INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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IUCR JOURNALS NEWS

Cryo-electron microscopy and IUCrJ



(left to right) Richard Henderson, Werner Kühlbrandt and Sriram Subramaniam.

IUCrJ (www.iucrj.org), the only journal to carry the name of the International Union of Crystallography, was launched in January 2014 with a simple mission: to attract high-quality science papers of broad scientific significance from across the full breadth of the scientific communities that use structural information.

We are pleased to announce the journal will start accepting articles in cryo-electron microscopy (cryoEM) within the Biology and Medicine section. CryoEM is proving to be a powerful tool for structural biologists for studying large molecular machines and membrane protein complexes at high resolutions.

Three of the world leaders in cryoEM - Richard Henderson (MRC, Cambridge), Werner Kühlbrandt (MPIBP, Frankfurt) and Sriram Subramaniam (NIH, Bethesda) - are joining the editorial board of IUCrJ to serve the cryoEM community and provide leadership for the enthusiastic acceptance of the journal by this expanding field.

On the occasion of the launch of cryoEM in IUCrJ, Richard Henderson said 'There has been a quantum leap in the power of single particle cryoEM due to recent improvements in microscopes, detectors and computer programs. It is entirely appropriate that the IUCr should become the home for cryoEM in the same way as it has nurtured X-ray and other crystallographies since its foundation in 1948.'

IUCR JOURNALS NEWS

Have you published open access?



Since the launch of **Crystallography Journals Online** in 1999, the IUCr has had a policy of providing free access to the full texts of certain types of articles (for example, CIF Applications, Prefaces, Editorials, Letters to the Editor, Book and Software Reviews, Crystallographers, Notes and News, Addenda and Errata, and New Commercial Products); this policy will continue. In addition, a number of services including tables of contents, e-mail alerting, and the provision of supplementary material (*e.g.* CIFs, structure factors and other structural data) are free of charge to both subscribers and nonsubscribers.

It is also worth mentioning in this article that the IUCr has an active policy (http://journals.iucr.org/services/archivingpolicy.html) concerning the long-term preservation and access to publications in its journals. The charge made to authors for open-access (OA) publication includes a contribution to the cost of the long-term preservation and access of the publication.

OA is a rapidly evolving landscape and there exist a number of benefits to publishing your work OA including possibly higher visibility of publications, the possibility of higher citation rates and improved access to literature for scientists in the developing world.

The IUCr publishes two journals that are fully (gold) OA, *i.e.* all articles are made available free of charge to the reader. An OA fee is charged to authors of articles published in these journals to cover the costs of peer review, journal production, and online hosting and archiving. These journals are IUCrJ and *Acta Crystallographica Section E: Crystallographic Communications*. All the remaining journals - *Acta Crystallographica Sections A*, *B*, *C*, *D* and *F*, *Journal of Applied Crystallography* and *Journal of Synchrotron Radiation* - are hybrid OA journals, which means they are traditional subscription journals in which some of the articles are OA.

Authors publishing an OA article in one of our gold OA or hybrid OA journals will be asked to pay an OA fee - also called an article processing charge or APC - upon acceptance of their article for publication. Note that authors will be asked to confirm that they can pay the OA fee, or that they have a payment waiver, at the submission stage. Discounts and waivers are available in particular circumstances; you can find out more by visiting http://journals.iucr.org/services/oa/openaccess_full.html. Payment is simple; authors may pay by credit card, cheque or voucher. Please note that purchase order and invoicing arrangements are also available on request. For more details of how to pay, go to the web pages of the individual journals.

Authors of OA articles will not be asked to transfer copyright to the IUCr, but will instead be asked to agree during article submission to an OA licence. This licence is a Creative Commons Attribution (CC-BY) Licence, which provides for the re-use of the article in whole or part provided there is attribution for the article.

By following this link http://scripts.iucr.org/cgi-bin/citedin?search_on=openaccess you can see a complete list of OA articles in Crystallography Journals Online.

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

IUCR ACTIVITIES

IUCr sponsored prizes



Asgar Abbas Kazrani (IIMCB, Warsaw, Poland) won a travel grant to ECM29 as his prize for giving the Best Student Presentation at the 17th Heart of Europe Bio-Crystallography meeting (Berlin, Germany; September 2014).

The IUCr Journals/CCG poster prize at the Spring BCA meeting (York, UK; March/April 2015) went to Christoph Zehe (U. Bayreuth, Germany). Photo credit: Carl Schwalbe, *Crystallography News*

From left, Lorena Tremiño-Agulló (Inst. Biomed. Valencia-CSIC, Spain), Mercedes Ramirez Escudero (IQFR-CSIC, Madrid, Spain) and Ikni Aziza (CNRS-Marseille U., France) who received poster prizes at the 5th International School on Biological Crystallization (Granada, Spain; May 2015). The prizes were presented by Richard Giegé (centre) and Claude Sauter (right).

Caleb Chappell (Western Kentucky U., USA) beside his winning poster at ACA2015 (Philadelphia, PA, USA; July 2015).

Anton Brausemann (centre) (Albert-Ludwigs-U. Freiburg, Germany), Eleonora Conterosito (U. Piemonte Orientale, Alessandria, Italy) and Matteo Alvaro (inset) (U. Pavia, Italy) receive their poster prizes from IUCr President Marvin L. Hackert at ECM29 (Rovinj, Croatia; August 2015).

At the India-Bangladesh Structural Chemistry Conference (Kolkata, India; September 2015), poster prize winners M. H. Mesbah Ahmed (centre) (Jagannath U., Dhaka, Bangladesh), Rima Paul (right) (Pandu College, Guwahati, India) and Pritam Gosh (inset) (CSIR-Central Mechanical Engineering Research Institute, Durgapur, India) were presented with a year's free access to *Acta Cryst. C*, an IUCr2017 polo shirt and a certificate by Michele Zema, IUCr Outreach Officer.

Eugeny V. Alexandrov (centre) from Samara State U., Russia won the IUCr Journal-*Acta Cryst. B* Poster Prize at the 2nd ICSU/IUPAC Workshop on Crystal Engineering (Como, Italy; August/September 2015). Presenting the prize and certificate are, from left to right, *Acta Cryst. E* Co-editor Petra Bombicz and *Acta Cryst. B* Co-editors Andrew D. Bond, Pierangelo Metrangolo and Janusz Lipkowski.

IYCR LEGACY

Celebrating the International Year of Crystallography in Argentina

The Argentinian Association of Crystallography (AACr; www.cristalografia.com.ar), founded in 2004, is dedicated to promoting crystallography all over the country as well as to bringing together groups working in this area of knowledge and/or groups employing it as a tool in their research. To celebrate IYCr2014 and also its 10th anniversary, the AACr organized not only academic activities, but also educational, promotional and dissemination ones.



10th Annual Meeting of the AACr.

The academic activities included the 10th Annual Meeting of the AACr and two satellite events, an Advanced Course on the Atomic Pair Distribution Functions Technique: Fundamentals and Applications and the 6th AACr School: Synchrotron Radiation Techniques for Materials Science, which took place in Mar del Plata in October and November 2014 (http://intema.gob.ar/cristalografia/principal.html). These had been preceded by the International School on Fundamental Crystallography - 4th MathCryst School in Latin America, held in La Plata from April 27 to May 3, 2014 (www.crystallography.fr/mathcryst/laplata2014.php).

An IUCr-UNESCO OpenLab was held in La Plata and Buenos Aires, May 5-10, 2014, in partnership with Agilent Technologies and OlexSys. A report was included in a previous issue of the *IUCr Newsletter* (www.iucr.org/news/newsletter/volume-22/number-2/argentina-open-lab).



Final round of the 2014 Argentinian Crystal-Growing Competition and some winning projects.
The AACr invited high-school students in the country to participate in its first crystal-growing contest (www.cristalografia.com.ar/index.php/concurso-de-crecimiento-de-cristales). The contest's Facebook page (www.facebook.com/ConcursoCrecimientoCristalesArgentina) has attracted >2300 likes! Previously, teachers of the establishments concerned were invited to participate in free Crystallography and Crystal Growth training sessions (www.cristalografia.com.ar/index.php/concurso-de-crecimiento-de-cristales/jornadas-para-docentes). In total the AACr organized 38 days, trained 1106 teachers and visited all the provinces. The award ceremony was held during the opening ceremony of the 10th Annual Meeting of the AACr. Out of a total of 139 entries to the Worldwide Crystal-Growing Competition 2014, 29 were from Argentina, winning three gold, two silver and one bronze medal and receiving five honorary mentions.



The first prize in the adult category was awarded to Gabriela Aloras, an artist from El Bolsón, Río Negro. A National Art Contest - cristalizARTE - was launched to inspire artists of all ages by crystallography. Several radio stations and newspapers featured the contest and published interviews with the organizers. To see the winning entries please visit http://fisica.cab.cnea.gov.ar/cristalizarte/index.php/novedades.



A National Photo Contest was held, open to photographers and researchers/scholars from the disciplines of physics, chemistry, biology, geology and materials science (www.cristalografia.com.ar/index.php/concurso-fotografia). Photo contests were also organized in Ushuaia ('Getting close to crystallography and discovering a new world') and (for schoolchildren) Bariloche ('Crystallography in action').



Diego Lamas participates in a radio show.

Numerous fairs, exhibitions, celebrations and dissemination talks took place all over the country (www.cristalografia.com.ar/index.php/actividades/divulgacion), including an International Book Fair in Buenos Aires and a Week of Science in Santa Rosa (Province of Santa Fe) and Santiago del Estero (Province of Santiago del Estero).



Brochure for promotion of the IYCr and our national crystal-growing contest.

The IYCr was promoted in Argentina using a website (www.cristalografia.com.ar/2014) and Facebook page (www.facebook.com/ForoArgentinoCristalografia2014). A brochure to promote the Year and the national crystal-growing competition was produced, along with material on crystal growing for teachers and students. National and regional newspapers, national science journals and radio and TV shows featured interviews with Argentinian crystallographers.

The IYCr in Argentina was an unforgettable experience. Many members of our association participated enthusiastically in all the activities and in this way it was possible to bring crystallography to all the provinces of our country. We would like to express our sincere appreciation to the IUCr for its auspices and financial support. Finally, we would like to mention that many of the above-mentioned dissemination activities are being conducted again this year 2015: talks all over the country, the national crystal-growing competition for high-school students, the short training courses for teachers, participation in fairs and exhibitions, etc.

This is an abridged version of a report submitted by Diego Lamas, AACr Immediate Past President and coordinator of IYCr activities (the full version can be seen at www.iycr2014.org/about/reports)

IYCR LEGACY

Introducing the IUCr's new Outreach Officer



The IUCr is very pleased to announce that Michele Zema, who acted as the IUCr Project Manager for the International Year of Crystallography (IYCr2014), has been appointed to the new post of IUCr Outreach Officer. In this role, Michele will continue many of the outreach programmes started for IYCr2014, such as the OpenLabs initiative, as well as coordinating IUCr's education activities, including reaching out to schools, colleges and the general public.

IYCR LEGACY

IYCr Legacy Fund

The IYCr Legacy Fund has been established to enable the continuation of many initiatives successfully launched during IYCr2014 (http://www.iycr2014.org/legacy). The aim of the fund is to support the following:

- to continue promotion of the fundamental role crystallography plays in the different branches of science, including chemistry, mineralogy, physics, biology, medicine, materials science, cultural heritage and geosciences;
- to target governments by interacting with them and advising on the design of policies that will support the establishment and operation of crystallography teaching, ranging from modernising existing crystallography teaching material in schools and universities to developing closer collaborative ties with crystallography centres across the world as well as synchrotron and other large-scale facilities;
- to continue to increase awareness of the way crystallography underpins most of the technological developments in modern society, and also its role in art and cultural heritage, via public conferences, sponsorship of poster exhibitions highlighting the usefulness and marvels of crystallography and by the commissioning and submission of articles to the press, television and other media on the contribution crystallography makes to the global economy.

'Of course, a lasting legacy from the International Year of Crystallography is not just related to outreach activities taking place during the year. It is also about creating lasting initiatives in our schools, colleges, universities and other places of learning to continue the message about the importance of crystallography. We want to see a nation of youngsters being inquisitive about crystallography and governments enabling schools and colleges with opportunities to teach crystallography alongside the core science disciplines currently featured. This can't happen overnight; however, with the launch of the IYCr Legacy Fund we stand a real chance to accomplish these goals, by continuing many of the initiatives launched during the Year'. Peter Strickland, Executive Managing Editor, IUCr.

Donate to the IYCr Legacy Fund at www.iycr2014.org/legacy/legacy-fund.

IYCR LEGACY

Crystals - Artwork of Nature: a Touring Exhibition through Austria in IYCr2014



On the occasion of the International Year of Crystallography (IYCr), proclaimed by United Nations (UN) for 2014, a touring exhibition through Austria was organised. Visiting all federal states, its aim was to disseminate knowledge of this science and show the relevance for our daily lives, for research and economy. Supported by the Austrian Ministry of Science, the Austrian Mineralogical Society, the Faculty of Geo- and Atmospheric Sciences of the U. of Innsbruck and PANalytical B.V. Austria, the touring exhibition was organised and executed by the author of this report, a crystallographer and science communicator.

Exhibition



Some impressions of the exhibition with examples of graphics, models, experiments and demonstration material.



Some visiting school classes.



Novel models, photographs and computer graphics were used to illustrate the internal structure of crystals and their physical appearance and properties. For effective communication, specially developed experiments, visualisations, activity stations and a lot of hands-on material were employed. The content was adapted to regional and seasonal conditions at the respective sites. Primarily, the exhibition was visited in the course of interactive tours provided by the author, thus achieving a maximum degree of personal care and support, response to individual questions and adaptive adjustment to the situation - so

ultimately 'reaching' people. Via an, at first glance, aesthetic access (for this reason, the title 'Crystals - Artwork of Nature' was chosen), knowledge of the following core contents was effectively imparted to the visitors:

- basic knowledge of crystallography, geo- and material sciences
- relevance to our daily lives
- related education, economy and research.

The Tour

Because of the assumed high communication potential concerning IYCr in cities with universities and major museums, it was a declared aim of the project to visit places and regions with no related local infrastructure. The tour stops are summarised below:

- 04.04.2014 - Long Night of Research, Vienna
- 21.05. - 18.07.2014 - Federal Library, St. Poelten, Lower Austria
- 18.-26.09.2014 - Town Hall, Leoben, Styria
- 22.09.2014 - Birthplace of crystallographer Felix Machatschki, Arnfels, Styria
- 30.09.2014 - Nature Museum Salzkammergut, Ebensee, Upper Austria
- 01.-03.10.2014 - Town Hall, Gmunden, Upper Austria
- 04.10.2014 - Long Night of Museums, Vienna
- 04.-05.10.2014 - Mineral fair 'Mineralium', Wiener Stadthalle, Vienna
- 07.-10.10.2014 - Vinatrium, Deutschkreutz, Burgenland
- 22.-25.10.2014 - Town Hall, Schattendorf, Burgenland
- 04.-07.11.2014 - Carinthian College of Education, Klagenfurt, Carinthia
- 08.11.2014 - Annual Meeting 'Min&Geo' of the Carinthian Society of Natural Sciences, PHK Viktor-Frankl-Hochschule, Carinthia
- 14.-17.11.2014 - Museum Fronfeste, Neumarkt am Wallersee, Salzburg
- 20.-23.11.2014 - Scholar Center, Frauenkirchen, Burgenland
- 28.-30.11.2014 - Forum, Rum, Tyrol
- 11.-14.12.2014 - Castle, Kittsee, Burgenland
- 17.-18.12.2014 - Elementary School Bregenz Schendlingen, Vorarlberg

In conclusion, all 9 federal states of Austria and 13 cities were visited by the touring exhibition. A total of 224 school classes received an interactive guided tour, there were 442 hours of personally guided tours and approximately 15,000 visitors reached in personal contact (conservative estimate). Some tour stations were located right at the national borders of Austria (Arnfels: Slovenia, Schattendorf: Hungary, Kittsee: Slovakia, Bregenz: Germany). There were a good number of visitors from abroad who were served with multilingual tours. The message of IYCr was therefore also carried to other nations, especially in the often neglected border regions. The interest among the population was very high and the touring exhibition very well visited. The coverage in radio, print and online media was very satisfactory. Most prominent events were reported to IYCr headquarters with positive feedback.

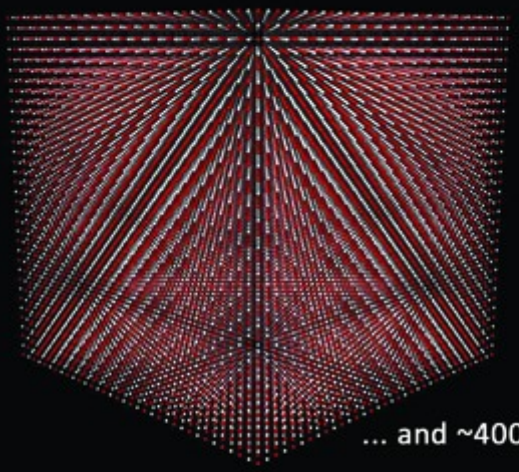
In addition to the touring exhibition, the author conducted numerous other activities in Austria to bring crystallography closer to the public. These include school and kindergarden projects, public talks, philatelic contribution, other exhibitions and outreach activities. More information and photos can be seen at www.r-krickl.com/kristalle.

Finally, there are still some ongoing major outreach activities, such as the construction of the world's largest crystal structure model (registered with Guinness Book of Records). It will be used for science communication in public spaces in November 2015 to honor the 100th anniversary of the Braggs' Nobel Prize (http://worldrecord.r-krickl.com/en/) (see below).

Robert Krickl

The world's largest crystal structure model

To honour the 100th anniversary of the Braggs' Nobel Prize



NaCl-type

42 875 balls

11.8 km sticks

3.09 m edge length

... and ~400 tubes of glue!

Record attempt registered with GUINNESS WORLD RECORDS®

Inauguration: Vienna City Hall, Austria
27 October–30 November 2015



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IYCR LEGACY

2015 Wisconsin Crystal-Growing Competition



Map showing the locations of participating schools in Wisconsin, USA. Ten schools out of 25 participated in the contest for the second time.

The 2nd crystal-growing competition among Wisconsin high-school students aged between 14 and 18 has been successfully conducted. The contest, which perfectly aligns with the Wisconsin Idea, inspired participation of over 550 students and teachers from 25 schools across the state and one school from Moscow, Russia. Students from seven WI schools received prizes at an award ceremony held on May 22, 2015, at the Chemistry Building, UW-Madison.



Judges evaluate crystals and artwork submissions.

To promote the contest we set up a booth at the Wisconsin Society of Science Teachers Conference in March 2015 to inform the public about the crystal-growing contest, crystallography and education at the UW-Madison Chemistry Department. A web site provided the information necessary to register for the competition, to learn about crystals and to learn the details of the crystal-growing procedure. There were links to the related national and international events.

The main goal of the contest was to grow large blue crystals of cupric sulfate pentahydrate. The crystals were evaluated for size and quality by a committee comprising six PhD chemists and one chemistry graduate student. The high-school students submitted 44 crystals that had won their local contests. New for this year was a contest-inspired art competition for which 11 submissions of drawings and mixed media were sent in. All winners were recognized with certificates, books, T-shirts and cash prizes. The best crystals and drawings are on permanent display in the Chemistry Department, and can be seen at www.iycr2014.org/about/reports/activities-for-schoolchildren/2015-wisconsin-crystal-growing-competition.



Contest winners who attended the award ceremony: six students and their teacher. The organizer is on the right.

Additional contest goals were to motivate students to learn about solution chemistry, compound solubility, purification, crystallization and optical microscopy. The students adopted an advanced vocabulary and learned to work in teams, keep detailed records of their progress, communicate with their teammates and follow good laboratory practices.

All participants of this important scientific outreach activity were invited to tour the UW-Madison campus, the Chemistry Department and the Molecular Structure Laboratory. They were also invited to the award ceremony that featured several high-profile speakers. Assistant chair Mark Ediger described the significant role of the department on campus. John Moore presented a lecture with experiment demonstrations to illustrate what it is like to be an undergraduate student in this department. A guest speaker from U. of North Carolina at Charlotte, Dan Rabinovich, spoke about crystals and crystallography on postage stamps. Paula Piccoli described the contest and its significance and then Ilia Guzei awarded the prizes. Over 70 students, teachers and parents attended the award ceremony.

The Wisconsin Crystal-Growing Contest is now an annual event; for details of the 2016 contest, please go to http://xray.chem.wisc.edu/WICGC_2016.html. On, Wisconsin!

Ilia A. Guzei, Organizer

Letters from students, teachers and leaders of the science clubs participating in the 2015 Wisconsin Crystal-Growing Competition

...This is way cooler than I thought...

Thank you so much again for organizing this event. I think the crystal growing competition is a good opportunity to introduce students to work in the laboratory. Aqueous solutions of copper sulfate are pretty safe to work with and the crystallization conditions allow enough permutations to provide a challenge to the students to find appropriate conditions for growing seed crystals and competition crystals. The students were intrigued by the intense color of the solution alone and literally blown away by the beauty and size of the crystals. We luckily had enough material that they even ventured into growing little crystal gardens. The students had fun, learned to work accurately and cleanly and follow instructions. They learned from their mistakes making adjustments to improve results. They learned to relate results to crystallization conditions and modify conditions to improve results.

My favorite quote: 'This is way cooler than I thought!' All of them were looking forward going into the 2016 competition with so much more experience.

Michael Ruf, coach of a student team, Verona, Wisconsin
I'd also like to thank you for again hosting the Crystal Growing Competition. I also organize a major academic competition and I know how time-consuming it can be, but it is also very rewarding. I want you to know that all of my students gave this competition two thumbs up and they very much enjoyed their visit to UW. Several students commented that they would have liked to stay overnight and take more tours. I am hoping that this competition continues to be an annual event and you continue to have the awards before summer as it easier to get the kids there.

Tim Cox, Berlin High School Chemistry, Wisconsin
At DC Everest High School, I run the crystal growing competition as an afterschool enrichment activity. This year is the second year we have participated in your contest. The students and I think it is great. Students love the intra-school competition. The students that participate are highly motivated students, and love a challenge. Thank you for running this statewide competition. It is a great learning activity for our students. The documentation you provided for instructions for the contest are very clear and user friendly. I do not have any suggestions for changes other than to please include us again.

Thank you for providing us with this opportunity.

Ann Wiernik, Chemistry Teacher, DC Everest Senior High School
I just wanted to tell you that I had a lot of fun doing the Crystal Growing Contest. It was a highly rewarding experience because I was able to create my own experiment within the experiment. It was hands-on and watching the crystals grow under different conditions was very interesting. In my opinion, any chance to learn and have fun while doing one is an opportunity that should not be passed up.

Thank you for organizing this.

Abby Schuett, high-school student, Fond du Lac, Wisconsin

IYCR LEGACY

The importance of the IYCr2014 resolution

The International Year of Crystallography - 2014 - was an extraordinary one for our science. Across the world, hundreds of activities highlighted the importance of our subject, and brought it, perhaps for the first time, to the notice of schoolchildren, teachers, the general public, politicians and policy makers. The formal milestones of the year occurred during major international events around the globe: the Opening Ceremony in Paris, France, in January 2014; regional summit meetings in Karachi, Pakistan (April), Campinas, Brazil (September), and Bloemfontein, South Africa (October); and the Closing Conference in Rabat, Morocco, in April 2015. From each of these events came a formal communiqué (http://iycr2014.org/declarations), often highlighting the challenges that face our science and its practitioners, especially early-career scientists, in our modern, busy world.

However, the final resolution, carrying the title that was the theme of the Rabat conference - **Crystallography for the next generation** - is different. It is optimistic in outlook, and carries a strong commitment to securing the future of crystallography, from representatives of several International Scientific Unions and international non-governmental agencies. The resolution embraces the needs to enhance the stature of crystallography, to build capacity in developing regions of the world, and to extend further the public understanding of science in general and crystallography in particular.

It is, of course, right that such a commitment be given by the senior officers of such bodies, and it is to be hoped that this commitment will be seen, heard and acknowledged by science directors and policy makers around the world. However, it is also right that individuals, who have been touched and inspired by the International Year of Crystallography, should have the opportunity to endorse publicly these goals and the specific actions identified in the resolution. This can be done through an online form (http://iycr2014.org/declarations/legacy-endorsement) that allows individuals to add their names to the list of those who support the IYCr2014 resolution goals and actions. Already more than 250 individuals have shown their support. Please take a few moments to read the resolution in detail (http://iycr2014.org/declarations/legacy-endorsement) (as published in the last issue of the IUCr Newsletter), recognise its importance, and - if you agree with these objectives - add your own name to the list. The next generation of crystallographers will thank you for it.

Michele Zema, IUCr Outreach Officer (mz@iucr.org)

IYCR LEGACY

CCDC OpenLab Kenya, 7-11 September, 2015





The IUCr-UNESCO-CCDC OpenLab Kenya entitled 'An Introduction to Computational Chemistry and *In Silico* Visualization. A Workshop for Sub-Saharan Africa Scientists' took place at Kenyatta U. and at the U. of Nairobi in Kenya during the week of 7-11 September, 2015, organized by Juliette Pradon of the Cambridge Crystallographic Data Centre (CCDC) and Lewis Whitehead of the Novartis Inst. of BioMedical Research, with the local support of Evans Changamu from Kenyatta U. and Solomon Derese from the U. of Nairobi. Patricia Gitari (d-orbital Ltd), formerly at Kenyatta U. and member of the committee for the African Crystallographic Association, was the local representative of the IUCr.

Nearly 90 attendees, with a range of nationalities (including Kenyan, Nigerian, Eritrean, Ethiopian, Ugandan and Congolese), backgrounds (chemistry, physics, biology) and levels (MSc, PhD and postdoctoral students; university lecturers; academic, governmental and industrial researchers) were introduced to molecular modelling in structural chemistry, medicinal chemistry and drug discovery. The Cambridge Structural Database (CSD), which is the world's repository for organic and organometallic small-molecule crystal structures, was introduced by Juliette Pradon, as well as the software suite which

allows its 800,000 crystal structures to be accessed, searched and analysed. Solomon Derese raised awareness of the Mitishamba database and its relevance to Kenya and beyond, inviting all to contribute their natural products where possible. Participants learned how to search the CSD, from simpler text/numeric searches to more advanced substructure searches; how to analyse the search results numerically and graphically; how to visualise molecules and investigate their packing arrangements; and how to analyse the intramolecular geometry of molecules and their intermolecular interactions using the knowledge base afforded by the wealth of quality crystal structures in the CSD. These sessions demonstrated how such crystallographic databases have value not only for research but also for teaching purposes. The teaching data set of the CSD proved to be a particularly useful resource for lecturers to visually illustrate key structural chemistry concepts such as stereochemistry, aromaticity, hapticity, VSEPR molecular shapes and ring conformations for the benefit of their undergraduate students. An introduction to modelling in drug discovery was also given, focusing on the hit identification phase and demonstrating the usefulness of computers in this field and the range of modelling techniques applicable to specific problems. Participants also had the opportunity to hear from Lewis Whitehead about several past challenges in medicinal chemistry and to themselves apply the CSD System to these challenges. Finally, Patricia Gitari, as the local representative of the IUCr, raised awareness among the participants of the various past and future IUCr activities in the world and more particularly in Africa.

The feedback from participants of this OpenLab was very positive, with many enthusing that they wished it was longer. Looking ahead, future editions of this workshop in East Africa would benefit greatly from having a practical session on a powder and single-crystal diffractometer, and a broader crystallographic education session to help participants understand how structures deposited in the CSD are solved. Once technical expertise on diffractometers has been formed locally, it would be of great benefit to establish a regional centre of diffraction studies, open to all Kenyan and regional institutions, where diffractometers would be available to solve crystal structures. The formation of an African Crystallography Association, once Kenya and other African nations become a member country of the IUCr - as Cameroon has recently done and others surely will do after the first Pan-African Crystallography Conference to be held in Cameroon next year - will shape the advancement of crystallography in Africa and contribute to its recognition as benefiting the entire continent.

Juliette Pradon and Patricia Gitari

Testimonial

I had a great experience and an awesome time during the OpenLab. The facilitators (Dr Pradon and Dr Whitehead) were really good, natural and had vast knowledge. It was a golden chance to receive some training on subjects not covered by our academic curriculum and to refresh some concepts. I also learnt about other databases such as CrystMet and ICSD. Dr Gitari gave a presentation about the IUCr, its activities and IYCr2014, which were previously unknown to me. I gained a lot of knowledge, which will be vital in my research work (especially the Acta journals) and my future chemistry endeavours.

In my project, I seek to develop a water purification material from siliceous (clay) nanoparticles. As maybe one university in Kenya has an XRD machine - and the chances are that it is not functioning - I had to source the XRD services from a geology company, which was very costly and meant I had limited access to the machine. I feel that the IUCr can make a great impact in the development of crystallography in Kenya by holding more OpenLabs, helping universities and other learning institutions to acquire X-ray diffractometers, providing access to XRD data interpretation software, encouraging universities to include crystallography in their curricula and funding postgraduate projects.

David Marikah (chemistry masters student, Jomo Kenyatta U. of Agriculture and Technology, Juja, Kenya), participant

IYCR LEGACY

PANalytical OpenLab Mexico, 29 September - 2 October, 2015



XRD practical session with Jorge Pablo Gonzalez.



High-school students enjoying a crystallographic activity.



Visit to Amparo Museum.
The first IUCr-UNESCO OpenLab Mexico (www.iycr2014.org/events/openlabs/iycr2014-openlab-mexico) partnered by PANalytical was held in November 2014 at the Inst. of Geology of the U. Nacional Aut□ónoma de Mé□xico. In 2015, PANalytical Mexico, together with the Institute of Physics of the Benemerita U. Autónoma de Puebla (BUAP), the Mexican Society of Crystallography (SMCr) and the IUCr, organized the second edition of the IUCr-UNESCO OpenLab Mexico (www.iycr2014.org/events/openlabs/panalytical-openlab-mexico) and Practices of X-Ray Diffraction and Fluorescence to promote crystallography in Mexico once again.

The program of the IUCr-UNESCO PANalytical OpenLab Mexico 2 consisted of a four-day seminar to give the participants access to an update about how crystallography has been developed in Mexico and about different and new applications related to the X-ray diffraction technique through presentations by 13 national crystallographers and Christina Hoffman, from Oak Ridge National Laboratory (TN, USA), who gave a lecture about Crystallography for deciphering the structure-property relationship in modern materials.

The program started with an introduction to the activities of the SMCr by its Public Relations Secretary, Lauro Bucio, who also talked about Application of the Rietveld method in the cement industry. Indeed most of the lectures focused on special applications of powder X-ray diffraction techniques, such as High-resolution XRD and reciprocal space mapping in semiconductors (Miguel A. Vidal), Crystallography in gemology (Juan Carlos Cruz), Graphic representation for the crystal structures of ceramic materials (Sylvain Bern□ès), Amorphous material determination by the *K*-factor method, X-ray diffraction and beyond and in situ methods (Jorge Pablo Gonzá□lez), Polymorphism in proteins (Abel Moreno Carcamo), Crystallography in earth science (Teresa Pi Piug), the Debye ring (Luis Fuentes Cobas), Dielectric ceramics: structural control of their properties (Ulises Salazar) and Surface impurities on selenite giant crystals from Naica, Mexico (Maria Elena Montero). This certainly gave a broad overview of the potentialities of the methods and inspired the young researchers with such a range of research topics.

In addition, three practical sessions were organized, which included basic and advanced measurements using the Empyrean X-ray diffractometer and the small but powerful Epsilon 1 XRF spectrometer. The sessions were led by Jorge Pablo Gonzalez and Alejandro Magno Villa (both from PANalytical Mexico), who demonstrated the analytical flexibility of the XRD technique through the use of different accessories, and the practicality of an XRF benchtop system.

Places were limited to 80 people. We received applications from about 120 people, showing a high interest in crystallography in the country.

In the spirit of promoting intra-regional cooperation, the IUCr supported travel and accommodation expenses for Elvis Garc□ía, a student from the U. of Guatemala, and Scarlett Garc□ía, a student from the U. of Costa Rica, to attend the OpenLab (read their testimonials below). The main objective was to support the emerging countries of Central America by inviting students to an important event that they don't always have the opportunity to attend.

PANalytical offered coffee breaks and lunch every day of the event, and a folkloric show and dinner on October 1. Forty-seven high-school students from the Freinet Prometeo Inst. visited the OpenLab venue to participate in a couple of crystallographic activities.

As part of an optional social activity, 30 OpenLab attendees along with BUAP/PANalytical personnel visited the Amparo Museum in downtown Puebla on 30 September to view exhibitions of pre-Hispanic and colonial objects.

The objective of promoting crystallography in Mexico was once again achieved, and we are very pleased to announce that everyone was delighted with the contents of this year's program, such that we were asked about next year's OpenLab dates and location. Therefore, in order to continue to promote

crystallography in Mexico and give the opportunity to all the people who took the time to apply, we are aiming to organize a similar event in 2016.

I would like to give special thanks to Maria Eugenia Mendoza, Ulises Salazar, Leonel San Román, Lauro Bucio, Juan Carlos Madrid, Jorge Gonzalez, Alejandro Villa, and Michele Zema from the IUCr, who supported the organization of this event.

Looking forward to the next OpenLab!

Luis Miguel Martinez, Marketing Specialist, PANalytical Mexico

Testimonials



This event was very rewarding and I think all of us (attendees and invited speakers) received from this event something more than mere knowledge in the field of crystallography by hearing presentations from each of the doctors, specialists in their areas. As a student I think these events are a very useful tool in our training because besides gaining more knowledge, they guide us, and they can be a key factor at the time of choosing a master's or doctorate in our areas. And even more when they are promoting Latin American participation as was the case of this OpenLab. I deeply thank the IUCr for the opportunity to participate in this conference, and all the attention we received from members of PANalytical Mexico, BUAP, the Mexican Society of Crystallography and all other members who participated to make this event possible.

Scarlett García, Student, U. of Costa Rica



I would like to express my gratitude for the opportunity to attend the OpenLab …. The lectures were high level and interesting, with useful content to apply in my engineering career. These lectures about the latest technologies allow me to have a broader view of what I can bring to my country to develop the area of research and development in mineralogy and crystallography in the fields of archaeology, gemology (Guatemala is one of the leading exporters of jade worldwide), exploration and characterization of new materials applied to the building segment.

Elvis García, Student, U. of Guatemala

MEETING REPORT

1st Crystallography Olympiad held in Poland

Poznań, Poland, June 2014



Participants of the 1st Crystallography Olympiad in Poland, caption refers to steps (s) numbered bottom up. A. Deptuch (s2) with her 1st Prize (air ticket), A. Gładysiak (s1) 2nd Prize, M. Zieliński (far left on s3) 3rd Prize, E. Michalski (far right on s2), Chairman of the Organizing Committee. (Photo by R. Paszkowski)

To celebrate IYCr2014 and to accentuate other anniversaries, including 'The Jan Czochralski Year 2013', the Committee of Crystallography in Poland organized the 1st National Crystallography Olympiad, modeled on other Olympiads (Mathematics, Physics, Chemistry). The Crystallography Olympiad was designed for university students, although high school students were also accepted. The tournament consisted of two stages. At the first level, the schools selected the candidates. The Finals were held in Wroclaw on 25 June, 2014, in connection with the Annual Polish Crystallographic Meeting ('Crystallographic Conversations'). The 29 finalists had to solve 60 test questions and to answer 5 open questions in 2 hours. The questions covered all fields of crystallography, including geometrical crystallography and symmetry, diffraction methods and structure analysis, growth and properties of crystals, crystal and structural chemistry, macromolecular crystallography, and other aspects of crystallography including history. The Olympiad was organized and a committee that included M. Jaskolski, A. Koziol, R. Przenioslo and D. Stroz, chaired by E. Michalski, prepared the examination questions. The winners were A. Deptuch (Krak□ów), A. Gładysiak (Poznań) and M. Zieliski (Warsaw). Rigaku/Testchem generously sponsored the prizes - the 1st Prize, a one-week visit to Japan - as well as Panalytical, Bruker and Agilent - the 2nd/3rd Prize received notebook/tablet. In a sense, however, all the participants including the Organizers are the winners because the Olympiad turned out to be a success and helped to popularize crystallography in Poland.

We plan to make the Olympiad an annual event and hope that other countries will organize Crystallography Olympiads, with the ultimate goal of having an International Crystallography Olympiad.

Mariusz Jaskolski

MEETING REPORT

23rd Slovenian Croatian Crystallographic Meeting

Logar Valley, Slovenia, June 2014



Plenary Lecturers (from l to r): T. Balić-Žunić, M. Đaković, G. Gunčar, I. Radosavljević Evans and J. S. O. Evans.

The 23rd Slovenian-Croatian/Croatian-Slovenian Crystallographic Meeting held in June 2014 in the beautiful Logar Valley was dedicated to the celebration of the International Year of Crystallography. There were 58 participants from Austria, Croatia, Denmark, Germany, Great Britain and Slovenia. Five plenary lectures were presented : 'Structural chemistry of functional materials: mobility in the solid state' (I. Radosavljević Evans, Durham U., UK); 'Functional inorganic materials: synthesis, structure, properties and methods development' (J. S. O. Evans, Durham U., UK); 'From molecular structure to crystalline solids: non-covalent interactions as a structure directing force in supramolecular assemblies' (M. Đaković, U. of Zagreb, Croatia); 'Crystallography in mineralogy in the 21st century' (T. Balić-Žunić, U. of Copenhagen, Denmark); and 'A structural view of nanobodies' (G. Gunčar, U. of Ljubljana, Slovenia).

One of Slovenian-Croatian meetings' advantages is that all participants give an oral presentation, providing young scientists the opportunity to present their work in a friendly but professional atmosphere. Thirty-three short oral contributions addressed contemporary topics in crystallography comprising data acquisition and interpretation in areas such as macromolecules, organic, organometallic and inorganic compounds, crystal architecture, metallurgy, solid solutions, phase transitions, small-angle scattering, nanocrystallography, structure and properties, synergy of diffraction, microscopy and other methods, history and nomenclature.

The meeting was organized jointly by the Faculty of Chemistry and Chemical Technology, U. of Ljubljana, and the Croatian Crystallographic Association under the auspices of U. of Ljubljana, and promoted by the Slovenian Chemical Society. There was no registration fee. Therefore we thank the sponsors, donors and advertisers: Agilent Technologies, Ansar-analitika and Bruker, Chemass, Incoatec, Lek-Sandoz, Mikro+polo, Renacon and PANalytical, and Scan.

More information about the meeting, including the Gallery, can be found on http://slocro23.fkkt.uni-lj.si.

Anton Meden and Stanko Popovic

MEETING REPORT

Biocrystallography Workshop in Białystok

Białystok, Poland, July 2014



Group photo of the Workshop participants. (Photo courtesy S. Wojtulewski)

A workshop entitled 'Biocrystallography for the High-throughput Era' was held in July 2014, at the U. of Białystok, Poland. The program included lectures on such aspects of macromolecular crystallography as: crystallographic fundamentals (M. Jaskolski, Poland); the future of structural biology (W. Minor, USA); molecular replacement (H. Fernandes, Poland); anomalous phasing (Z. Dauter, USA); macromolecular refinement (M. Gilski, Poland); Bayesian reasoning and structure validation (B. Rupp, USA) ; protein cloning and purification (R. Jedrzejczak, USA); protein crystallization (K. Brzezinski, Poland); and bioinformatics (B. Nocek, USA).

Most of the lecturers also taught tutorial sessions, during which the students gained hands-on experience in bioinformatics aspects of crystallographic studies, HT protein expression, purification and crystallization, efficient X-ray data collection and processing, phasing, model refinement, and validation. The focus was on high output rather than throughput. The 24 pre- and postdoctoral students from four countries found the workshop highly successful and they appreciated gaining practical experience, often using their own projects. With the help of the experts, several participants were able to crystallize their proteins, process their data and solve difficult structures. The success stories contributed to a high level of satisfaction among the participants. The best posters were presented by J. Loch (1st prize) and M. Wierzbicki (2nd prize), they were awarded with a copy of the 'Biomolecular Crystallography' handbook by B. Rupp. The principal organizer, K. Brzezinski, is to be applauded for planning and implementing a remarkably productive workshop.

Mariusz Jaskolski

NOTICE

German Crystallographic Society Annual Conference

Stuttgart, Germany, 14-17 March, 2016
www.dgk-conference.de

The 24th Annual Conference of the German Crystallographic Society is scheduled to take place from 14-17 March, 2016, at the U. Stuttgart, Germany. An international and national delegation of renowned scientists will present and discuss the following topics:

- Aperiodic and periodic complex materials
- Biostructures I: Challenges in macromolecular crystallography
- Biostructures II: Hot new structures of biological macromolecules
- Biostructures III: Protein function and regulation
- Biostructures IV: Protein-nucleic acid interactions
- Computational and theoretical crystallography
- Total scattering (PDF)
- Complementary methods for structure determination
- Coordination polymers and weak interactions
- Crystallography, crystal chemistry and application of layered materials
- Inorganic structural chemistry: syntheses and structure
- Inorganic structural chemistry: properties and applications
- Lightning talks by young crystallographers
- Spectroscopic methods in crystallography
- Structural chemistry under non-ambient conditions
- Liquid crystals and their applications
- Time-resolved crystallography
- Storage and battery materials
- Molecular structural chemistry: syntheses, structure and applications.

Abstracts should be submitted in English and online by 31 December, 2015. Up-to-date information can be found on our conference website www.dgk-conference.de.

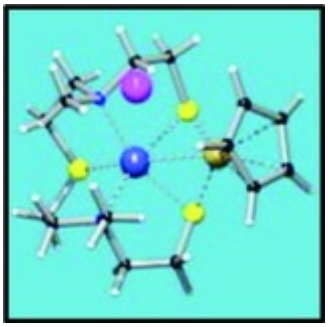
Robert E. Dinnebier and Thomas Schleid

MEETING REPORT

The Zürich School of Crystallography

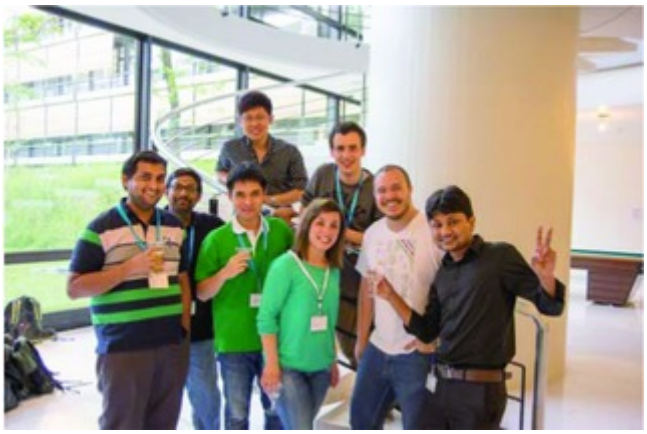
Bring Your Own Crystals

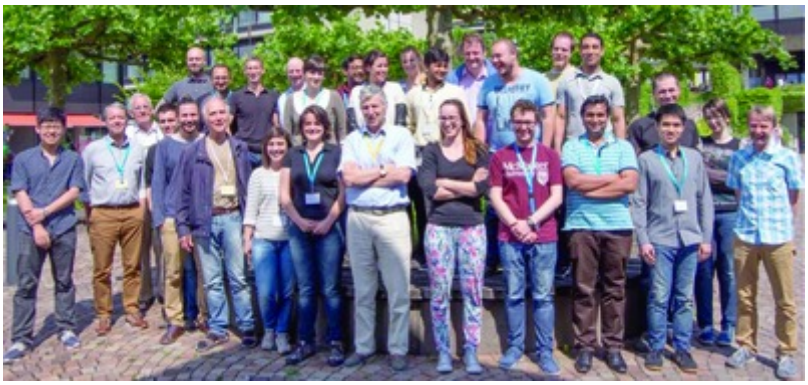
Zürich, Switzerland, June, 2015











Participants at the Zürich School of Crystallography.

The sixth Zürich School of Crystallography was held in the Dept. of Chemistry at the U. of Zürich (UZH). Within five minutes of the opening mixer starting, we knew the school would be an outstanding success: the 19 participants and 10 tutors were all chatting with each other enthusiastically. After 13 days of intense theory and practical sessions on all aspects of small-molecule single-crystal X-ray crystallography, the participants were still excited, although tired, and the final banquet finished with lots of book-signing by the tutors, photography, and the occasional tear because new friends were going their separate ways.

We maintained our usual 2:1 student:tutor ratio and participants always comment very favourably on the personalised friendly attention they receive. The 19 participants this year comprised 1 MSc and 15 PhD students, 2 postdocs and 1 researcher from industry. They came from 12 countries: Australia, Canada, Croatia, Germany, Israel, Portugal, Russia, Slovenia, Sweden, Switzerland, Thailand and the United Arab Emirates. The 10 tutors were from the Universities of Basel, Bern, Geneva, Zürich, the EPFL Lausanne, the ETH Zürich and the Institute of Physics, Prague. This year we had two second-generation participants: PhD students whose supervisors were PhD participants themselves at one of our first schools.

The central goal of the School is to equip each participant with enough knowledge of the theory and practice of X-ray diffraction and single-crystal small-molecule structure determination so that they can competently determine their own structures when they return to their home laboratory. With this in mind, the practical sessions and example structures are designed to allow the participants to see behind the button-pushing, to learn about the actual procedures going on when various operations are performed, and to interpret whether or not the results obtained are appropriate. We used the *Olex2* software this year and found it to be didactically suitable in the School environment, readily understood by the participants and replete with a wide range of functionality and options.

The daily schedule alternated lecture blocks and practical work so that the participants could readily associate the theory with the practical aspects. The practical work included access to five diffractometers at the UZH and ETH Zürich campuses and a fully equipped computer classroom. The

participants worked on two real-case example data sets, with which they learned to use the software and to recognise and resolve unexpected difficulties with structures. Each participant then determined the structure of the compound they had provided crystals of in the lead-up to the School. The 'bring your own crystal' concept is highly motivating because the participants work on the structure of a compound of specific interest to them. All these structures were completed successfully. On the final day, each participant gave a ten minute presentation on their own structure. Everyone sat a two-hour written exam, either to obtain ECTS credit points or to self-test their knowledge. Each day concluded with a short discussion where participants could express their feelings about their experience that day. The breaks offered relaxation in the pleasant environment of the university campus. Interesting discussions with the tutors often continued over the evening meal and beyond.

The half-day excursion was to the Swiss Light Source and SINQ neutron spallation facility of the Paul Scherrer Institute. The participants are always very impressed when they see the immensity of the facilities. This year, we were able to collect data live and astonishingly quickly from one of the participant's samples at one of the SLS PX beamlines.

The questionnaire filled in by the participants provided very positive feedback about the quality of the School, the friendliness and approachability of the tutors, and the organisation and the venue. Participants often say they would like a longer less intense school so they can digest the content better and wish to work on additional structures. Unfortunately, this is not really feasible given the accommodation costs and the availability of the tutors, who generously donate two weeks from their hectic schedules, and to whom we are most grateful. Each participant received a certificate and a copy of 'Crystal Structure Refinement, A Crystallographer's Guide to *SHELXL*' by Peter Müller, kindly donated by the IUCr and OUP. The personal impressions of one of the participants are given below. Our next School is scheduled for June, 2017.

We are very grateful for the generosity of the sponsors and supporters: Dept. of Chemistry of the U. of Zürich, Swiss Society of Crystallography, Cambridge Crystallographic Data Centre, European Crystallographic Association, IUCr, Oxford University Press, Rigaku Corp., Dectris Ltd, Bruker AXS, Oxford Cryosystems, Paul Scherrer Institute, Hotel Coronado, Zürich, the Chemistry Platform of the Swiss Academy of Sciences, MiTeGen, and the Contact Group for Research Matters (BASF, Novartis, Roche, Syngenta).

Tony Linden and Hans-Beat Bürgi, School Directors

The Zürich School of Crystallography 2015 - Report from a participant

Given the fact that several Croatian crystallographers attended the ZSC in past years, it has a somewhat famous status among the Croatian crystallographic community. When applying for the school I had no doubt in my mind that it will be an intense course, maybe even exhausting at times, but definitely worthwhile. All of my expectations were met.

So far I have been preparing crystals and using solved crystal structures in my work, but it was always someone else doing the measurement and solving the structure for me. Due to its complexity, single-crystal analysis never seemed to be an easy-to-master technique and even though one could use the software just by clicking the buttons and not worrying about what is all there in the black box behind, it is still not trivial and, personally, this was the only technique I always felt intimidated by. Having completed the ZSC course, I now feel confident about performing the analysis myself and I am sure I will be able to recognize and even solve problems I find on the way.

The course was a well-organized mix of lectures and tutorials given by the ten tutors, all of whom were very helpful, friendly and always ready to answer any of the student's questions. At the end of each day we had a half-hour student session where students gave their feedback on the day and could ask for

repetitions or program modifications. Practical sessions involved learning how to measure, solve and refine crystal structures. I found the lectures and practical sessions to be well balanced. Also, since students came from many different fields of chemical research and had different uses for solving crystal structures, I found it was very useful for all to learn through solving not only prepared example structures, but also their own structures of pre-sent crystalline compounds.

The course also included a visit to the Paul Scherrer Institute and the Swiss Light Source with a demonstration of a single-crystal measurement on one of our own crystals, which allowed us to see up-close how it all works. Impressively, the measurement took only six minutes.

Apart from the lectures, the social component of the school was just wonderful. Students and tutors socialized at every breakfast, lunch break and dinner. There was also a barbecue which was a lot of fun and a great dinner party at a Chinese restaurant at the very end of the course. I thought it was wonderful to have so many different people from all around the world getting along so well and enjoying their time together.

To conclude, I think the ZSC is definitely worthwhile. In one of his review papers, Peter Müller wrote that a crystallographer's training is similar to that of a Jedi knight, where practical knowledge passes down from the master's mouth to the apprentice's ear and is not something easily learned from a textbook. I believe that the ZSC, with its intensity and two students per tutor ratio, definitely provided the students with the most important tricks of the trade. All students need to do now is to solve structures and gain their own experience.

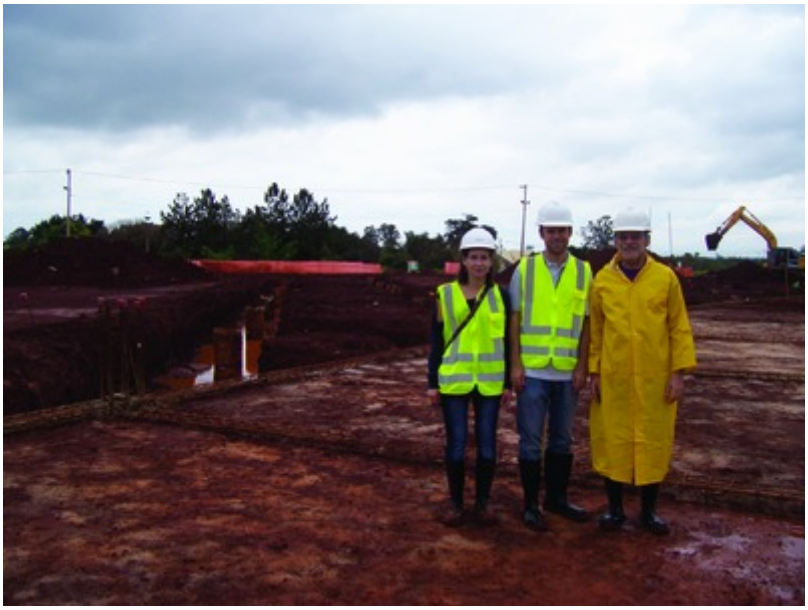
I really enjoyed the ZSC and I will make sure to recommend it to anyone in need of crystallographic knowledge.

Marina Ratkaj, PLIVA Croatia Ltd, Zagreb, Croatia

MEETING REPORT

IUCr High-Pressure Workshop 2015 in Brazil

Campinas, Brazil, September, 2015



SIRIUS storage ring and the nano-focus beam line under construction visited by A. Olejniczak, N. Souza-Neto and A. Katrusiak.



Participants of the IUCr HP Workshop in Campinas, 2015, gathered before the LNLS hall.

The 14th Workshop of the IUCr Commission on High Pressure was held 12-15 September, 2015, at the Brazilian Synchrotron Light Laboratory (LNLS) in Campinas. 75 participants from 14 countries attended. The workshop was focused on recent advances in high-pressure techniques and research at synchrotron, neutron and laboratory-based facilities. Lectures covered structural phase transitions and their kinetics, new materials synthesis, earth and planetary science, soft and biological matter, physical and chemical properties, and theory and computation. The lecturers included K. Dziubek (Deposition of data), M. Zaworotko (High-pressure application of porous metal-organic materials), L. Miyagi (Synchrotron radial diffraction studies in the diamond anvil cell), S. Hunt (Apparatus for controlled strain-rate deformation), H. Marquardt (Elasticity measurements of FIB-prepared single crystals by Brillouin spectroscopy and X-ray diffraction), J. Haines (Guest insertion and polymerization in zeolites), N. Brooks (Probing membrane

structure and dynamics), D. Paliwoda (A new phase of ferrocene), R. Wentzcovitch (Spin-crossover systems in the deep mantle), K.-M. Ho (Crystal structure predictions using adaptive genetic algorithm and motif search methods), K. Umemoto (Volume isotope effects in ice,) V. Solozhenko (Boron-phosphorus system), A. Cairns (Designing next-generation negative compressibility materials), S. Deemyard (Lithium isotopes at low temperature), M. Pravica (Novel fluorine chemistry under extreme conditions using hard X-ray photochemistry), M. Probert (Routes to more polymorphs and phase changes), R. Miletich (Mechanisms and pathways of pressure-driven structural transitions), Y. Le Godec (Synchrotron portable large-volume high-P/T/stress/tomography cell for extreme chemistry), S. Redfern (New challenges for mineral physics of the deep earth), R. Conceicao (Clay minerals, volatiles transport to the mantle and internal heating of the Earth), J. A. Lima Jr (Crystalline amino acids), J. Smith (Fast compression/decompression of materials in diamond anvil cells), R. Bini (Pressure-induced reactivity in molecular crystals: complementary structural and spectroscopic experiments), Ch. Murli (Hydrogen-bonded organic molecular solids), A. Gomes (Resonance high-pressure Raman spectroscopy in nanocarbon materials), G. Finkelstein (Magnesiow□stite using single-crystal synchrotron methods), M. Marcondes (Hybrid experimental/theoretical thermodynamics and thermoelasticity of materials) and O. Kurakevych (New silicon and carbon materials by in situ high pressure synthesis).

Best poster awards went to Z. Konopkova (Time-resolved studies using X-ray diffraction at synchrotrons) and Marcelo Nobrega (High-pressure study and oligomerization of 2-aminoterephthalate/Ni-Al layered double hydroxide composites).

The workshop was held after the 1st Latin American Crystallographic Association (LACA) Meeting in S□ão Paulo, promoted by the LACA jointly with the 22nd Sociedade Brasileira de Cristalografia (SBC Meeting), and before the 25th RAU (LNLS Annual Users Meeting), promoted by LNLS.

The workshop was sponsored by Agilent Technologies, Quantum Design, MCI | Princeton Instruments, Dectris, Almax-EasyLab and Huber, with support from the IUCr and Brazilian funding agencies FAPESP and CAPES.

High-pressure studies in Campinas will be enhanced with an ultra-low emittance synchrotron source (SIRIUS), currently under construction.

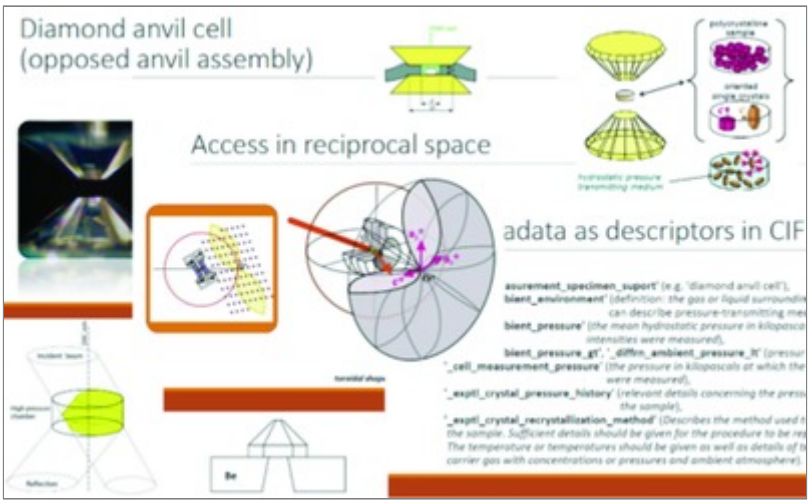
The next IUCr HP Workshop will be held in Seoul, 20-23 September, 2016, at Yonsei U., with the Organizing Committee chaired by Y. Lee.

N. Souza-Neto, Chair of the Organizing Committee, and A.J. Katrusiak, Chair of the IUCr HP Commission and Program Committee

MEETING REPORT

Metadata for raw data from X-ray diffraction and other structural techniques

Rovinj, Croatia, August 2015
www.iucr.org/resources/data/dddwg/rovinj-workshop



Montage of slides from Kamil Dziubek's presentation (illustrations courtesy of Ronald Miletich-Pawliczek, U. Vienna).

> *'Thank you for organizing such an inspiring workshop on what was nominally a rather dry subject.' Andreas Förster, Dectris*

Indeed, the term 'metadata' - often described as 'data about data' or 'information to help you understand the data' - is generally held to be a dry topic, of importance to digital librarians and data analysts, but irrelevant or even an obstacle to the real business of science. This two-day satellite workshop of the 2015 European Crystallography Meeting demonstrated emphatically that this is far from the truth. Some 20 expert speakers from Europe, Australia and the USA (two presenting remotely over the Internet) surveyed the central importance of detailed and high-quality metadata to the interpretation, validation and use of experimental data.

The workshop was organized by the IUCr Diffraction Data Deposition Working Group (DDDWG) in association with the Croatian Association of Crystallographers. J. Helliwell, Chair of the DDDWG, explained how it had been working over the past four years to analyse the prospects for routine deposition of raw experimental data, and had become aware that storage capacity for the vast amounts of raw data being generated at modern synchrotron and neutron facilities is almost the least of our worries. For these data to be re-used, it is essential that all details of the experimental arrangement are documented and retrievable - this is where 'metadata' comes into play.

L. Kroon-Batenburg and W. Minor, among others, highlighted the very low level of standardisation in storing basic information about orientation, exposure, oscillation axis *etc.* in the header of each image. The workshop renewed calls for agreement on a minimum set of such metadata that should be recorded in every image. H Bernstein and A. Förster illustrated how the necessary definitions already existed in the imgCIF dictionary, and could effectively be carried over to the HDF5/NeXus files that are becoming the norm in high-volume imaging.

J. Hester and B. McMahon, both active in the Committee to maintain the IUCr CIF data exchange standard (COMCIFS), discussed the importance of identifying *concepts* that needed to be recorded, and the relative lack of importance of the chosen storage format. While multiple formats do in practice hinder interoperability, there is no fundamental barrier to creating concordances and translation tools to build seamless data management systems in which crystallography is but one of many contributing disciplines.

Current and evolving practice in data capture and management was described across a range of large-scale facilities accommodating a variety of techniques and sciences: the European Synchrotron ESRF (A. Götz, G. Leonard), the Inst. Laue-Langevin (M. Blakeley), and the UK STFC and Diamond Light Source at the Rutherford Laboratories (B. Matthews and P. Aller). S. Coles spoke about the challenges of data management in home laboratories and medium-scale service providers such as the UK National Crystallography Service. In all these locations, all the data from an experiment must be handled in the context of resource management, provenance, validation and bulk storage, all of which require ever greater volumes of metadata that should conform to widely accepted standards.



Workshop participants enjoying a coffee break.

The importance to databases of carrying extensive metadata throughout the scientific process was described by S. Ward (CCDC) and J. Westbrook (PDB), while T. Terwilliger developed the theme of 'The Living PDB', where deposited structures could be revised, improved and continuously updated in the light of new scientific developments. M. Wall emphasised that exciting new science potentially lay in the diffuse scattering in the images that is largely ignored when deriving structures solely from the Bragg peaks. K. Dziubek outlined the additional metadata that were needed to perform a complete analysis of structures collected under high pressure and other non-ambient conditions.

In an intriguing presentation, N. Johnson demonstrated that plausible diffraction images could be manufactured. In principle, such artificial images could be produced to support fraudulent experimental results. Here, again, rich metadata describing the full provenance of the images and the context in which they were collected could help in forensic analysis of suspect data. Indeed, quite apart from worries about fraud, the more metadata that are available for cross-comparison, the more the data can be analysed (or reanalysed) for consistency, and the more trust can be placed in the scientific deductions that use the data.

The same considerations had encouraged the development by the IUCr of *checkCIF* as a validation tool in the publication of crystal and molecular structures. There was a strong feeling in this workshop that the time was rapidly approaching for the crystallographic community to work on a similar 'checkCIF'

mechanism for the validation and evaluation of experimental data - perhaps a topic for the next DDDWG Workshop?

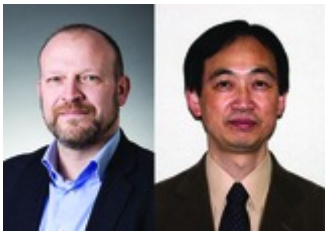
Perhaps most noteworthy is that the work of the DDDWG has become so much more urgent as raw data sets become increasingly available in the scientific environment. When this workshop was first planned, rather few images were being stored on publicly-accessible platforms. Now, one may find raw data sets in repositories such as Australia's Store.Synchrotron, on the NIH BD2K website www.proteindiffraction.org/ run by W. Minor's group, on the shared resource site Zenodo, and in the powder pattern database maintained by the International Centre for Diffraction Data. Whether this growth will turn into a deluge of diffraction data sets is still unclear; what is certain is that the best use of such data sets will depend on metadata developments such as those explored during those two sunny days in Rovinj.

Videos of all the presentations are available at the Workshop website http://tinyurl.com/diffraction-metadata. We are grateful to all our speakers for their outstanding presentations and contributions to the discussion, to the Croatian Association of Crystallographers for hosting the event, and to the IUCr and industrial sponsors for providing the necessary funding.

Brian McMahon and John R. Helliwell

AWARDS AND PRIZES

Gregori Aminoff Prize 2016



Poul Nissen (left) and Chikashi Toyoshima (right). Photos courtesy of The Royal Swedish Academy of Sciences.

The Royal Swedish Academy of Sciences has awarded the Gregori Aminoff Prize in crystallography 2016 to Poul Nissen, Aarhus U., Denmark, and Chikashi Toyoshima, U. of Tokyo, Japan. 'The prize winners have developed new technology to crystallize and determine the structure of membrane proteins in their natural environment. The major breakthrough is that these studies have broadened our understanding of the mechanism that transports ions through cell membranes, as well as the structural states that occur in this very complex system. Determination of the structure of membrane proteins has played a very important role in the development of modern medicine.' The prize includes 100.000SEK.

Paul Nissen, born in 1967, obtained his PhD at Aarhus U. in 1997 followed by a postdoctoral period at Yale U. In 2000 he returned to Aarhus U. where he is now Professor of Protein Biochemistry, as well as Director of the Danish Research Inst. of Translational Neuroscience and the PUMPkin Centre.

Chikashi Toyoshima, born in 1954, obtained his DSc degree in 1983 from U. of Tokyo, Japan. After a postdoctoral period at Stanford U., USA, and U. of Cambridge, UK, he returned in 1989 to Japan and is now Professor of Protein Biochemistry and Director of the Center for Bioinformatics at U. of Tokyo.

Professors Toyoshima and Nissen have determined crystal structures of several key members of the P-type ATPase family and established structures of essential intermediates in their ion transport cycles, information which has led to the detailed description of molecular mechanisms of these important ion translocation systems.

The P-type ATPases constitute a major family of membrane ion pumps found in all kingdoms of life. They catalyse the chemical-driven translocation of a range of different cations over biological membranes, including Ca^{2+}, K^{+}, Na^{+} and H^{+}, as well as several transition and post-transition metals. The ion concentration gradients generated by P-type ATPases across biological membranes provide driving forces for many other biological processes, but also play prominent roles in cell signaling and regulation.

P-type ATPases are large multi-domain integral membrane proteins that undergo distinct conformational changes along the ion transport cycle and are therefore particularly challenging for crystallographic work. Toyoshima solved the first crystal structure of a P-type ATPase in 2000, the structure of the Ca^{+2}-ATPase SERCA. To accomplish this he developed novel crystallization techniques allowing three-dimensional protein crystals to be grown within a phospholipid environment. He subsequently determined the SERCA Ca^{+2}-ATPase structure in several trapped conformational states of the transport cycle. This work provided the initial description of the structural basis for ion transport by a P-type ATPase.

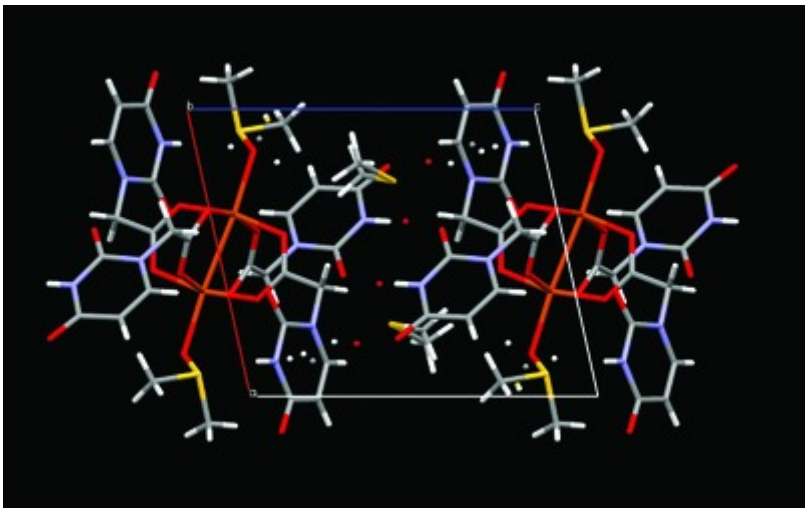
Nissen has also studied trapped conformational states of SERCA but in addition determined structures of P-type ATPases of other subfamilies including the Na^{+}/K^{+}, H^{+}, and most recently copper and zinc P1B-type ATPases. His work also includes the development of novel strategies for trapping and crystallizing intermediates in the ion transport cycle of P-type ATPases. The independent and largely complementary work of these two scientists has led to fascinating insights into these molecular machines; the structural basis for the dramatic structural changes seen between different intermediates of the ion transport

cycle; the sophisticated fine tuning of ion binding and release; the establishment of selectivity for specific ions; the dynamic formation of ion excite and entrance channels; and the molecular basis for how chemical energy from ATP is utilized to drive the structural transformations

NOTICE

The CCDC celebrates the 800,000th structure in the Cambridge Structural Database

Essential resource for scientists worldwide hits another record



The 800,000th structure. This particular structure is a di-copper paddle wheel with four bridging uracil-1-methylcarboxylate ligands and two dimethyl sulfoxide molecules occupying the apical positions. These dimeric entities are able to involve the entire uracil residue in base-pairing interactions to provide supramolecular sheets. Di-copper paddles have been used since ancient times as pigments and fungicides and are today used in organic syntheses as catalysts or oxidizing agents. A simpler copper paddle wheel structure, namely copper acetate monohydrate, was critical in the development of modern theories for antiferromagnetic coupling. Uracil is one of the four nucleobases in the nucleic acid of RNA and it was originally discovered by Alberto Ascoli in 1900. View online at http://dx.doi.org/10.5517/cc1jj92f. Ref: Khaled Hassanein, Oscar Castillo, Carlos J. G□ómez-Garcí□a, F□élix Zamora, Pilar Amo-Ochoa, *Crystal Growth and Design*, 2015, DOI: 10.1021/acs.cgd.5b01110.

The Cambridge Crystallographic Data Centre (CCDC) announces that the Cambridge Structural Database (CSD) has passed the milestone of 800,000 expert-curated experimental crystal structures with the addition of a novel metal-organic paddle-wheel structure from researchers in Spain.

The CSD is the world's only comprehensive and up-to-date knowledge base of crystal structure data. It is an essential resource used every day by scientists worldwide for drug discovery, materials science, formulations studies, and structural chemistry research and education.

The CSD's 800,000th entry is a metal organic copper structure (CSD refcode: TUWMOP), published by K. Hassanein, O. Castillo, C. J. G□ómez-Garcí□a, F. Zamora and P. Amo-Ochoa in Crystal Growth and Design. Knowledge of this structure, coupled with the wealth of structures in the CSD, will inform the design of new materials, and will be used to predict new crystal structures and validate X-ray data.

Pilar Amo-Ochoa, from the Inst. de Ciencia Molecular (ICMol), Spain, said, 'We are delighted that our structure, tetrakis[μ-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)acetato]-bis(dimethyl sulfoxide)-dicopper(II) dimethyl sulfoxide solvate, is the 800,000th entry in the database. We use the CSD in order to know the number of structures containing paddle-wheel type copper(II) units with ligands of biological

interest. Being able to have access to and share the very latest novel metal-organic structures with the world is fundamental to our understanding of these frameworks and complexes.'

'The remarkable growth of the CSD is testament to the ongoing commitment of the crystallographic community to share their results to benefit scientists everywhere,' commented Colin Groom, Executive Director of the CCDC. 'Fifty years on from the first crystal structure collection, we are reaping the benefit of this unique data resource by learning more and more about the wonderful interplay between molecular conformation and molecular interactions.'

Robin Rogers, Editor, *Crystal Growth and Design*, added, 'I have always been a big fan of the power of the CSD and what it brings to the scientific community, and indeed was very pleased when my own structure was celebrated in 1999 as the 200,000th structure in the CSD. One of my primary goals in founding *Crystal Growth and Design* with the ACS has been to forge strong collaborations with the CCDC. I am delighted that one of our papers contains the CSD's 800,000th entry and I will continue to work for seamless cooperation between our authors, reviewers and readers and the invaluable services provided by the CCDC.'

The Manager of the CCS, Suzanna Ward, commented, 'It is exciting that the 800,000th entry has been shared through the CSD so soon after we hit 3/4 million entries. This demonstrates both the sheer number of crystal structures published annually in scientific articles as well as the growth in otherwise unpublished structures being shared through the CSD as Private Communications.'