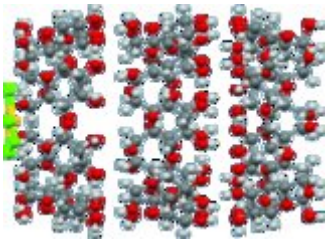
PDB ID 4kzx.
The structures of three complexes of the small ribosomal subunit define three steps in mammalian translation and initiation and reveal the dynamics of the interaction in the P site of the ribosome [I. B. Lomaken, *Nature* (2013), **500**, 307-311, doi: 10.1038/nature12355].

Many predatory bacteria synthesize a large spike-shaped multi-molecular machine with which they inject toxins into other species and destroy them. A recent structure determination reveals the details of piercing tips of the spike [M. Shneider *et al.*, *Nature* (2013), 500, 350-353, doi: 10.1038/nature12453].

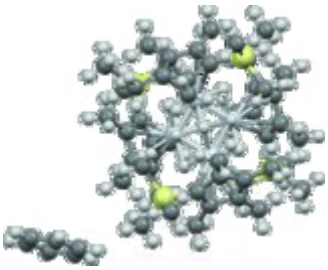


CSD No. 895701.
Just as Dorothy Hodgkin determined the correct structure of penicillin in the 1930s with a single-crystal structure determination, an acrimonious debate over the actual structure of the 2-norbornyl cation has been resolved by X-ray crystallographic demonstration that the carbonium ion is a bridged structure with 'non-classical' geometry [F. Scholz, *Science* (2013), **341**, 62, doi: 10.1126/science.1238849].

The computationally designed and crystallographically verified structure of a multi metal ion oxide, with properties of a solid oxide fuel cell cathode, was reported by M. Dyer *et al.* [*Science* (2013), **340**, 847-852, doi: 10.1126/science.1226558]. The oxide consists of specific composition of Y, Ba, Ca, Fe and Cu that has a 60 Å cell side and 148 atoms in the unit cell.



CSD No. 918417.
Recent crystallographic structures of new materials with economic potential include a cyclodextrin offering a 'greener' method for gold recovery [J. F. Stoddart, *Nat. Commun.* (2013), **4**, doi: 10.1038/ncomms2891], mesoporous single crystals of semiconducting titanium dioxide [E. J. W. Crossland *et al.*, *Nature* (2013), **495**, 215-219, doi: 10.1038/nature11936], a metal-organic framework that enhances fuel efficiency [J. R. Long *et al.*, *Science* (2013), **340**, 960-964, doi: 10.1126/science.1234071], and a complex binary solid having reproducible electronic and magnetic properties prepared by combining fullerenes with a metal triethyl phosphate cluster [X. Roy *et al.*, *Science* (2013), **341**, 157-160, doi: 10.1126/science.1236259].



CSD No. 937386.
A trinuclear titanium polyhydride cluster that cleaves and functionalizes N_2, forming N-H bonds essential to converting abundant N_2 molecules in the air into a chemically usable form essential to life, has been prepared. Single crystals reveal the long-sought mechanism [T. Shima *et al.*, *Science* (2013), **340**, 1549-1552, doi: 10.1126/science.1238663].

In July 2013, survey articles highlighted proton conduction in metal-organic frameworks (MOFs), and van der Waals heterostructures constructed of two-dimensional atomic crystals appeared in *Science* (2013, **341**, 354, doi: 10.1126/science.1239872) and Nature (2013, **499**, 419-425, doi: 10.1038/nature12385), respectively. Crystallographic studies continue to reveal the structures of modern materials that are responsible for unusual properties and phenomena.

AWARDS AND PRIZES

Kolos Medal and Lecture Award



Philip Coppens.

Philip Coppens has been awarded the Kolas Medal from the Polish Chemical Society and the Dept. of Chemistry of the University of Warsaw. Professor Coppens delivered the Kolos Lecture on September 16, 2013 during the LVI Conference of the Polish Chemical Society in Siedlce, Poland.

AWARDS AND PRIZES

2012 PANalytical Award



Thomas Bennett.

The inaugural PANalytical Award of 2012 was presented to Thomas Bennett, Dept. of Materials Science at the U. of Cambridge, UK. The prize was based on a research article published in *Physical Review Letters* (2010), 104, 115503, entitled: 'Structure and Properties of an Amorphous Metal Organic Framework'. As first author on the publication Dr Bennett received the PANalytical Award trophy, a certificate and £5,000 sterling.

The PANalytical Award initiative was launched to identify and encourage exceptional young researchers who have never held a professorship and use laboratory-scale X-ray equipment as their primary analytical technique. A key feature of Dr Bennett's work is his use of X-ray total scattering data (PDF), in combination with data from scattering electron diffraction and optical microscopy and computer pictures of the metal-organic framework under investigation.

AWARDS AND PRIZES

ACA2014 Awards

Patterson Award to John Helliwell



John Helliwell.

John R. Helliwell has been selected to receive the 2014 ACA Patterson Award for his pioneering contributions to the development of the instrumentation, methods and applications of synchrotron radiation in macromolecular crystallography. Professor of Structural Chemistry at the U. of Manchester, UK, John received his undergraduate degree in physics from York U. (with Michael Woolfson and Peter Main) and a PhD in protein crystallography at Oxford (with Margaret Adams). He was mentored by Charlie Bugg and Guy Dodson in the laboratories of Dorothy Hodgkin and David Phillips.

John was involved in the first experiments that used synchrotron radiation for macromolecular structural studies and he has dedicated his career to exploring new applications of synchrotron radiation and has worked tirelessly to improve synchrotron and neutron facilities worldwide. He contributed to solving the phase problem by, among other things, introducing longer wavelength radiation to expand anomalous scattering applications for phasing to a wider range of scatterers. He is also recognized for having pushed forward the development of Laue methods for time-resolved studies and other applications, both in X-ray and neutron crystallography.

He led the design and realization of the first synchrotron beamline (SRS, Daresbury) dedicated to protein crystallography (1981) and of the first synchrotron radiation wiggler instrument (1984). Other notable initiatives at SRS were in longer wavelength anomalous dispersion (Howard Einspahr), weakly scattering crystals (Steve Ealick), microcrystal diffraction (Britt Hedman and Keith Hodgson), virus crystal diffraction (Michael Rossman) and Laue diffraction (Keith Moffat). In the late 80s and into the 90s he led the European working group for macromolecular crystallography for the ESRF Foundation Phase report and became Vice Chair and then Chair of the ESRF Science Advisory Committee.

In 1995 he first demonstrated sharpened crystal mosaicity in microgravity-grown protein crystals. In 2001-2002 he determined the first *de novo* structure of apocrustacyanin A1, solved with softer X-rays. In 2005 he initiated *ab initio* structure determination by MAD phasing of powder diffraction data and discussed the potential for extending the method to structures of large molecules containing anomalous scatterers.

He is the author of a classic book on protein crystallography, *Macromolecular Crystallography with Synchrotron Radiation* (Cambridge Univ. Press, 1992) and is a founding editor of the *Journal of Synchrotron Radiation*. He was president of the ECA (2006–2009) and served as Editor-in-Chief of the IUCr journals (1996–2005).

He has traveled widely to promote and support crystallography internationally, and has fostered several synchrotron and neutron projects in the US and served on many advisory and board panels to review synchrotron projects at the APS. His special relationship with American crystallography and the crucial

contributions he has made to improve synchrotron radiation applications from the very dawn of the synchrotron era were key for his selection as the 2014 Patterson award recipient. John will receive the award at the 2014 ACA meeting at Albuquerque, NM.

Chiara Pastore
Taken from ACA RefleXions, Summer 2013

AWARDS AND PRIZES

Etter Early Career Award to D. Borden Lacy



D. Borden Lacy.

D. Borden Lacy (Vanderbilt U. Medical Center) is a structural biologist and biochemist. Some of her outstanding achievements include the determination of the structure of the botulism neurotoxin during her graduate studies at UC Berkeley, broadly enabling both basic and applied research targeting this pathogen. Her postdoctoral studies with John Collier were equally productive and are best described as a tour de force examination of the molecular basis of anthrax toxin pathogenesis. She has already trained a number of students and has contributed to a number of courses. She has served on multiple committees both within and outside the university. She has won the Burroughs Wellcome Award for the study of the pathogenesis of infectious diseases, as well as several NIH grants. She has received numerous fellowships and awards during her training years, and is known for being a caring mentor and a role model for women in science. She truly embodies the spirit of Margret C. Etter.

Eric Ortlund, Emmanuel Skordalakes

NOTICE

Visa assistance for travel to the United States

With the upcoming 23rd Congress of the International Union of Crystallography in Montreal in 2014, many international visitors may be also interested in visiting the US.

The US National Committee for Crystallography is housed within the US National Academy of Sciences (NAS). The NAS also hosts the International Visitors Office (IVO), which may be able to assist you in obtaining a US visa. (www.nationalacademies.org/visas/)

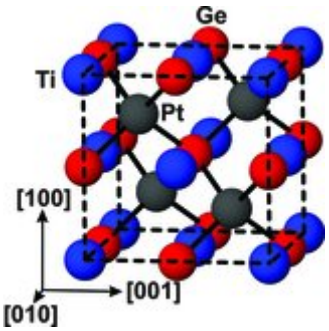
The IVO has a web page with information on how to apply for a US visa (http://sites.nationalacademies.org/PGA/biso/visas/PGA_048013) that every scientific visitor should read before planning a trip here. Amongst the useful suggestions to be found on the web page are: information on who needs to obtain a visa to enter the US; suggested timeframe for the visa application, at least 3-4 months in advance of your trip, to allow ample time for visa interview scheduling and for the administrative processing following your visa interview; to bring to the interview a copy of your most current CV with a list of your publications to help demonstrate your credentials; and to provide an accurate email address for consulate communications in the event your visa cannot be issued the same day.

Visa processing delays often depend on the applicant's nationality and background, but most of the time the US visa application process works well and is completed reasonably quickly. If your visa has not been processed and more than 21 days have passed since your application has been submitted and the interview completed, the IVO has a questionnaire for you to fill out.

We hope to see you in Montreal.

REGIONAL NEWS

Science coming out of the Zürich School of Crystallography



The recent paper in *Acta Crystallographica* B**69**, 457-464, *TiGePt - a study of Friedel differences* by Ackerbauer *et al*. (2013), is a product of the Zürich School of Crystallography held in June 2011. The objective of these two-yearly schools is to teach 20 young participants, mostly PhD students, the basic notions of crystallography by a combination of lectures and practical classes in which each student solves their own crystal structure.

This study arose in a singular way. The crystal of TiGePt used for structure determination by Ackerbauer *et al*. (2012) (*Chem. Eur. J.* **18**, 6272-6283) was submitted to the Zürich School of Crystallography [Linden & Bürgi (2008) *Acta Cryst.* A**64**, C30 and www.chem.uzh.ch/linden/zsc] by one of the 20 student participants (S.-V. Ackerbauer) as her project study. Diffraction measurements (Mo *K*α radiation) were made by the school organizers and the student had to solve and refine the project structure, once two example structures provided by the school had been completed. The intermetallic compound TiGePt is atypical in its chemical composition and symmetry compared with most crystals submitted by the other student participants. At an *R* value of 1.1%, the study of TiGePt was still producing furrowed brows amongst the ten highly experienced tutors and the student. The values of statistics concerning the fit of Friedel opposites looked weird. In particular, it was not entirely clear whether the space group was non-centrosymmetric or not, and in the hustle and bustle of the school, there was no time to pursue these problems further. A lively e-mail discussion was undertaken following the school and its results are presented in the paper.

The X-ray single-crystal diffraction intensities of the intermetallic compound TiGePt were analysed. These showed beyond doubt that the crystal structure is non-centrosymmetric. The analysis revolves around the resonant-scattering contribution to differences in intensity between Friedel opposites *hkl* and *hkl*. The following techniques were used: $R_{\rm merge}$ factors on the average (A) and difference (D) of Friedel opposites; statistical estimates of the resonant-scattering contribution to Friedel opposites; plots of $2A_{\rm obs}$ against $2A_{\rm model}$ and of $D_{\rm obs}$ against $D_{\rm model}$; the antisymmetric D-Patterson function. Moreover, it was possible to show that a non-standard atomic model was unnecessary to describe TiGePt. Two data sets were compared. That measured with Ag *K*α radiation at 295 K to a resolution of 1.25 Å^{-1} is less conclusive for absolute-structure determination than the one measured with Mo *K*α radiation at 100 K to the lower resolution of 0.93 Å^{-1}.

Hans-Beat Bürgi, Howard Flack and Anthony Linden

REGIONAL NEWS

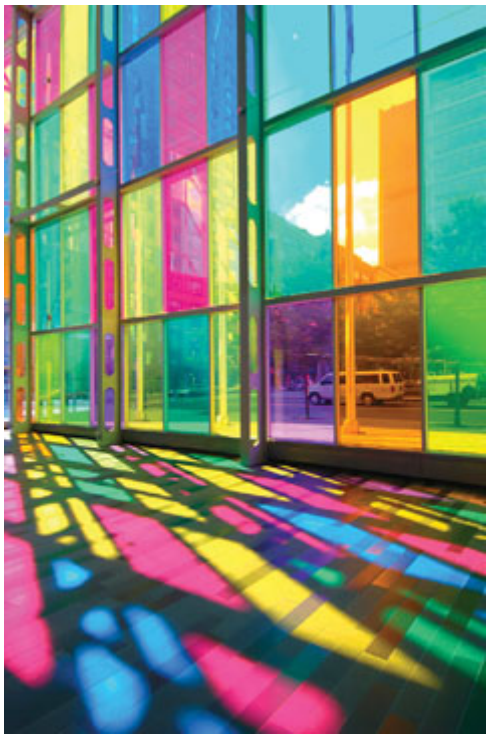
BCA Council Officers

	**President (2015)** David Keen david.keen@stfc.ac.uk
	**Vice President (2013)** David R. Allan david.allan@diamond.ac.uk
	**Acting Secretary (2013)** Claire Wilson claire.wilson@diamond.ac.uk
	**Treasurer (2014)** Pamela Williams pamela.williams@astx.com

FEATURE ARTICLE

Celebrate crystallography in Montréal – the IUCr 2014 scientific program is now online!

Celebrate crystallography in Montréal – the IUCr 2014 scientific program is now online!



The scientific program for the 2014 IUCr Congress has now been announced and it promises to be one of the glittering centerpieces in the International Year of Crystallography. The congress website (www.IUCr2014.org) now lists titles and descriptions of each of the Microsymposia, with more details such as chairs and speakers being added as they are confirmed. You will soon be able to submit your contribution through the congress website's *Call for Abstracts*, which is targeted for release by November 1, 2013. In addition to the Plenary and Keynote speakers, the 2014 session chairs will invite over 300 speakers to Montréal, and will need to select another 300+ speakers from the submitted abstracts – a significant increase from the previous Congress. When you submit, please indicate that you would be willing to give an oral presentation if asked. Let's give them lots to choose from.

The venue for the meeting, Montréal's Palais des congrès, is huge, but everything is located on two levels, directly connected by an escalator. The sessions are all on one floor, and posters, exhibitors, and coffee on the other. More than half the exhibit spaces have already been sold, but we still have some choice locations available. Both exhibit and sponsorship opportunities are available through IUCr2014.org.



The subway system – The Metro - stops at the Palais, and underground passages lined with shops and restaurants spread throughout the downtown area. Stepping outside, you are minutes away from hundreds of restaurants and bars, and dozens of hotels. You will be impressed with Montréal in the summer. Don't forget to check out the tours and excursions being offered in conjunction with the Congress. The committee has tried to ensure that interesting options exist for delegates and their travel companions alike.

There will be many exhibits and events proudly celebrating the International Year of Crystallography around the world in 2014, and we would very much like to make Montréal the focal point of the IYCr during the Congress. Members of the International Program Committee and others will be presenting short public lectures on various aspects of crystallography. In the public area in the foyer of the Palais there will be posters and exhibits. The Executive Committee of the IUCr is organizing a microsymposium on the IYCr.

We want more. Let us know what you have planned for the celebration. Have you generated teaching materials? Posters? Videos? Demonstrations? Let's make an effort to share our contributions with our professional colleagues as well as the general public. You can contact any member of the Local Organizing Committee either directly or through our Conference Manager Michèle Bourgeois-Doyle (her contact information is on the website). You can also get in touch with Michele Zema, the Project Manager for IYCr2014 (iycr2014@iucr.org) or Louise Dawe (ldawe@wlu.ca), the Canadian representative on Martha Teeter's ACA IYCr task force. We will make every effort to include your contributions in the Montréal celebrations.

EDITORIAL

Editorial



William Duax



Judy Flippen-Anderson

Judy Flippen-Anderson has accepted an appointment as corporate secretary of the American Institute of Physics. Judy generously agreed to become the editor-in-chief of the newsletter when I became president of the IUCr in 2002. She graciously allowed me to return as co-editor with her in 2006. Although Judy will no longer be on the staff of the IUCr newsletter her impact upon it will remain. Among her many valuable contributions as editor, Judy was instrumental in promoting timely publication and fostering fiscal responsibility. We will do our best to stay on the course Judy has set for us. We wish her success in her new position and all her endeavours on behalf of the crystallographic community.

William Duax