

# INTERNATIONAL UNION OF Crystallography

NEWSLETTER

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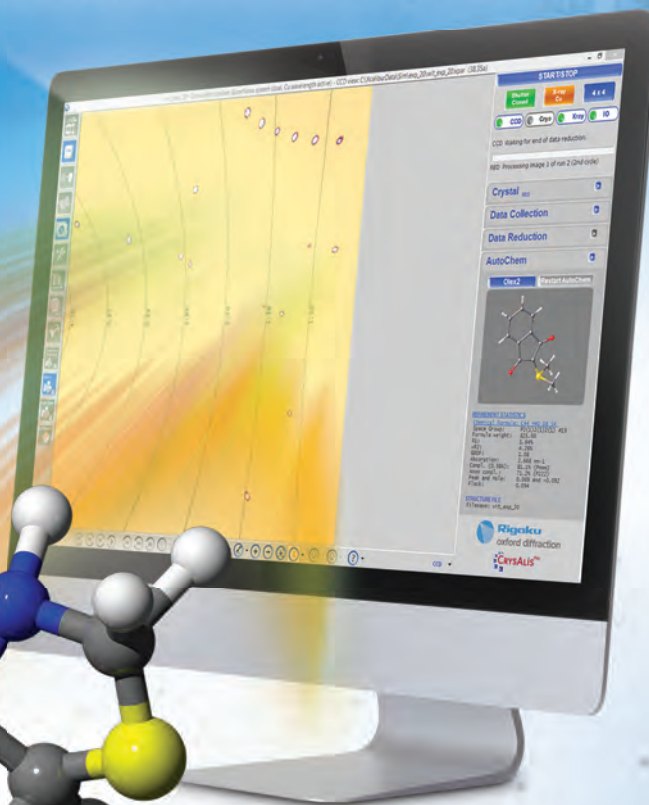
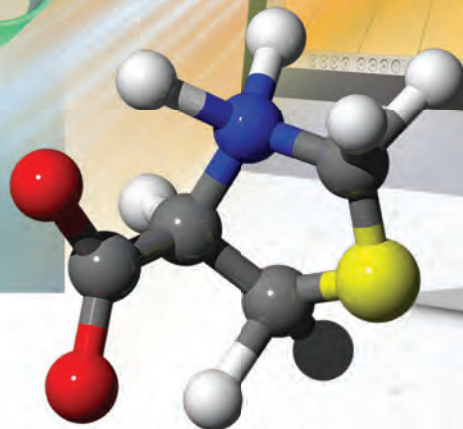
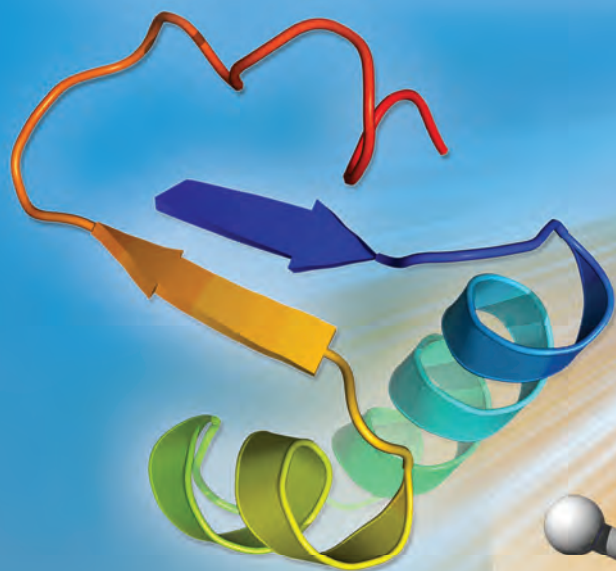


## Meeting of the Brazilian Crystallographic Association and Latin American Crystallographic Association



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## TABLE OF CONTENTS

LETTER FROM THE PRESIDENT.....	1
IUCr JOURNALS.....	3
IYCr LEGACY.....	5
IUCr2017.....	10
CRYSTALLOGRAPHIC MEETING REPORTS.....	12
AWARDS, NEWS AND NOTICES.....	22
MILESTONES.....	23
BOOK REVIEWS.....	24
INDEX TO ADVERTISERS.....	2
CRYSTALLOGRAPHIC MEETINGS CALENDAR.....	24

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**On the Cover:** Images from the XXII Meeting of the Brazilian Crystallographic Association (ABCr) and First Regional Meeting of the Latin American Crystallographic Association (LACA). See article on pages 17–18.

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Marvin L. Hackert

Summer is rapidly approaching and soon many of us in academics in the northern hemisphere will be enjoying a rather more relaxed schedule and the opportunity to see colleagues we often only see once or twice a year when we attend scientific conferences. The focus of this column is going to be a bit different in that I want to comment on some of the behind-the-scenes efforts that take place to support crystallography and crystallographers, which many of us are not even aware are happening.

The Finance Committee (FC) monitors the financial health of the IUCr and makes recommendations to the Executive Committee (EC) of the IUCr for action. The FC met March 21–22 in Leuven. Many good things are happening in our community, but the financial challenges we face are significant. Many improvements have been made to our journals, new editors have stepped up to serve, reviews are happening faster, Open Access use continues to grow, new tools have been developed, the IUCr Journals website has been updated, etc., but subscription revenue is down. The reality is that there is not a direct correlation between the number and quality of pages we publish in our IUCr journals and our subscription revenue, which is more dependent on what is happening in the publishing industry and library subscription budgets in general.

In many ways, we are victims of our own success. The IUCr EC made the decision to launch several new initiatives in conjunction with IYCr2014 and fund those activities by spending down some of our reserves. IYCr2014 was a tremendous success by many measures, but in particular in the increase in public awareness and in the areas of education and outreach. The IUCr organized just over a dozen OpenLabs during 2014. These have been very successful and have helped train many future crystallographers all over the world. The programme is so successful, that we have organized almost that many again since 2014 (reports from two appear on pages 5 and 7 in this issue). The number of scientific meetings with a crystallographic focus is also up. With the addition of LACA we now have four Regional Associates, and great progress continues to be made in Africa. A recent check of the IUCr website lists no fewer than 18 meetings that have been granted IUCr sponsorship in the latest batch considered, making a total of 39 supported meetings in 2016.

Of course, it takes funding to continue to support all these good activities in our community. With subscription revenue down, the FC is reviewing a number of options to recommend to the EC to increase revenue and better our world-wide crystallographic community. Last year the FC recommended that the EC consider the establishment of an IUCr Associates Programme. It was felt that a voluntary IUCr Associates Programme with a modest dues structure would help accomplish the dual goals of promoting a sense of professionalism to better serve our community and supporting worthy activities. Key aspects of the Associates proposal are that it would be voluntary, would help promote our profession, and could provide tangible benefits, all with a modest dues structure. All the National Committees for Crystallography were consulted about the plan to get their feedback and input. The results were overwhelmingly positive, but several valid concerns were raised which were reviewed by the FC in March. The proposal has been modified with the benefits more clearly defined and has been forwarded to the EC for their consideration.

I would be remiss if I did not mention that this FC meeting turned out to be far more adventurous than one would normally expect for a meeting focused on budgets. On the morning of March 22<sup>nd</sup>, we learned of the two bombs that killed several people at the nearby Zaventem airport near Brussels and another explosion that killed over 20 people at the Maelbeek metro station. While we all had one eye on work and we did finish IUCr business, the other eye was tracking the news.

*continued on Page 2*

With the airport closed, all trains around Brussels shut down, and hotel rooms and rental cars rapidly in short supply, many of us were pondering how and when they were going to get home – even wondering if we would have a place to stay that evening. Three of us (S.N. Rao, Mike Glazer and myself) decided to try and get east of Brussels where local trains were still running. From there we would catch a train to Lille and hopefully catch a Eurostar out of Paris *en route* to London. Taxis and rental cars were in short supply, but our good friend and General Secretary/Treasurer of the IUCr Luc Van Meervelt offered to drive us to Kortrijk to catch a train. That worked, we made it to Lille, and got a seat on the Eurostar to London later that evening. As an example of turning lemons into lemonade, we were seated with a young classics major and for most of the trip to London she was a very receptive audience learning all about crystallography and how it has benefited society.



A relieved Marv Hackert, S.N. Rao and Mike Glazer in Lille knowing they had seats on the Eurostar to London.

ICSU (International Council for Science) is another organization of importance to the IUCr. ICSU was founded in 1931 as a non-governmental organization whose mission is to strengthen international science for the benefit of society. ICSU seeks to break the barriers of specialization by promoting and supporting international interdisciplinary programmes of common concern to all scientists. The IUCr is a scientific union and was formally admitted to ICSU in 1947. The principal source of ICSU's finances is the contributions it receives from its members along with grants and contracts from UN bodies, foundations and agencies. The IUCr was successful in obtaining an ICSU grant for 30K euros to support our initiatives in Africa. ICSU also has triennial meetings with their next General Assembly taking place in Taipei in October 2017.

The Adhering Bodies of the IUCr are the National Academies or National Crystallographic Societies. This is important because this is how a country's representation within the IUCr is determined and this varies from country to country. In the USA, the US National Committee for Crystallography (USNC/Cr) represents US crystallographers in the IUCr through the National Academy of Sciences with support and oversight by BISO (Board on International Scientific Organizations). Indeed, the USNC/Cr is one of about 18 National Committees supported by BISO, which strives to strengthen US participation in international scientific cooperation. I recently returned from a meeting of BISO where I learned that many of our goals for the IUCr (support for interdisciplinary research, capacity building, etc.) and struggles (funding, communication, diversity representation, etc.) are shared by many other international unions. I will

be sharing some of the ideas I learned with the EC when we next meet face-to-face in Denver in July.

This spring a very successful "International School on Crystallography for Space Sciences" was held April 17–29 in Puebla, Mexico (see article on Pages 17–18). The school was organized by Maria Eugenia Mendoza (Puebla), Juanma Garcia-Ruiz (Granada, Spain), Mariano Mendez (COSPAR), Gueliermo Tenorio (INAOE, Mexico) and Hanna Dabkowska (IUCr EC). The school was co-sponsored by IUCr and COSPAR and attended by about 30 students, mostly from Latin-America, but also from North-America and Europe. The IUCr EC was also represented by Wulf Depmeier. The group of lecturers was truly international and they taught and discussed items spanning the full range from crystallization, methods of crystal characterization, mineralogy/crystallography of remote places on Earth, such as the Popocatepetl volcano, and real space objects such as Moon, Mars, comets, or asteroids. Follow-up events will be organized around the world.

I do hope that many of you will be able to attend one or more of our four Regional Associate Meetings: ACA (Denver, CO, USA, July 22–26); ECA (Basel, Switzerland, August 28–September 1); LACA (Merida, Mexico, October 23–27); and AsCA (Hanoi, Vietnam, December 4–7). You can find information on IUCr XXIV in Hyderabad in 2017 on pages 10–11, we will hear a lot more about the plans at the next EC meeting. I have mentioned this frequently, but I cannot emphasize too much how important it is for the future health of our organization that we recognize the need for diverse representation in all phases of the IUCr – that starts with the nomination of delegates, nominations for officers and Commission members to be voted on in Hyderabad.

A reminder, that the IUCr is inviting nominations for the Ewald Prize for outstanding contributions to the science of crystallography. The Prize is presented once every three years during the IUCr Congress. Davide Viterbo is the chair of the Selection Committee. Nominations may be submitted electronically until the end of August. The Nomination Form and the names of the Selection Committee can be obtained from [www.iucr.org/iucr/ewald-prize](http://www.iucr.org/iucr/ewald-prize).

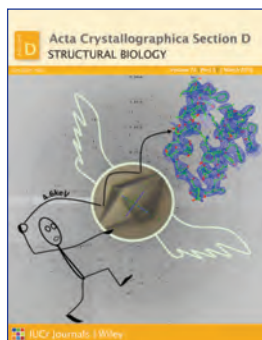
Thank you for your continued support of our collective mission to support and advance crystallography around the world. As always, my heartfelt thanks to the many of you who do so much for the IUCr. Please do not hesitate to contact me or any member of the EC with your concerns, comments or suggestions for how the IUCr can work more effectively to serve you.

MARVIN L. HACKERT ([m.hackert@austin.utexas.edu](mailto:m.hackert@austin.utexas.edu))

## INDEX TO ADVERTISERS

ANTON PAAR GMBH <a href="http://www.anton-paar.com">www.anton-paar.com</a> .....	C3
BRUKER AXS <a href="http://www.bruker-axs.com">www.bruker-axs.com</a> .....	C4
DECTRIS <a href="http://www.dectris.com">www.dectris.com</a> .....	6
HUBER DIFFRAKTIONSTECHNIK GMBH & Co. KG <a href="http://www.xhuber.com">www.xhuber.com</a>	4
MOLECULAR DIMENSIONS LTD <a href="http://www.moleculardimensions.com">www.moleculardimensions.com</a> .....	15
OXFORD CRYOSYSTEMS <a href="http://www.OxfordCryosystems.co.uk">www.OxfordCryosystems.co.uk</a> .....	23
RIGAKU <a href="http://www.rigaku.com">www.rigaku.com</a> .....	C2
STOE + CIE GMBH <a href="http://www.stoe.com">www.stoe.com</a> .....	13

## Advances in experimental phasing



The proceedings of the 2015 CCP4 Study Weekend on Advances in Experimental Phasing, held on January 8–9, 2015 at the U. of Nottingham, UK, have been published in the March 2016 issue of *Acta Crystallographica Section D, Structural Biology*.

Crystallographic phasing using experimental approaches remains an important, and often the only successful, route for solving crystal structures, especially for structures with novel folds. These are often large and complex assemblies diffracting to limited resolution, but also those likely to provide

the most novel biological insights. Speakers from academia and several synchrotron facilities were invited to cover both practical aspects, such as sample preparation and data collection strategies, and computational aspects, relating to the analysis and use of diffraction data from derivatized or anomalously scattering crystals. A session on radiation damage was included to remind experimentalists of the unavoidable side effects of using X-rays for diffraction data collection, while a final session on evolving methods provided a forum for ideas for (perhaps) solving the phase problem employing unconventional approaches.

The Guest Editors, Charles Ballard, Airlie McCoy and Thomas Schneider, hope that the speakers' papers will inspire young and seasoned crystallographers alike. The issue is open access at <http://journals.iucr.org/d/issues/2016/03/00/>. ♦

## Making a difference

BY JONATHAN AGBENYEGA, IUCR BUSINESS DEVELOPMENT MANAGER (JA@IUCR.ORG)



In April 2016, the IUCr's publishing partner John Wiley & Sons hosted its annual Executive Seminar for a number of their society partners looking at the changing landscape of our scholarly communication ecosystem. The one-day event took place at the impressive London, UK offices of the Royal Society of Chemistry at Burlington House.

This year's seminar was built around the theme of *Making a difference*. Wiley chose this theme in part because of the number of society partners telling them that one of the greatest challenges of running a successful publishing programme is measuring impact. Many partners have asked questions like "How can we demonstrate the impact that scientific and scholarly research has on government policy?" and "What does the Open Research movement mean for our journals?"

To answer these questions, Wiley put together a diverse panel of experts: thought leaders in research communications and experts in public engagement with science and policy, who offered insight and practical strategies to help us improve our voice in the decisions that affect how research is funded, communicated and understood.

Other areas where Wiley society partners focused discussion covered publishing impact: how we can improve and sustain the impact of the work we publish, and how we can improve downloads and usage of our papers. Interesting research shows that publishing via Gold open access can influence (in a positive way) the number of times your work is downloaded and the number of times it is read.

Marketing reach and how societies can maximise value of membership was also hotly debated, particularly how to encourage members to remain active once they have joined and how societies can then improve the service they provide to their members by understanding interests and activities.

Given the relatively small size of some of the society partners, some concerns were expressed around technology service

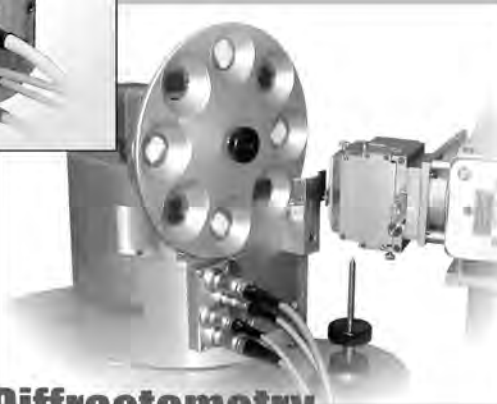
and how smaller organisations can keep up with some of the bigger players. Here Wiley representatives discussed some of the projects they are working on to help societies disseminate content more effectively, for example, apps for scientists to create their own special issues based on their individual interests. It is not only content that is king; services and other types of resource help our communities improve their research output. Wiley touched on some of these initiatives and then on ways to actually monitor the effectiveness of these activities.

The afternoon started with a fascinating and thought-provoking lecture and ensuing discussion on the importance of affecting policy from a representative at the Strategic Society Centre. The discussion took a very hands-on approach to how we should be more aware of the role we play in communicating science to politicians and policy makers. What certainly came out of the discussion was a need for scientists as a body to be more dynamic and effective in getting their point across; for example, if we don't say anything then nothing changes, and a good story can make a policy. One comment that I thought resonates with the state of crystallography teaching in our universities was, "Nature fills a vacuum, so if we spot a void that is important – fill it". We need to talk about these issues and frame them in a way in which society can make sense of it and then effect change.

One organisation called [senseaboutscience.org](http://senseaboutscience.org) is working with scientists, policy makers and the public at large to improve scientific communication, discussion and understanding. With initiatives such as #askforevidence they are empowering individuals, organisations and governments to seek out the truth about claims they have come across. For example, a recent study into the various detox remedies you can find on the shelves of supermarkets found that the best remedy is actually your liver and kidneys!

On the train heading back up to Chester that evening I had a lot to keep me occupied, from thinking about how I must take greater care of my liver and kidneys to how we can talk about science and share some of the wonderful things we are doing to change the world to a much wider part of society. ♦

# SPEED...



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## Rigaku OpenLab Cambodia 2, Phnom Penh, Cambodia, January 11–15, 2016

BY BUN KIM NGUN, LOCAL ORGANIZER AND MICHELE ZEMA, IUCr REPRESENTATIVE

The first edition of the IUCr-UNESCO Rigaku OpenLab Cambodia, organized during the International Year of Crystallography 2014, represented the first opportunity for Cambodian researchers and students to receive some exposure to crystallography. That event was hosted by the Inst. of Technology of Cambodia (ITC), where the first X-ray powder diffractometer (MiniFlex II) in the country had just been installed, thanks to a donation from Rigaku Corp. Participation in that case was limited to some undergraduate and post-graduate students from the Dept. of Geo-resources and Geotechnical Engineering of the ITC and two representatives of the private sector (one from mining and another from the cement industry). However, during the OpenLab, delegates from the Ministry of Industry, Mine and Energy of the Cambodian Government and from the UNESCO Office in Phnom Penh visited the new crystallography laboratory at ITC and appreciated the many opportunities that it could offer in terms of research projects and service to local industries. Following the OpenLab in 2014, the first graduate theses appeared, reporting on the use of X-ray powder diffraction (XRPD), and some collaborations with the cement and mining industries were initiated.

To build on this enthusiasm generated by the first edition, the IUCr and UNESCO, together with ITC and Rigaku Corp., decided to organize a new OpenLab to further disseminate and raise awareness about the importance of crystallography, and emphasize how Cambodian society would benefit from a proper crystallography education at the academic level, especially in the formation of a new class of top managers of both academic and governmental institutions, who would take part in policy-making decisions. The new OpenLab would also make use of the new X-ray fluorescence instrument installed at ITC.

The IUCr-UNESCO Rigaku OpenLab Cambodia 2 was held at ITC on January 11–15, 2016. More than 250 participants attended the Opening Section on January 11, which was hosted by OM Romny, Director General of ITC, and Anne Lemaistre, UNESCO Head of Office and Representative in Cambodia, in the presence of delegates from the Ministry of Education, Youth and Sport; the Ministry of Industry and Handicraft; and the Ministry of Environment of the Cambodian Government. Moreover, lecturers and students from public universities such as the Dept. of Chemical Engineering and Food Technology/ITC, the Dept. of Mechanical Engineering/ITC, the Dept. of Chemistry/Royal U. of Phnom Penh (RUPP), the Dept. of Biology/RUPP, the Dept. of Bioengineering/RUPP and the National Institute of Education attended the session, together with representatives from the private

sector, such as Renaissance Minerals Ltd, Kampot Cement and Cambodia Cement Chakrey Ting Factory.

The ceremony was chaired by BUN Kim Ngun, Deputy Head of the Dept. of Geo-resources and Geotechnical Engineering at ITC and Coordinator of the OpenLab Cambodia. Welcome remarks by OM Romny and Anne Lemaistre were followed by speeches by **Gautam R. Desiraju** (*Bringing people and countries together with the message of science*), Immediate Past President of the IUCr and Chair of the 24th IUCr Congress and General Assembly (Hyderabad, 2017); **Pinak Chakrabarti** (*Promoting communication and cooperation in the Asia-Pacific region: the role of the AsCA*), President of AsCA; **Ian D. Williams** (*Establishing scientific collaborations among SE Asian countries*), Hong Kong U. of Science and Technology; and **Michele Zema** (*The contribution of the IUCr to the development of scientific education, research and infrastructure*), Outreach Officer at the IUCr. **Taisuke Yoshiki**, representative of Rigaku Corp., showed the strong involvement of Rigaku in promoting education and innovation.

An open discussion on “*How can crystallography education contribute to Cambodian society through science and technology development?*” involved all participants in the afternoon of the same day. This was followed by a series of dissemination lectures: Gautam R. Desiraju told “*the story of three crystals*” (i.e. salt, sugar and diamond), Pinak Chakrabarti introduced the concepts of molecules and interactions, Ian D. Williams highlighted the complementarity of powder and single-crystal X-ray diffraction techniques, and Serena C. Tarantino, U. of Pavia, Italy, suggested a way of exploiting local resources to produce inorganic polymers as an alternative to cementitious materials for structural applications.

The Practical Section of IUCr-UNESCO Rigaku OpenLab Cambodia 2 was started on January 12. Pinak Chakrabarti opened it with a broad overview of symmetry in crystals and X-ray diffraction methods. Then, Ian D. Williams, Michele Zema and Serena C. Tarantino alternated at the teacher’s desk to give

a full course on the fundamentals of crystallography with particular emphasis on diffraction theory and the basics of XRPD. This led on to the XRPD practical session on sample preparation



Practical Section.

and data acquisition, held by Yue Bing (Rigaku Corp.) on the afternoon of January 14. On January 15, X-ray fluorescence spectrometry was introduced by Hisashi Homma (Rigaku Corp.), with lectures and tutorials on sample preparation (powder and bulk metal), data acquisition and quantitative analysis. Hands-on training was done on geological and metallurgical materials, using powder or pressed pellets as well as bulk metal samples.

At the end of the day, certificates were awarded to all participants at the closing ceremony of the OpenLab Cambodia 2 by BUN Kim Ngun. The participants were very enthusiastic about the OpenLab activity. ♦



Opening Section of IUCr-UNESCO Rigaku OpenLab Cambodia 2.

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## IUCr-UNESCO Bruker OpenLab Uruguay 2, Montevideo, Uruguay, February 23–29, 2016

BY LEOPOLDO SUESCUN, MARIO MACÍAS AND NATALIA ALVAREZ, LOCAL ORGANIZERS

The second edition of the Bruker OpenLab Uruguay, “Resolución de estructuras cristalinas por difracción de rayos X de monocristal” (<http://iycr2014.org/events/openlabs/bruker-openlab-uruguay-2>), was held in sunny Montevideo in February 2016 taking advantage of the Bruker D8 Venture diffractometer installed in 2014 at Facultad de Química, U. de la República. The event was organized by Leopoldo Suescun, Mario Macías and Natalia Alvarez from Laboratorio de Cristalografía, Química del Estado Sólido y Materiales (Cryssmat-Lab), Cátedra de Física, DETEMA and DEC Facultad de Química, and was supported by the IUCr (through the IYCr2014 Legacy Fund), Bruker, Comisión Académica de Posgrado (CAP) of U. de la República and Teclab (Bruker’s representative in Uruguay). The OpenLab brought together 44 participants (young professors, PhD, MSc and undergraduate students) from Argentina (4), Bolivia (1), Brazil (4), Chile (3), Costa Rica (2), Perú (2) and Uruguay (28) who had the chance to learn the fundamentals of crystallography and their application to single-crystal X-ray diffraction (SC-XRD). All participants had the chance to experience all the processes of SC-XRD, from crystal selection and mounting to CIF preparation, with practice samples and data. They were also provided with temporary licenses to Bruker APEX3 software and the Cambridge Structural Database (CSD) to complete their structural analysis and learn about databases. Additionally, 17 very excited participants brought single crystals and were able to select and mount them, collect their own data, and perform the structure determination and refinement of the structures with the assistance of Tutors, Lecturers and fellow participants. One structure solved and refined during the OpenLab has already been submitted to the CSD and included in a manuscript accepted by *Tetrahedron Letters* (Victoria de la Sovera *et al.*, <http://dx.doi.org/10.1016/j.tetlet.2016.04.072>).

The program included 18 hours of Lectures and 12 hours of Practical sessions on the fundamentals of crystallography, taught in Spanish by the local Lecturers Leopoldo Suescun, Álvaro W.

Mombrú and Ricardo Faccio (all from Facultad de Química) and Javier Ellena (Instituto de Física de Sao Carlos, U. de Sao Paulo, Brazil) and in English by Hamilton B. Napolitano (U. Estadual de Goiás, Brazil). Additionally, it included 3 hours of Lectures and 2 of practice on crystallization and single-crystal selection and mounting taught by Iván Brito (U. de Antofagasta, Chile) and 14 hours of Lectures and 10 hours of Practical sessions on application of single-crystal diffractometry taught by Bruce Noll (Bruker AXS, USA). Three hours of the program were also devoted to advanced applications of SC-XRD to characterization of materials taught by Serena Tarantino (U. di Pavia, Italy) and Michele Zema (U. di Pavia, Italy/IUCr). B. Noll and the Tutors Mario Macías and Natalia Alvarez devoted many hours helping the participants select and mount their crystals, performing crystal evaluation and data collection setup and guiding the data processing and structure determination process of organic, metal-organic and mineral samples. The intense program included a welcome reception hosted by Teclab and Juan Carrau Winehouse (maker of Cristalizado, the wine of the IYCr2014).



Left: Participant Sebastián Martínez (Uruguay) finishing his presentation on the structure he solved during the OpenLab. Right: Organizers and five of the six international Lecturers during the closing of the OpenLab: M. Zema (Italy/IUCr), S. Tarantino (Italy), M. Macías (Organizer), L. Suescun (Organizer), B. Noll (Bruker, USA), H. Napolitano (Lecturer, Brazil), N. Alvarez (Organizer), I. Brito (Lecturer, Chile).

Sunday morning was devoted to problem solving where all Lecturers and Tutors sat with the students to finalize their refinements and prepare their CIF files. Sunday afternoon was also busy with more than 20 participants and tutors working on their problems until the evening. The final day of the program was de-


*continued on Page 9*



Top left: Javier Ellena (Brazil) lecturing on the use of CSD search software. Top right: Participants Lorena Martínez, Alejandro Peixoto, Victoria de la Sovera, Anna Burgueño, Carlos Rojas, Jaime Franco, Florencia Luzardo and Daiana Ferreira (all Uruguay) with Prof. Ellena during the Sunday morning problem-solving session. Left: Participants Brayan Solano (Costa Rica), Carlos Rojas (Uruguay) [back], Mario Pacheco, Victoria Pereyra (Uruguay), Naviana Leiva (Bolivia) [middle], María Bardanca and Daiana Ferreira (Uruguay) follow explanations by Bruce Noll on the use of APEX3 software in the diffractometer room.



Participants of the IUCr-UNESCO Bruker OpenLab Uruguay 2.



IUCr-UNESCO **OpenLab** Rigaku OpenLab Bolivia  
La Paz, Bolivia  
September 12–16, 2016

**VENUE**

Facultad de Ciencias Puras y Naturales, Cota Cota Campus, Universidad Mayor de San Andrés, La Paz, Bolivia

**BACKGROUND**

During the General Assembly of the Latin American Crystallographic Association (LACA) meeting, formally the first meeting of LACA, which took place in São Paulo, Brazil, in September 2015, Wilma and Julián Ticona Chambi, two very enthusiastic young scientists from Universidad Mayor de San Andrés (UMSA), La Paz, Bolivia, put forward the idea of organizing a crystallography event in Bolivia, the first of its kind. This proposal was warmly received by LACA in the context of the collaborative spirit that permeates the organization and its mission to promote and expand crystallography in the region, and it was suggested to run the event under the umbrella of the very successful program of the IUCr-UNESCO OpenLab initiative. Julián had already participated in the Rigaku OpenLab Colombia, held in 2014. The idea was enthusiastically supported by the IUCr and Rigaku, who have arranged the delivery of a second powder diffractometer, in addition to the old one, already available at UMSA.

**THEME**

Although the main theme of the OpenLab will be powder diffraction, several lectures on single-crystal X-ray diffraction will be included in the program. The plan is to organize an event centered around single-crystal X-ray diffraction in 2017.

**CONFIRMED LECTURERS**

Santiago García-Granda (Spain), Graciela Díaz de Delgado (Venezuela), Miguel Delgado (Venezuela), Diego G. Lamas (Argentina), José Antonio Henao (Colombia), Rigaku technical representative (Brazil)

**LOCAL ORGANIZING COMMITTEE**

María Eugenia García (Chair), *Vice-Dean of Facultad de Ciencias Puras y Naturales, UMSA*  
Luis Morales Escobar, *Head of the Chemistry Program, UMSA*  
Giovanna Almanza Vega  
Carlos Santelices Gómez  
Saúl Cabrera Medina  
Julián Ticona Chambi  
Macquiver Pilco  
Fania Humerez  
Naviana Leiva  
Mery Laura  
Representative from Universidad Técnica de Oruro

**TECHNICAL COMMITTEE**

Oswaldo Ramos  
Mario Blanco Cazas  
Wilma Ticona Chambi

**INTERNATIONAL COMMITTEE**

Santiago García-Granda, IUCr representative (Spain)  
Michele Zema, IUCr representative (UK)  
Diego G. Lamas (Argentina)  
Miguel Delgado (Venezuela)  
Akihiko Iwata (Brazil)



Participants at an intensive two-day mini-course on the Fundamentals of Crystallography at UMSA in January 2016. A similar event will be held at UMSA on September 8–9, 2016, i.e. immediately before the OpenLab, to help students with little crystallography background.

For more information, please visit

[www.iycr2014.org/openlabs](http://www.iycr2014.org/openlabs)

## 2016 IUCr Crystal growing competition for schoolchildren

The IUCr Crystal growing competition is open to all schoolchildren and aims to introduce students to the exciting, challenging and sometimes frustrating world of growing crystals. This initiative was originally launched in 2014 as part of the celebrations for the International Year of Crystallography and has now reached its third edition.

### How to participate?

The winners will be those who most successfully convey their experiences to the panel of judges in a video report.

Each contribution should clearly show or mention the experimental work carried out by the participants during the growing of their single crystals (compounds and methods used are free of choice). Furthermore the contribution should reflect in a creative way on the experimental work and theoretical background and/or applications. It is strongly recommended to use English subtitles when applicable and to provide the name and school of the participants along with their photos at the end of the video.

Videos should be submitted at <http://www.iycr2014.org/participate/crystal-growing-competition-2016/submit-entry>.

### Important dates

- Closing date for submissions: 20 November 2016
- Notification of winners and launch of 2017 edition: 27 January 2017

### Rules

- The competition is open to students of primary or secondary schools; maximum age 18.
- Videos submitted to local competitions during 2016 may be also submitted to the IUCr competition.
- Duration of video: strictly no longer than four minutes.
- Format: mpeg, avi or mov, or hosted on a public video platform (e.g. YouTube, Vimeo)
- Language: mother language of participant or English.
- A maximum of two entries per category per school is permitted.
- The judging panel will be nominated by the IUCr. The decisions of the judging panel are final.



### Categories

- Under 11 (primary school)
- 11–15 (high school middle forms)
- 15–18 (high school upper forms)

### Prizes

The winning contributions in each category will receive 'Young crystal growers' certificates and medals.

### Criteria for evaluation

A panel of judges will evaluate the entries. The following six criteria will be used: creativity, aesthetic value, description of working plan and experimental work, clarity of explanations, scientific background, and safety.

For more information, please visit [www.iycr2014.org/participate/crystal-growing-competition-2016](http://www.iycr2014.org/participate/crystal-growing-competition-2016). ♦

## IUCr-UNESCO Bruker OpenLab Uruguay 2

*continued from page 7*

voted to presentations from 15 of the students who had solved their own problems and an exam taken by 21 participants who will receive academic credit for their participation in the OpenLab. An anonymous evaluation form was submitted for the students to give their opinions on different aspects of the OpenLab. Except for the unanimous feeling that the course was very intense, most comments were positive and some helpful remarks were given that will help organize future schools of this kind in Latin America. A detailed report of the opinions of participants given in the evaluation form can be obtained from <http://cryssmat.fq.edu.uy/OpenLab/evaluationbyparticipants2.pdf>. ♦



(l-r) Denise Espindola, Micaela Todoroff and Agustina Villalba (Escuela de Educacion Secundaria N° 2 Luis Federico Leloir, Comandante Nicanor Otamendi, Buenos Aires, Argentina) proudly show the bronze medal they won in the 2015 competition (11–15 age group). For the full results, please visit [www.iycr2014.org/participate/competition-winners/2015-winners](http://www.iycr2014.org/participate/competition-winners/2015-winners).



[www.iucr2017.org](http://www.iucr2017.org)

# 24<sup>th</sup> Congress and General Assembly of the International Union of Crystallography Hyderabad International Convention Centre 21 - 28 August 2017, Hyderabad, India



## Plenary Lectures

- **Susumu Kitagawa** - Crystallography of dynamic structures and properties of porous coordination polymers / metal - organic frameworks
- **John Spence** - Crystallography with X-ray lasers
- **Giacomo Chiari** - Crystallography in art and cultural heritage

## International Program Committee

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The next **IUCr Congress in 2017** will be a state-of-the-art international convention set in the unique ambience of India. We extend a warm welcome to crystallographers from all across the world!

The program will be cutting edge with plenaries, keynotes, microsymbiosia and posters, commercial exhibits, satellite meetings, workshops and official meetings of the IUCr. The organization and arrangements for this meeting are already well under way. The HICC is the first convention center of its kind in South Asia and compares with the best in the world in infrastructure, technology and service. It has all the floor space to conduct an IUCr Congress and is a Green Globe certified convention center. The Novotel, adjacent to HICC is a 5-star hotel and the Congress has been able to secure 200 rooms here at a most competitive rate for the convenience of registrants.

The program committee of 34 international experts has met in March 2016 and have chalked out a schedule of 3 plenaries, 39 keynote lectures and 120 microsymbiosia. The inauguration will take place on the evening of 21 August 2017 followed by seven full days of scientific sessions. The closing ceremony is on the evening of 28 August.

Workshops (half and full day) will be held on 21 August in the HICC and are free for all registered participants. Five satellite meetings are already confirmed and will take place just before or after the Congress.

This Congress will offer several new features for registered participants. These would include spot presentations by investigators and awards of ad hoc research grants, interactions between students and established crystallographers, electronic posters, electronic abstracts linked to IUCr journals and open access for all IUCr journals during the duration of the meeting, depending on budgetary factors. We will offer free registrations to scientific sessions for company representatives based on the generosity of their financial contributions. Gourmet complimentary lunches will be served to all registered participants for seven days.

The scope of the Congress is expanding towards disciplines related to crystallography and with a strong presence in the industrial sector. Hyderabad is an important pharmaceutical district in India, with more than 100 pharmaceutical industries located both within the city and its environs. We expect wide participation from these companies as well as from firms elsewhere in India and are working on a two-day registration package to facilitate their attendance. The package will be available to all participants to attend the Congress for any two consecutive days of their choice.

Hyderabad is centrally located in India with easy access via hubs in the Gulf and South East Asia. Non-stop flights from North America to Delhi ply daily. All participants will need to obtain conference visas to enter India. Please refer to our web page for details. Several hotels within easy shuttle distance of HICC will be identified as official hotels for the Congress. These hotels, which include chains like Lemon Tree, Radisson and Westin, are clean and efficiently managed. Affordable serviced apartments close to HICC and suitable for students and senior scientists are also available.

As the International Year of Crystallography 2014 sought to bring people and countries together through the message of science, we will aim for at least one participant from each of 25 countries in Asia, Africa and South and Central America, who have been previously unrepresented in IUCr Congresses. Delegates will be chosen so as to effectively spread the idea of crystallography in their respective nations. This Congress is therefore offering, in addition to all the rest, new networking opportunities amongst scientists and crystallographers from more than 80 countries. This will create immense outreach for academia and industry with emerging countries. It is also hoped to arrange satellite meetings or meetings within the Congress for regional groupings of countries, say the Indian sub-continent or South East Europe or South America. The IUCr is also playing an active role in the organization of the Congress for the first time.

The Local Organizing Committee welcomes scientists, students and representatives from companies for what is already promising to be a magnificent occasion.

**G.R. Desiraju**, *Chair (Indian Institute of Science, Bangalore)*

**R.K.R. Jetti**, *Vice Chair (Mylan Laboratories, Hyderabad)*

**J.A.R.P. Sarma**, *(Formerly from GVK Biosciences, Hyderabad)*

**K. Biradha**, *(Indian Institute of Technology, Kharagpur)*

**M. Zema**, *(International Union of Crystallography and University of Pavia)*

**C. Malla Reddy**, *(Indian Institute of Science Education and Research, Kolkata)*

**R. Banerjee**, *(CSIR-National Chemical Laboratory, Pune)*



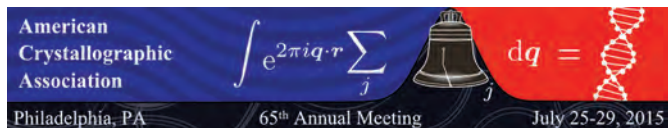
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## ACA 2015

Philadelphia, PA, July 2015  
[www.amerocrystalassn.org/](http://www.amerocrystalassn.org/)

EXERPTED FROM *REFLEXIONS*, FALL 2015

The following report is a digest of more complete reports of the 2015 ACA Meeting in Philadelphia published in the *ACA Reflexions* of Fall 2015.

The meeting began with workshops on Serial Crystallography Data Analysis, Rietveld Refinement, and Small Angle Scattering. The Opening Reception was hosted by the exhibitors on Saturday evening.

The B. Warren Award for 2015 was presented to Laurence Marks. Gregory Petsko received the M.J. Buerger Award, and Yan (Jessie) Zhang received the Margaret C. Etter Early Career Award. Juan Manuel García-Ruiz delivered a plenary lecture “The Impact of Crystals and Crystallography in Art and Culture” and screened his documentary film “The Mystery of the Giant Crystals” filmed in the Naica mine in Mexico where transparent single crystals of gypsum as long as 11 meters were discovered. Cora Lind-Kovacs and Robin Rogers chaired the Transactions Symposium, Crystallography for Sustainability.

The ACA’s annual Awards Banquet featured the Past President’s Address by Martha Teeter. The 2015 Class of ACA Fellows was introduced at the banquet by ACA President Chris Cahill. The fellows are Zbigniew Dauter, David Eisenberg, Hakon Hope, John Helliwell, Tom Koetzle, and David Rose. Cahill presented the ACA Service Award to Ilia Guzei. The ACA honored this year’s 14 Poster Award Winners.

### Warren Award

The B. Warren Award was awarded to Laurence Marks, Professor of Materials Science and Engineering at Northwestern U., for “his contributions to electron crystallography and surface science, using both electron and X-ray diffraction.” Marks and his students have used electron microscopy to examine a number of metal oxide surfaces and have developed techniques that allow exquisite structural descriptions of these systems. He provided an atlas of elegant reconstructed surfaces that have been found and structurally characterized for different lattice planes from a single material, SrTiO<sub>3</sub>, and described several order-disorder transitions.



Laurence Marks

Brian Toby

### Buerger Award



Gregory Petsko

The M.J. Buerger Award for 2015 was awarded to Gregory Petsko, Arthur J. Mahon Professor of Neurology and Neuroscience at Weill Cornell Medical College, USA. The award citation reads, “Petsko has made contributions of exceptional distinction to the study of proteins and enzyme mechanisms by X-ray crystallography, to the application of Structural Biology to

the medical sciences, to the training and education of researchers and undergraduate students, to the mentoring of a generation of Structural Biologists, and to the research community in general, through service on government and other advisory boards and committees, and through his unique communication skills to the broader scientific community and the lay public.” Petsko’s Award lecture was at times moving and inspirational as it featured the career of Tom Alber who passed away from Lou Gehrig’s disease. Tom, Greg’s first graduate student at MIT, later became professor at the U. of California, Berkeley and was a renowned crystallographic presence in his own right. Not incidentally, Greg now directs an institute dedicated to the elucidation and potential treatment of neurological diseases, one of which ultimately claimed Tom’s life. In addition to his expressed admiration for Tom, Greg’s lecture was rich with praise for the many collaborators and students who marked his research career. He reserved particular appreciation for his long-time research partner Dagmar Ringe and collaborator Ilma Schlichting. Many of the methods used today were invented in Greg’s laboratories at MIT and Brandeis U. The lecture included an extended discourse on how these approaches were employed to work out the enzymatic pathway of P450 and the importance of concepts like the glass transition temperature and the intrinsic flexibility of proteins and enzyme active sites. The methodologies initiated and developed in Greg’s laboratory have been recognized as major contributors to our understanding of enzymatic catalysis. Indeed, in enzymology today, a knowledge and detailed understanding of the underlying molecular structure as derived by X-ray crystallography is the first imperative. Greg finished his talk by suggesting that caution in interpreting cryogenic structures was certainly in order, and that it would be appropriate if all macromolecular structures deposited in the Protein Data Bank were to be accompanied by structures determined at room temperature, and suggested that this might be possible using the free electron laser source.

Alex McPherson

### Transactions Symposium: Crystallography for Sustainability

The symposium focused on crystallographic research related to reducing energy consumption, protecting the environment, or providing greener synthesis of materials. L. MacGillivray (USA) discussed the solid-state synthesis and photodimerization of resorcinol co-crystals and showed that halogens or hydrogen bonding could be exploited to produce photostable co-crystals. T. Friščić (Canada) described mechanochemical solid-state synthesis without any solvents. H. zur Loye (USA) has developed a low temperature two-step hydrothermal method to prepare hybrid materials with improved yield. A. Huq (USA) showed how powder neutron diffraction can elucidate the pathways of lithium, hydrogen or oxygen atoms in energy materials and determine site occupancies, including those responsible for ionic conductivity. The distribution of vacancies and anisotropic displacement parameters of light atoms that indicate the direction of ionic movement, can give insights into underlying mechanisms and help optimize materials. P. Kalifah (USA) described powder diffraction studies of semiconductors that catalyze solar water splitting. H. Kleinke (Canada) described studies of thermoelectric materials that convert waste heat into electricity. Advanced thermoelectrics are heavily doped, narrow-gap semiconductors with heavy elements and complex crystal structures. Holger’s group uses crystallography to correlate compositional changes with



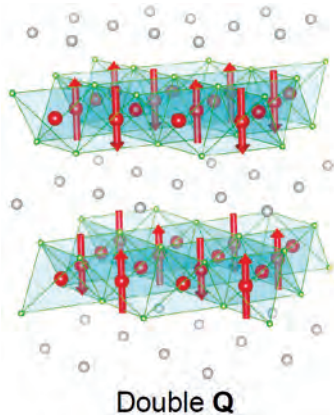
Transactions Symposium speakers (l-r): Cora Lind-Kovacs, Ashfia Huq, Holger Kleinke, Anja Mudring, Len MacGillivray, Tomislav Friščić, John Helliwell, Hans-Conrad zur Loye, and Robin Rogers.

thermoelectric properties. They have tripled the thermoelectric figure-of-merit of some materials.

*Cora Lind-Kovacs and Robin Rogers*

### 1.1.1: Crystallography of Emergent Phenomena

The session showcased crystallographic determinations of the structures of ‘complex’ materials having properties that emerge from the collective interaction of the components of the complex. K. Taddei (USA) combined X-ray and neutron powder diffraction to follow phase transitions from high to low symmetry and back in iron-based superconductors as a function of temperature and composition. The result was a complex phase diagram with two types of magnetism competing against superconductivity and each other. The two prevailing theories may explain the observed magnetism: either the physics is dominated by local-type interactions or by delocalized band-like physics. Since the latter implies wave-like states that might destructively interfere, Mössbauer spectroscopy was used as a local probe to look for ‘nodes’ where the component wavefunctions cancel one another out, so that there is no effective magnetic field. Exactly 50% of the iron sites were shown to be non-magnetic as predicted by the magnetic wave-like model. This highlighted the importance of combining careful diffraction experiments with complementary local probes.



*Jared Allred*



Crystallography of Emergent Phenomena session speakers ((l-r): Efrain Rodriguez, Jai Prakash, Jared Allred, Keith Taddei, Huibo Cao, and Hemamala Karunadasa.

### 1.1.3: Application of SANS/SAXS to Structural Biology

W. Heller (USA) reported on small-angle neutron scattering (SANS) studies of the Sinbidis Virus, Light Harvesting Complex II, Bacterial Photosystem I, and antimicrobial peptides, to illustrate how contrast variation methods using isotopic exchange and

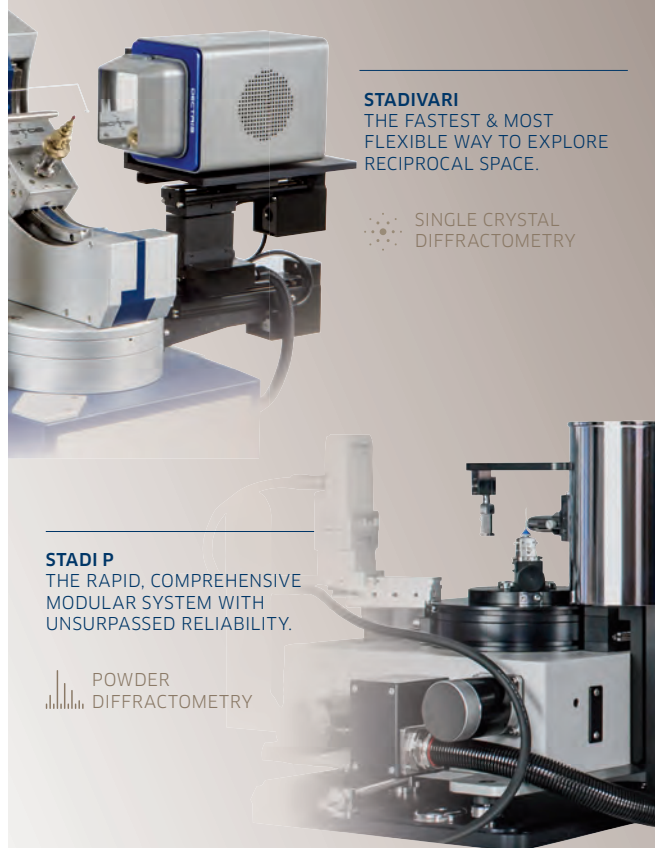


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neutron scattering experiments achieve insights not accessible by other approaches. S. Sinha (USA) presented research on the structure and function of a key component of the autophagy nucleation complex that is involved in the degradation and recycling of damaged or harmful cytoplasmic components. Combining bioinformatics, X-ray crystallography, SAXS, circular dichroism, and molecular dynamics revealed the presence of a transient structure that changes into an ordered arrangement upon binding to a partner. N. Sekulic (USA) described contrast variation studies of centromeric mononucleosomes. Centromeres, vital to the proper segregation of chromosomes, are defined by a variant histone protein called CENP-A and slightly A-T rich repetitive DNA sequences. Using analytical ultracentrifugation and SANS contrast variation, a more extended conformation of CENP-A derived nucleosomes in solution was determined relative to the canonical form. These results reveal the role of DNA in the physical basis of how the CENP-A histone distinguishes centromeres from the rest of chromatin. J. Trehwella (Australia) described studies of proteins from HIV, including HIV reverse transcriptase and matrix (MA) interacting with calmodulin. Complementary information from solution scattering, crystallography, hydrogen-exchange mass spectrometry, and fluorescence provide insights into the structure and dynamics of these proteins. A. Round (France) reported on innovations at the synchrotron SAXS beam line BM29. In situ crystallization of glucose isomerase was performed to show that crystals could be grown and transported within the droplets, allowing for the study of nucleation in different additive conditions. S. Krueger (USA) applied SANS and contrast variation to the study of disordered proteins in two-subunit complexes. Using the program SASSIE, Monte Carlo sampling of backbone dihedral angles within protein models was used to generate ensembles of energetically relevant conformations for the disordered regions of the complex, using structural models that satisfy the contrast variation data. J. Curtis (USA) gave a progress report on the CCP-SAS initiative, an NSF-funded joint UK/USA collaboration to produce a new generation of open-source software to facilitate the atomistic modeling of macromolecules using SANS/SAXS data.

*Kushol Gupta and Alvin Acerbo*



Application of SANS/SAXS to Structural Biology session speakers (l-r): Adam Round, William Heller, Jill Trehwella, Nikolina Sekulic, Joseph Curtis, Susan Krueger, and Sangita Sinha.

## 1.2.1: From Fingerprinting to Full ID: PXRD

This session was intended to bring new aspects of the use of powder diffraction to a more general audience with support from Bruker AXS, PANalytical, and Rigaku/Oxford Diffraction. A. Brunskill (USA) demonstrated the power of PXRD to characterize compounds relevant to the pharmaceutical industry. S. Bates (USA) spoke of the ability of PXRD to perform quantitative analyses on component mixtures, emphasizing the use of the chemometric method. J. Quinn (USA) discussed the use of conventional PXRD instrumentation to perform Pair Distribution Function (PDF) studies for the analysis of non-crystalline ma-

terials. PDF can provide a new method of analysis in PXRD. R. Suryanarayanan (USA) is using PXRD to understand the chemistry and effects of pressing drugs into pellets. J. Britten (Canada) provided an overview of how one can use single-crystal diffractometers and area detectors to perform PXRD experiments.

*Richard Staples*

## 1.2.2: Engaging Undergraduates with Crystallographic Research

Speakers focused on how to incorporate X-ray crystallography into the undergraduate curriculum, and how to launch a successful research program at an undergraduate institution. A. Nazarenko (USA) uses crystals of sweeteners of everyday products to show non-chemistry majors how useful information on molecular structure may be obtained through X-ray crystallography. C. Phillips-Piro (USA) discussed using X-ray crystallography to study the interaction of unnatural amino acids with proteins and explored the key factors in setting up and running a protein crystallography lab at an undergraduate institution. J. Golen (USA) described acquisition of a diffractometer through the NSF-MRI program to establish a regional resource in south-east Massachusetts and gave examples of undergraduate research results that are being obtained. D. Johnston (USA) described using mini research projects, based on student proposals, to characterize coordination compounds with his inorganic chemistry class and undergraduate research students. P. Cook (USA) discussed the challenges he faced in setting up a macromolecular crystallography research program at an undergraduate institution. J. Tanski (USA) gave a description of his research program in titanium mediated asymmetric catalysis with crystal structures obtained at all stages of the project.

*Joe Tanski and Roger Rowlett*

## 1.3.1: Career Odyssey

The four panelists C. Lind-Kovacs, C. Beavers, C. MacElrevey, and S. Sheriff, described their careers, the responsibilities in their current positions and what has helped them succeed. C. Lind-Kovacs, a Professor at U. Toledo, USA who teaches undergraduates and mentors graduate students and postdocs, suggested that postdocs aspiring to an academic career should learn people-management skills and seek mentors who are more experienced than they are. When asked, 'What is one thing you wish you were taught in graduate school?' Cora replied, "Nobody taught me how to teach." What Cora especially likes about her job is flexibility to set her own schedule. C. Beavers is a beamline scientist at ALS. The one thing she wishes she was told in graduate school is, 'Graduate school is not about what you learn, it's about learning to learn and learning to network.' Christine says her job is never boring, allows her to meet new beam line users, and requires her to travel



Career Odyssey session speakers (l-r): Celeste MacElrevey, Christine Beavers, Smita Kakar, Cora Lind-Kovacs, and Steven Sheriff.

all over. C. MacElrevey is a pharmacokineticist at Nuventra Inc., a contract research organization and has established an LLC consulting company. She enjoys the 'variety' in her job and the satisfaction of helping others to achieve research goals. Celeste urges students to try new things and never give up. S. Sheriff, a senior research fellow at Bristol-Myers Squibb suggested that being flexible is important to survival. He also suggested that managing people is a part of any job and one should learn how to do that well. Steve enjoys doing science and discovering what is not known.

*Smita Kakar*

### 2.1.2: Crystal Engineering Form & Function

This session addressed current research in the field of crystal engineering with an emphasis on the relationship between the structure and the function of crystalline forms. N. Seeman (USA) created the field of DNA based nanotechnology and has won numerous prestigious awards including the Kalvi Prize of 2014. His lecture attracted a huge audience who got a glimpse of his outstanding work in generating wide-open and programmable structures based on self-assembled DNA-based building blocks. N. Bathori (South Africa) discussed pharmaceutical applications, showing some fascinating structures and clear trends between melting points and solubility, which promise to place us closer to a rational design of crystals with desired pharmaceutical properties. J. Benedict (USA) presented pioneering work on combining the modular and open structures of MOFs with the photoswitchable behavior of diarylethylenes. Jason presented a structurally challenging new family of switchable MOFs accomplished by a unique combination of organic synthesis and coordination-driven self-assembly.

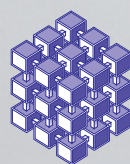
*Peter Wood and Tomislav Friščić*

### 2.1.3: General Interest I

This session highlighted recent developments in instrumentation and software technology. M. Ruf, (USA) described the APEX3 software package including the new structure solution and refinement plugin and improved twin-handling tools. A. Kleine (Germany) described their microfocus X-ray sources and scatterless pinholes and what it takes to upgrade existing systems to these technologies. E. Espes (Sweden) talked about liquid metal jet X-ray source technology and the use of a Ga-In alloy as the cup of liquid metal, that allow two wavelengths to be used in diffraction experiments on the same instrument. With brilliances close to those of first-generation synchrotron sources, protein data can be collected in-house to nearly the same resolution as synchrotron data (1.85Å vs. 1.75Å). C. Campana (USA) presented examples of analyses completed with the metal jet system on a Bruker D8 Venture. Z.-Q. Fu (USA) described shutterless data collection with a CCD detector to extract an ex-



General Interest I session speakers (l-r): Michael Ruf, Brian Toby, Emil Espes, Stacey Smith, Chuck Campana, Zheng-Qing Fu, Andreas Kleine. Photo courtesy of Stacey Smith.



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tremely weak native SAD signal. B. Toby (USA) highlighted the improved user interface and graphing capabilities of GSAS-II as well as the dual powder and single crystal and dual X-ray and neutron diffraction refinement capabilities.

*Stacey Smith*

#### 2.1.4: Publication Practices

This year's Publication Practices session focused on small-molecule crystal structures. Suzanna Ward (USA) drew attention to thousands of unpublished 'zombie' structures. She encouraged the use of the CCDC private-communication mechanism to bring the zombies to life. Information about zombie deposition at: [www.ccdc.cam.ac.uk/Community/Depositastructure/Pages/StructureDepositionInformation.aspx](http://www.ccdc.cam.ac.uk/Community/Depositastructure/Pages/StructureDepositionInformation.aspx).

S. Blake (UK) Section Editor at Acta Cryst., Section B, described significant restructuring of the contents, formats and focus of all IUCr Journals. For example *Section C*, which has been rebranded as 'Structural Chemistry,' now has lead articles, feature articles and scientific comment. It has a more flexible submission process that includes the use of Word and OpenOffice documents for the text. This removes an earlier requirement to include all text, including rich text, in the CIF, which led authors to publish elsewhere. T. Spek (Netherlands) urged that unmerged reflection data be deposited to permit any unusual features of the structure and claims of unexpected chemical features to be investigated in detail. Ton demonstrated his point with examples.

*Kimberly Lincoln and Larry Falvello*

To be continued in the next issue, Volume 24, Number 2.



## 18<sup>th</sup> Heart of Europe Bio-Crystallography Meeting

Kutná Hora, Czech Republic, September, 2015

BY WULF BLANKENFELDT

The 2015 Heart of Europe Bio-Crystallography (HEC) meeting took place under the auspices of the Czech Society of Structural Biology at the UNESCO World Heritage site of Kutná Hora in the Czech Republic. The HEC meeting provides Ph.D. students and postdocs from Austria, the Czech Republic, Germany and Poland with a platform to present their results to over 120 researchers representing 25 research groups. Principal investigators, while obliged to be present, leave the stage completely to their coworkers, creating an atmosphere of genuine collegiality that fosters lively discussions and nurtures excellent communication skills. HEC has become a favorite get-together for those who have attended the meeting before and has built a legacy with many of its former participants now running their own groups in bio-crystallography.

This year's participants enjoyed more than 30 scientific talks and had a chance to collect information about new products showcased by 11 industrial sponsors. The 2015 HEC lec-

ture, was given by Randy Read from the Cambridge Institute for Medical Research in the UK. Read, who is the mastermind behind the molecular replacement program PHASER, provided a thorough insight into maximum likelihood and impressed the audience with recent examples showing the power of its implementations. This year's HEC prize for best presentation was awarded to Andrea Schmidt from the group of Patrick Scheerer at the Charité - Universitätsmedizin Berlin. Her work on oxygen-tolerant [NiFe] hydrogenase secured for her a copy of Volume F of the International Tables donated by the IUCr and a travel grant for the 16<sup>th</sup> International Conference on the Crystallization of Biological Macromolecules (ICCBM-16) 2016 in Prague sponsored by the Czech Society for Structural Biology.

The organizers of HEC-18, Jan Dohnalek and his team from the Laboratory of Structure and Function of Biomolecules at the Institute of Biotechnology in Prague, did a fantastic job in welcoming their guests and introducing them to Kutná Hora,

a town that was once a rival of its neighbor Prague. Its former richness arose from an ample supply of now depleted silver ore, as the HEC participants saw in the splendor of the medieval city center and by daring an entertaining yet claustrophobic tour in the narrow shafts of a former silver mine. The meeting ended with a succulent feast of Czech specialties including a roasted suckling pig and dumplings and ample tastings of local brewery products.

At the end of September 2016, the HEC community will reconvene in the 13th century castle Burg Warberg close to the former German-German border, and will fill its walls with bio-crystallography at its finest. ♦





## XXII Meeting of the Brazilian Crystallographic Association (ABCr) and First Regional Meeting of the Latin American Crystallographic Association (LACA)

São Paulo, Brazil, September, 2015

BY IRIS TORRIANI

The Twenty-Second Meeting of the Brazilian Crystallographic Association (ABCr) was held jointly with the First Regional Meeting of the Latin American Crystallographic Association (LACA) and preceded by an International Center for Powder Diffraction Data (ICDD) course on Powder Diffraction. The one day course was held at the U. of Campinas (UNICAMP), sponsored by the ABCr, the Graduate School of Physics and the ICDD.

The course was prepared by Iris Torriani (IFGW-UNICAMP, Brazil) and Miguel Delgado and Graciela Diaz Delgado (U. of Mérida, Venezuela). Lectures were delivered by Eduardo Granado, Carlos Manuel Giles, and Martín Saleta (UNICAMP). Miguel Delgado and Graciela Diaz Delgado were responsible for the presentations related to the ICDD data bank.



Diego Lamas receives the award granted to Federico R. Napolitano (CNEA, Bariloche-Argentina) by the ICDD: 10 or more published patterns to the PDF (2014).

### Scientific Program of the ABCr/LACA Meeting

The ABCr/LACA Meeting was organized by a joint International and Local Committee. Three members of the ABCr Executive Council coordinated the tasks in São Paulo and Campinas (SP) and Belo Horizonte (MG).

Márcia C.A. Fantini (IF-USP) led the group, as President of ABCr and Provisional President of LACA; Iris L. Torriani (IFGW-UNICAMP), ABCr Treasurer, acted as Chair of the Meeting and Nivaldo L. Speziali (IF-UFMG), ABCr Teaching & Communications Secretary took care of webpage contacts, publications and participant registration with technical and logistic support from the staff of the IF-USP and members of the Executive Committee and Council of the ABCr. The support of the Brazilian Physics Society (SBF) is gratefully acknowledged by the organizers.



More than 128 participants attended the event, approximately 77% of those registered were researchers, professors and young scientists from Argentina, Brazil, Bolivia, Chile, Cuba, Colombia, Costa Rica, México, Peru, Uruguay and Venezuela. Participation of most of the young researchers was sponsored by the IUCr Bursary Fund.

The program included 3 Keynote lectures, 18 oral communications, and 3 poster sessions

1. Santiago Garcia-Granda (U. of Oviedo, Spain) presented the lecture *A controlled pressure/temperature set-up for synchrotron in situ studies of solid-gas processes and reactions: Structural deformation of ZIF-8*. He addressed the subject of porous materials, and their applications in catalysis. Garcia-Granda also commented on interactions between the IUCr and crystallographic entities in Latin America. He encouraged the participants to organize meetings, schools, and work-groups that promote crystallography at all levels. The number of Nobel prizes in Physics, Chemistry and Medicine and the International Year of Crystallography (IYCr2014) were also highlighted.

2. Abel Moreno Cárcamo (U. Autónoma de México), presented the lecture *The influence of Electric and Magnetic Fields on the 3D Structure of Protein*. He presented strategies developed for the crystallization of proteins from solutions and gels using electric and magnetic fields. The influence of the applied fields may be convenient for the observation of the processes of nucleation and growth of protein crystals. The experiments allow a choice to be made between the production of a large number of small crystals to be analyzed by powder methods or the production of single crystals for the use of conventional crystallography.

3. Mike Zaworotko (U. of Limerick, Ireland), delivered the lecture *Crystal Engineering of Task-Specific Materials*. Saworotko is investigating how composition and structure affect the properties of crystalline solids and designing strategies that will produce "functional" crystalline materials. He focused on Multi-Component Pharmaceutical Materials and Ultramicroporous Materials, and showed how molecular modeling together with crystal engineering can lead to the production of the proper material for a specific application.



Participants at the ABCr/LACA 2015 Joint Meeting - IF-USP, São Paulo, Brazil.



27 PhD students, postdocs and young staff members took part in the workshop. They learned about modern crystallographic techniques in the fields of diffraction, imaging, spectroscopy and remote sensing. Mineral growth patterns in the early Earth, other planets, moons, and meteorites, and the relevance of crystals to investigations of the origin of life were described. The students analyzed their own data as well as the data from the Discovery and Curiosity Missions. Portable diffractometers and spectrophotometers designed for these Missions were used during the field trip for remote analysis of volcanic rocks. The participants learned about the programs of COSPAR (M. Mendez) and the IUCr (H. Dabkowska).

On the opening day the nearby Popocatepetl volcano erupted, providing the students with an ample amount of volcanic ash to be analyzed. The planned excursion to this volcano, led by the vulcanologist Claus Siebe, was moved to the site of lava deposits from previous eruptions.

The crystallographic and crystal growth lectures were presented by J. Britten, J.R. Carvajal, H. Dabkowska, Y. Kimura, J.A. Manrique, C. Mavris, M.E. Mendoza, T.P. Puig, J.M. Garcia-Ruiz and F. Rull. The program featured talks about the Mars Missions (D. Blake on Curiosity, J. Vago on Exomars, and P. Söbren on future missions), the Hayabusa Mission (T. Nakamura), meteorite investigations, (R. Navarro-Gonzalez, F. Ortega and J. Urrutia), early minerals (M. van Zuilen) and interesting crystals (W. Depmeier and D. Page). Students worked with the instructors preparing samples and analyzing them using a portable diffractometer, Raman and infrared spectrophotometer and optical microscopy. The school ended with the presentation of the practical works performed by the students on their own samples or samples provided by the organizers. The detailed program of the workshop can be found at [www.inaoep.mx/cospar2016](http://www.inaoep.mx/cospar2016).



Round table discussion "Are there signs of life on Mars" round table discussion in Universum Museo de las Ciencias, Mexico City. Participants (from the left) David Blake (USA), Jose Franco (Mexico), Juan Manuel Garcia Ruiz (Spain), Jorge L. Vago (ESA) and Tomoki Nakamura (Japan).

The local organizing team lead by G.T. Tagle, M.E. Mendoza, R. Mujica, T.P. Puig and U. Salazar kept the group well fed and entertained with visits to Puebla City and the ancient pyramids in Cholula and Teotihuacan, a concert performed by the young Esperanza Azteca orchestra, a lecture about the Giant Crystals of Naica (J. Garcia-Ruiz), the Exomars mission (J. Vago), and a round table discussion on "Possibility of Life on Mars". The movie "The Martian" was screened and discussed with the experts involved in Mars exploration. There was also an opportunity to observe the crystal growth competition organized by R. Múica and M.E. Mendoza for Puebla school children. ♦

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Space workshop break



A dinner organized by Maria Eugenia Mendoza and Guillermo Tenorio Tagle for the participants of COSPAR-IUCr workshop in the famous China Poblana restaurant in Puebla.

## 9<sup>th</sup> AOFSSR Cheiron School

Hyogo, Japan September 2015

BY NAOTO YAGI

The 9<sup>th</sup> AOFSSR (Asia–Oceania Forum for Synchrotron Radiation Research) Cheiron School (<http://cheiron2015.spring8.or.jp/>), organized by AOFSSR, RIKEN, the Japan Synchrotron Radiation Research Institute (JASRI) and the High Energy Accelerator Research Organization (KEK), was held September 10–19, 2015 at SPring-8 in Japan and was attended by 60 students.

The AOFSSR is an association established in 2006 to enhance global cooperation in the Asia–Oceania region for synchrotron radiation research among member countries including Australia, China, South Korea, Singapore, Taiwan, Thailand and Japan and associated member countries New Zealand, Malaysia and Vietnam.

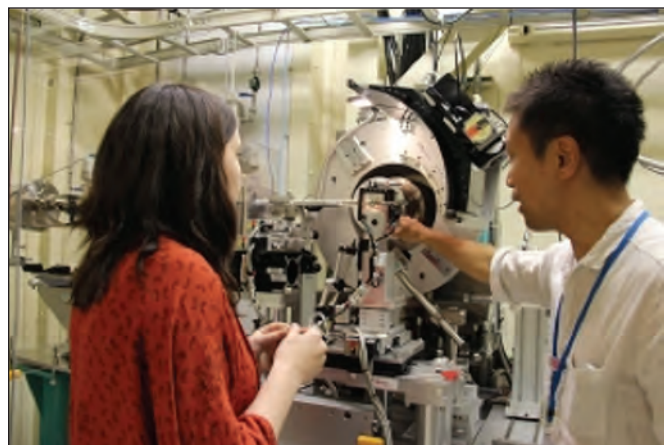
To develop human resources in synchrotron radiation science in the region, the AOFSSR Cheiron School was launched in 2007 at SPring-8. The school was named after Cheiron, an immortal god who was the master of many arts and sciences and the mentor of Greek heroes. His mentorship coincides with the policy of the school to provide each student with the appropriate knowledge and skills. The main aim is to provide useful and basic knowledge as well as perspectives of synchrotron radiation science and technology for graduate students, postdoctoral fellows, young scientists and engineers who wish to pursue their career in a field requiring synchrotron radiation and to join a synchrotron radiation facility in the Asia–Oceania region. Over the past 9 years, more than 500 young scientists have attended the school. In 2014, the school welcomed young scientists from Africa recommended by UNESCO in the context of the International Year of Crystallography (IYCr2014), and in 2015, with support and recommendation from the IUCr, two prominent young scientists participated from Africa and the Middle East. The school includes lectures, practicals, discussions with researchers/experts and site tours of SPring-8 and the XFEL facility, SACLA.

The introductory lecture, “*The school Overview of SR and the AOFSSR*” was delivered by Richard Garrett (ANSTO, Australia), and lectures related to crystallographic applications were pre-

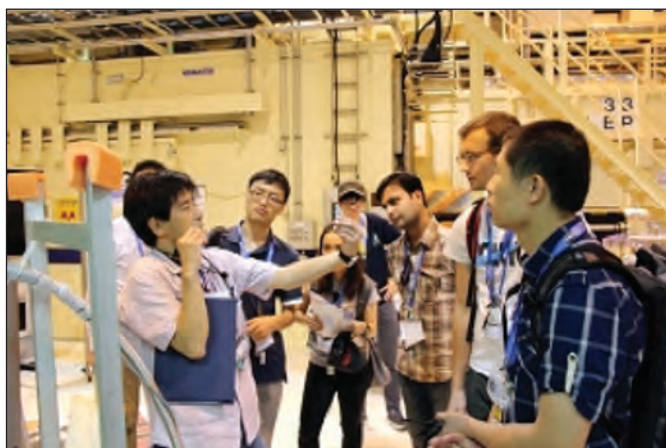


sented by David Attwood, UC Berkeley (X-ray optics), Mitchell Guss, U. of Sydney (protein crystallography) and Mark Dean, Brookhaven National Lab, (resonant X-ray scattering).

The students enjoyed discussions with the experts about their own problems in synchrotron radiation science and learned useful skills and knowledge in the practicals.



Beamline tour



Site tour.



Discussion with experts

## Advanced School on Experimental and Bioinformatics Tools for Protein 3D-structure Determination and Analysis

Varadero, Cuba, November, 2015

ROSSANA GARCÍA-FERNÁNDEZ, PEDRO A. VALIENTE AND CARLOS ÁLVAREZ VALCÁRCEL

The Advanced School: *Experimental and Bioinformatics Tools for Protein 3D-structure Determination and Analysis* (<http://protein-2015.uh.cu/index.html>) was organized by the Center for Protein Studies of the U. of Havana, the Cuban Section of Biochemistry and Molecular Biology, and the Center for Molecular Immunology under the auspices of the International Union of Biochemistry and Molecular Biology (IUBMB). It was held November 9–13, 2015, at Varadero Beach in Cuba.

Of the 52 participants, 33 were PhD or postdoc students that came to our course to hear case-study presentations, participate in a round-table discussion and discuss their results in poster sessions. All of the 52 participants, coming from 12 different countries, received funding, which covered the registration fees, transfer and accommodation in a resort.

An opening lecture delivered by Efstathios Gonos, member of the IUBMB Executive Committee for Congresses and Conferences, was followed by five lectures that covered experimental methods, such as small-angle X-ray scattering (SAXS) and X-ray crystallography to study proteins and protein–protein complexes. Late in the afternoon, a round table addressed undergraduate and graduate educational programs related to bioinformatics and techniques for protein structure determination. It was interesting to hear about related experiences in Canada, Cuba, Israel and the USA. At the end of the roundtable a Brazilian representative of the PosLatAm Program explained the opportunities that such an initiative is offering for young researchers and their institutions to strengthen and develop biophysics in Latin America. On the second day, lectures and discussions focused on molecular modeling and dynamic simulations and their contribution to the study of protein stability, function, conformation and interactions. On the third day, case studies in the Cuban biotechnological industry and other biomedical projects in which the contribution of structural and computational biology approaches has been decisive were presented. The last day featured Finally, two lectures about publishing scientific papers and the experiences of some of the lecturers who had served as journal editors.

At the end of the School, students and lecturers were surveyed for their views. The general comments were positive and encouraging; the discussion–evaluation of posters was one of the best-evaluated activities by all participants in this academic experience. Post-prize award went to Teresa

Nuguit, (U. of Hamburg), Aymara Cabrera (U. of Havana), Karella Delgado (U. of Calgary, Canada) and Edwin Reyes (U. Nacional de Colombia). The IUCr Journals prize was awarded to Dr Mey L. Reytor from the U. of Havana, Cuba.



Some of the Latin-American students - from Argentina, Chile, Colombia and Cuba - attending our School. Edwin Reyes (U. Nacional de Colombia), winner of one of the poster prize awards, is in the middle.

From left to right, the IUCr Journals poster prize winner: Mey L. Reytor (U. of Havana, Cuba), and two of the other four winners of poster prizes: Theresa Nuguit (U. of Hamburg, Germany) and Aymara Cabrera (U. of Havana, Cuba).



Participants at the entrance of Mercure Playa de Oro Hotel, venue of the School.

## Nangia Appointed Director of the CSIR-National Chemical Lab



Ashwini Nangia

Professor Ashwini Nangia (School of Chemistry, U. of Hyderabad) and well known within IUCr and in the international crystallographic community has taken over recently as the 11th director of National Chemical Laboratory (NCL), Pune. This flagship laboratory of the Council of Scientific and Industrial Research (CSIR) of the Government of India, has close to 200 scientists with around 400 students pursuing a PhD degree. NCL publishes over 400 research papers and files for 60 worldwide patents annually in the field of chemical sciences. It is a unique source of research education producing the largest number of PhDs in chemical sciences within India and its former students occupy prestigious positions all over the country.

Nangia is an alumnus of IIT Kanpur. After earning his PhD at Yale U. (1988), he worked in NOCIL Agrochemicals R&D Centre, Navi Mumbai for a year, before joining the University of Hyderabad in 1989 and started a research group in sesquiterpene synthesis. In 1994, he changed his research area completely and joined his colleague Professor G. R. Desiraju for a few years before he began independent research in crystal engineering in 1998, especially studies of very strong hydrogen bonds, interpenetrated organic crystal structures and the design of cocrystals for pharmaceutical development. He contributed very significantly to this new field and in particular, he began a now successful start-up Crystalin in the university campus in 2010 based on commercial applications of cocrystal technology ([www.crystalin.co.in/](http://www.crystalin.co.in/)). He has published some 250 papers and his recent paper in IUCrJ is representative (<http://journals.iucr.org/m/issues/2016/02/00/ed5007/index.html>). He has been invited to speak at many meetings across the world in recent times. He was on the Montreal Ewald prize jury and he is an invited speaker at the 2016 Gordon Conference on Crystal Engineering this June. He was a member of IUCr Commission on Structural Chemistry between 2008-2014, and has played a significant role in bringing the AsCA meeting to Kolkata, India in 2015 and the IUCr Congress to Hyderabad in 2017. He is a fellow (2009) of the Indian National Science Academy (INSA) which is the adhering body to IUCr.



National Chemical Laboratory (NCL), Pune, India.

NCL is a vast interdisciplinary research center with a wide research scope and specializes in polymer science, organic chemistry, catalysis, materials chemistry, chemical engineering, biochemical sciences and process development. The National Collection of Industrial Microorganisms is located there and is a microbial culture repository maintaining a variety of industrially important microbial culture stock. Nangia also now leads the NCL Venture Center, India's largest science business incubator. Nangia is the first in India to initiate a start-up based on crystallography and intends to expand collaborative interactions between NCL and industry in India and abroad, and to increase translational research in the generic pharmaceutical industry in particular. In a recent interview with the IUCr newsletter he said that "NCL needs to ramp up dialog with industry in general and the generic pharma industry in particular. It needs fresh thinking and newer perspectives on market translation". The Indian crystallographic community records its pleasure at having a crystallographer-chemist at the helm of this huge and important organization. ♦

William L. Duax, Editor

## ICDD 2016 Ludo Frevel Scholarship Recipients

The ICDD Ludo Frevel Crystallography Scholarship Committee has selected ten recipients for the 2016 Scholarship Program. These recipients were selected, on a competitive basis, from fifty-seven commendable applications received by the ICDD Scholarship Committee.

The recipients are: Anna Gres (Columbia, MO, USA), *Structural Basis of Stability of the Mature HIV-1 Capsid Core*; Seung Jun Hwang (Cambridge, MA, USA), *Photocrystallographic Observation of M-Cl Bond Activation and Cl-Cl Bond Formation of Fe(III) Complexes in the Various Geometries*; Bandi Malleshham (Hyderabad, Telangana, India), *Investigations on Local Structure and its Influence on Ferroelectric Properties of Complex Perovskite Oxides*; Andrew Martinolich (Fort Collins, CO, USA), *In Situ Crystallography of Solid State Chemical Reactions*; \*Elias Nakouzi (Tallahassee, FL, USA, 2015 recipient), *From Crystalline Nanorods to Self-Assembled Biomorphs*; Livia Prado (Fluminense Federal U., Rio de Janeiro, Brazil), *Surface Properties of Carvedilol Crystals: Combining X-ray Diffraction with Advanced Techniques*; Davin Tan (Quebec, Canada), *Rational Design of a Family of Organic Thermosolvent Crystals*; Daniel Taylor (College Park, MD, USA), *Reactivity and Oxygen Storage in Materials for Chemical Looping Processes*; Mark Weidman (Cambridge, MA, USA), *Engineering Transport Rates in Nanocrystal Superlattices using In Situ X-ray Scattering*; Julia Wind (Sydney, NSW, Australia), *A Combined Experimental and Computational Approach to Understanding and Developing New Solid-State Ionic Conductors*.

The ICDD will present each of these students with a check in the amount of \$2,500 to assist in the continuation of studies in their selected fields of crystallographic research.

Scholarship awards are made possible by donations from both individuals and corporations. One hundred percent of all donations to the scholarship fund are applied to student funding, as defined by the program's charter. The Ludo Frevel Scholarship Program is a registered non-profit charity, and all donations are tax-deductible. Please consider making a personal or corporate donation to the fund today! ♦

## Aloysio Janner (1928–2016)

BY TED JANSSEN



Image copyright C. van Ommen

Aloysio Janner passed away on 27 January 2016. He was born in 1928 in Muralto, Ticino, the Italian-speaking part of Switzerland. He was awarded his master's degree with a thesis under Pauli at the ETH Zurich, but during his PhD work Pauli died, so Aloysio finished his PhD with Thellung, at the U. of Zurich. Then he went to the Batelle Research Institute in Geneva, where he worked with Edgar Ascher.

One of their achievements was an analysis of the structure of space groups in terms of extensions in the mathematical sense. In 1963 he came to Nijmegen as head of the theoretical solid-state physics group. There his interest in the relation between structure and properties led him to study the symmetry of electromagnetic fields in terms of four-dimensional space-time groups. I was his first PhD student and we derived the first list of these groups.

In 1972 Aloysio met Pim de Wolff, who had found that the  $\gamma$ -phase of anhydrous sodium carbonate has a structure that does not have lattice periodicity but still has sharp diffraction peaks, which, however, require four indices in order to be indexed.

He proposed a four-dimensional space for the description of its structure. The symmetry groups he needed were exactly the four-dimensional groups in our work, now called superspace groups. Aloysio continued this research with Pim and me by generalizing this approach, called the superspace approach, to include other aperiodic structures, such as density-modulated and composite compounds, and quasicrystals. He was very happy that the result of this research led to international recognition. He received the Aminoff Prize of the Swedish Academy of Science (with Pim and me) and the IUCr Ewald Prize of the IUCr (with me). Furthermore, he was awarded honorary degrees from the Universities of Rennes, Geneva and Lausanne. After his official retirement he chose a different direction, though related to his earlier work. He studied the symmetry of snow crystals, and later of polytopes, biomolecules and viruses. These structures show scale symmetries similar to those of quasiperiodic tilings, like the Penrose tiling. He published several papers in this area as well.

Aloysio was a very enthusiastic and warm person. In the last ten years he did not travel much, but at every conference I attended in that period there were always people asking about him. He was always happy to discuss the problems he was working on, and his advice was very stimulating for his PhD students. Some of them were experimentalists because he thought that, just as experimental groups sometimes include theoreticians, a group of theoreticians could have experimentalists as members; they could carry out the research suggested by the calculations of the theoreticians. An example of the benefit of this approach was the solution of a very old riddle: the morphology of calaverite. This compound shows facets that cannot be indexed in the usual way with three indices. Aloysio and his collaborators showed that it is possible to index them with four indices. The reason behind this is that the structure is aperiodic, and the diffraction pattern also needs four indices to index it.

*continued on Page 24*



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A selection of future meetings. A more complete list is available at [www.iucr.org](http://www.iucr.org). Corrections and new listings are invited by the Editor.

## JULY 2016

- 3-8 ♦ ICCBM-16. 16<sup>th</sup> International Conf. on the Crystallization of Biological Macromolecules. Prague, Czech Republic. [www.iccbm16.org](http://www.iccbm16.org).  
22-26 ♦ ACA 2016. Denver CO USA. [www.amerocrystalassn.org](http://www.amerocrystalassn.org).

## AUGUST 2016

- 21-24 ♦ 12<sup>th</sup> International Conf. on Biology and Synchrotron Radiation (BSR). Menlo Park, CA, USA. <https://conf-siac.stanford.edu/bsr-2016/>.  
28-1 ♦ 30<sup>th</sup> European Crystallography Meeting (ECM-30). Basel, Switzerland. <http://ecm30.ecanews.org/2016.html>.  
28-2 ♦ 16<sup>th</sup> European Microscopy Congress (EMC2016). Lyon France. <http://www.iccbm16.org/>.

## SEPTEMBER 2016

- 21 – 25 ♦ 24<sup>th</sup> Croatian-Slovenian Crystallographic Meeting (CSCM24), Bol, Croatia. <http://cscm24.org/>  
25 – 2 ♦ 3<sup>rd</sup> European Crystallography School (ECS3), Bol, Croatia. <http://ecs3.ecanews.org/>.

## DECEMBER 2016

- 4-7 ♦ AsCA 2016. Hanoi, Vietnam. <http://asca.iucr.org/meetings>.

## OCTOBER 2016

- 30-5 ♦ 5<sup>th</sup> MaThCryst School/Workshop on Nanocrystallography. Havana, Cuba. <http://www.crystallography.fr/mathcryst/havana2016.php>.

## MARCH 2017

- 25-2 ♦ 16<sup>th</sup> BCA/CCG Intensive Teaching School in X-Ray Structure Analysis. Durham, UK. <http://community.dur.ac.uk/durham.x-ray-school/staff.htm>.

## AUGUST 2017

- 21-29 ♦ 24<sup>th</sup> IUCr Congress and General Assembly. Hyderabad, India. <http://www.iucr2017.org/>.

## Aloysio Janner (1928–2016)

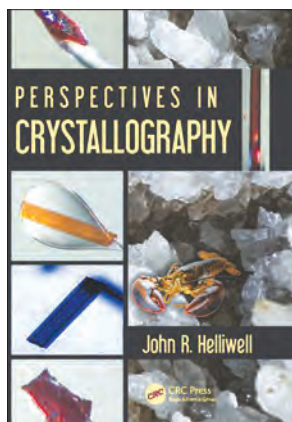
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Besides his research, he was active in other fields. He was the Dean of the faculty for several years, twice he (co-)organized the Conference on Group-Theoretical Methods in Physics, he was a member of an EPS Committee on Physics and Education, and Chair of the Committee on University, Industry and Public Authorities of the U. in Nijmegen. These tasks he also performed with much energy.

We have lost a great colleague. ♦

This obituary originally appeared in *Acta Cryst.* (2016). **A72**, 296-297, <http://dx.doi.org/10.1107/S2053273316001935>.

## BOOK REVIEWS



## Perspectives in Crystallography

John Helliwell, CRC Press, Boca Raton, FL, 2016, 171 pages, ISBN: 978-1-4987-3210-9

BY JOSEPH FERRARA

Helliwell's *Perspectives* is a collection of articles and lectures by the author celebrating the 100th anniversary of the first crystal structures (1912) and the UNESCO International Year of Crystallography. The book covers a broad range of topics in crystallography

from the author's perspective, hence the title. Some of the chapters have already been published in *Crystallography Reviews*.

Section 1 consists of a single chapter in which the author attempts to answer the question for the general public "What is crystal structure analysis?" Helliwell describes how the question was answered at several venues including his home institution, the U. of Manchester, and the Prisoners' Education Trust.

I found the next section very interesting. Chapter 2 succinctly describes the first diffraction experiments by the Braggs before and during WWI while Chapter 3 provides retrospectives by W.H. Bragg, W.L. Bragg, P.P. Ewald and D.C. Phillips on the work described in Chapter 2.

Section III is titled "Aspects of Crystallography Research" and consists of 4 chapters. Chapter 4 is a transcript of the au-

thor's Lonsdale Lecture at the 2011 British Crystallographic Association. I found the short biography of Kathleen Lonsdale at the beginning enlightening. I knew of her importance with respect to the early crystal structures of organics and the creation of the original *International Tables for Crystallography*, but I did not know the details of her life's story. The lecture then describes the history of the use of synchrotron radiation by the crystallographic community.

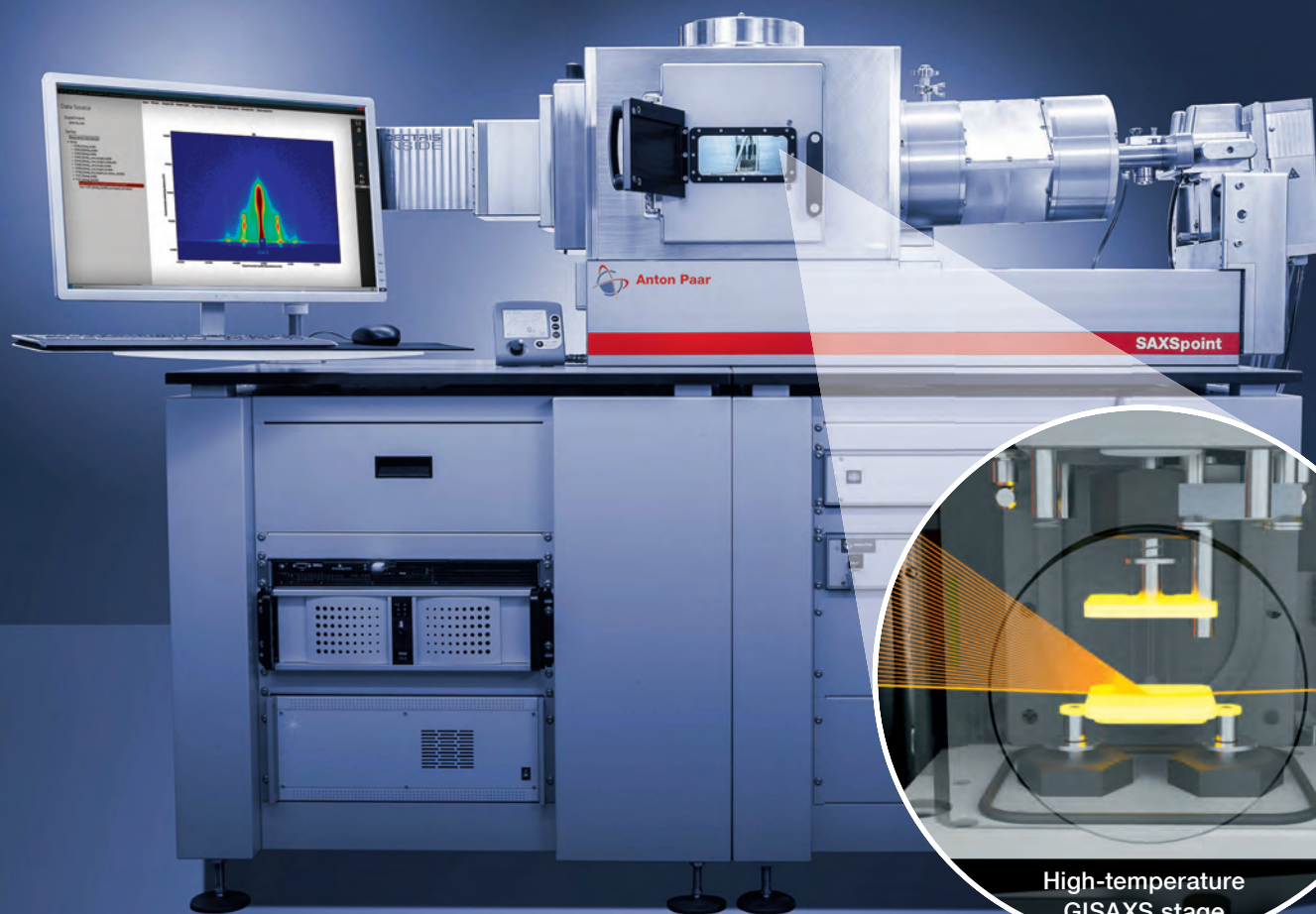
The next two chapters cover more specific topics: a comparison of several programs for predicting protonation versus X-ray diffraction results and the structural of crustacyanin. The last chapter in this section is a short prospective on the future of crystallography.

The last section and chapter looks at how crystallography has been a part, and will continue be a part, of the eight Millennium Development Goals set forth by the UN in 2000. One of the goals is to promote gender equality and empower women. The author points out that compared to other sciences, crystallography has more balance. Many of the goals are related to the alleviation of human pain and suffering—clearly crystallography excels through better a understanding of the world around us. ♦

# The world's brightest footprint



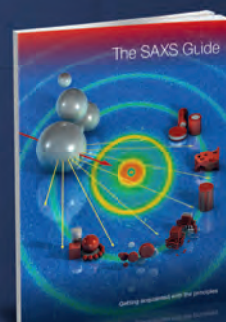
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## The all New D8 VENTURE Second Generation

**“There is nothing like a dream to create the future.” Victor Hugo**

At Bruker we had a dream: to create a diffractometer powerful enough to drive the science of the future. Now, with major advances in detector, source and software technology we have made this dream a stunning reality: the New D8 VENTURE.

**Contact us for a personal system demonstration**

[www.bruker.com/d8venture](http://www.bruker.com/d8venture)