INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

Volume 25 · Issue 1

Collected archival edition
Original article text and available illustrations

Contents

> Extraction incomplete: missing article positions 1.

IUCr journals news

2016 IUCr impact factor results 3

Charge density, photocrystallography and time-resolved crystallography: a tribute to Professor Philip Coppens 4

IUCr Main Editor appointments 7

Come and meet us in Hyderabad 9

IUCr activities

Mike Dacombe retires as IUCr Executive Secretary 10

IUCr bursary case studies 12

IUCr2017 Special Activities Programme 19

IYCr legacy

Rigaku OpenLab Bolivia, September 12-16, 2016 15

OpenLab Senegal, November 20 - December 2, 2017 17

Meeting report

13th International Conference on Quasicrystals (ICQ13) 28

Second Meeting of the Latin American Crystallographic Association 32

The Zürich School of Crystallography - Bring your Own Crystals 34

Awards and prizes

Tom Blundell awarded the 2017 Ewald Prize 38

Book review

International Tables for Crystallography, Volume A, Space-group symmetry. 6th edition 42

IUCR JOURNALS NEWS

2016 IUCr impact factor results



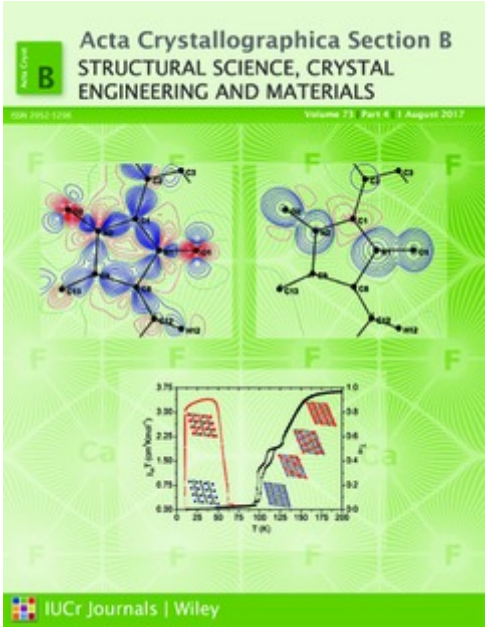
The 2016 impact factors have been released by Clarivate Analytics, and IUCr Journals (http://journals.iucr.org/) now occupy the top three positions in the Crystallography category.

IUCrJ, established in 2014, saw its impact factor increase to 5.8 from 5.3; *Acta Cryst. A: Foundations and Advances* to 5.7 from 2.3; and *Acta Cryst. C: Structural Chemistry* to 4.1 from 0.5. The impact factors of other journals also increased significantly: *Acta Cryst. F: Structural Biology Communications* from 0.6 to 0.8 and the *Journal of Synchrotron Radiation* from 1.9 to 3.0.

Editor-in-chief, Samar Hasnain, commented, 'We thank our authors, reviewers and over 200 editors and co-editors for their continued commitment to ensuring that the best crystallographic science is reported in IUCr Journals. We are particularly indebted to our authors who continue to place their trust in IUCr Journals. We look forward to building on this success and working towards further improvements in our impact and influence.' For more details, please see http://journals.iucr.org/services/impactfactors.html.

IUCR JOURNALS NEWS

Charge density, photocrystallography and time-resolved crystallography: a tribute to Professor Philip Coppens



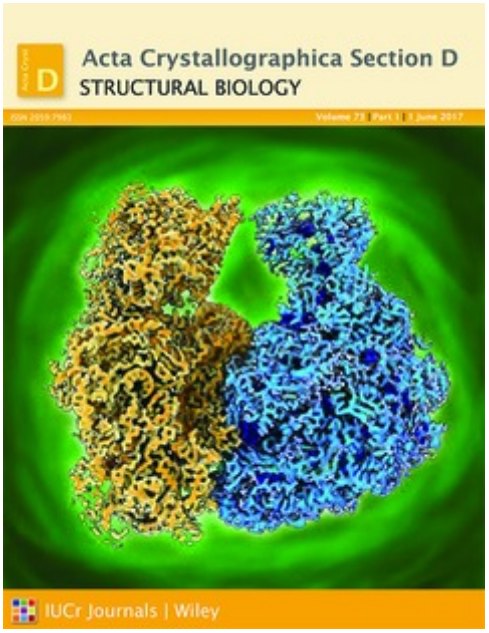
A lifetime of outstanding scientific achievements by Philip Coppens is celebrated in the August 2017 issue of *Acta Cryst. B* (http://journals.iucr.org/b/issues/2017/04/00/). Originally a tribute to his recent retirement, this collection of papers - approved by Philip - was submitted by former students, postdocs, close friends and collaborators. With Philip's unexpected passing in June 2017, this collection of manuscripts has now become a remembrance of his impactful scientific legacy.

Among the earliest of pioneers of the field of charge density, Philip demonstrated that accurate high-resolution X-ray diffraction was an unparalleled experimental method for mapping and modeling electron density in crystals. In both theory and practice, his contributions impacted every aspect of charge density: helium temperature experiments, data reduction, multipole modeling, combined analysis of charge and spin densities, derived electrostatic properties, multipolar data bases, and applications to chemical bonding and materials science. Much of Philip's later work involved the development and application of time-resolved X-ray diffraction methods to monitor light-induced transformations in small-molecule systems.

The contents range from high-quality charge- and spin-density studies (one of which is combined with X-ray absorption measurements), optimizing data and model quality, statistical analysis of the data, charge densities at high pressures, evaluation of pseudo-atom density models, measuring the charge density in unusual bonding situations, a further extension of Bader's theory by applying the Source Function to spin localization and polarization mechanisms, and development of new detectors allowing accurate powder diffraction measurements of charge-density quality, as well as in-house time-resolved studies down to millisecond resolution with a new gated detector, thus optimizing faster, in-house, dynamic studies.

The Guest Editors Claude Lecomte (who initiated this issue), Jason Benedict and Yu-Sheng Chen hope you enjoy reading this collection of manuscripts dedicated to the remembrance of Professor Philip Coppens (1930-2017).

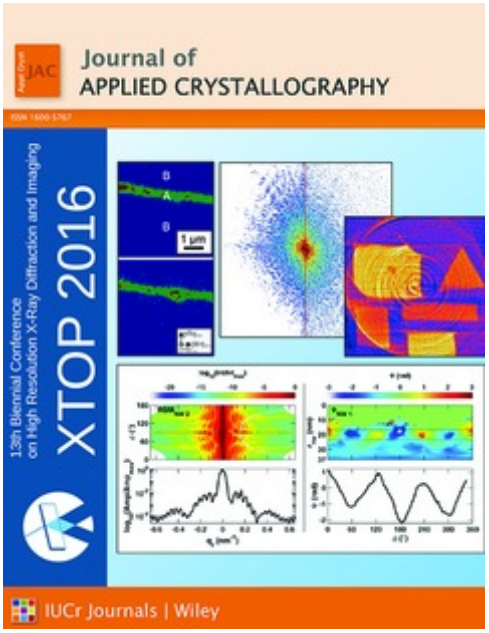
Proceedings of the CCP-EM Spring Symposium 2016



The Collaborative Computational Project for electron cryo-microscopy (CCP-EM; www.ccpem.ac.uk) supports users and developers in biological EM, and holds an annual symposium that reviews and highlights state-of-the-art developments in macromolecular cryo-EM. The proceedings of the 2016 Spring Symposium (Rutherford Appleton Laboratory, UK; May 2016) have been published in the June 2017 issue of *Acta Cryst. D* (http://journals.iucr.org/d/issues/2017/06/00.

Cryo-EM is currently in a golden age: multiple, symbiotic improvements in instrument technology have resulted in vastly improved signal-to-noise allowing a step-change in resolution and scale. Indeed, such is the pace of development that the term 'resolution revolution', first coined in 2014, is fast becoming a cliché. This has propelled cryo-EM into the mainstream, evidenced by the exponential rise in the number of new EM-derived structures and high numbers of new researchers in the field. These new methods have opened a rich tranche of new biological systems to explore, including those that were well hidden from the bright light of other structural biology disciplines. As such, this inaugural edition, edited by Tom Burnley, Paula da Fonseca and Randy Read, focuses on emerging methods - the how, and highlights applications - the why. The methods and applications presented in this open-access issue provide a glimpse of what can be expected in the coming years for cryo-EM.

XTOP 2016



The latest virtual special issue of the *Journal of Applied Crystallography* (open access at journals.iucr.org/special_issues/2017/xtop2016/) features a selection of original contributions from the 13th Biennial Conference on High-Resolution X-ray Diffraction and Imaging (XTOP 2016), which was held in Brno, Czech Republic, in September 2016. The topics of the published articles cover the broad spectrum of problems discussed during the conference, highlighting in particular four specific X-ray techniques: X-ray Bragg diffraction, small-angle scattering and reflectivity, X-ray diffraction imaging, and coherent (phase-sensitive) X-ray imaging.

IUCr Journals sponsored two Student Poster Awards at the meeting, which were won by Jinxing Jiang (NIMS, Tsukuba, Japan) for his poster 'Visualization of inhomogeneous layers and interfaces in ultrathin films by X-ray reflectivity', and Rajkiran Tholapi (U. Hamburg, Germany) for 'Effect of indentation-induced strain on epitaxial Fe layers'.

The next XTOP meeting will take place in Bari, Italy, in 2018.



Jinxing Jiang (left) and Rajkiran Tholapi (middle) accept their IUCr Journals Student Poster Awards from IUCr Executive Committee member Radomír Kužel.

IUCR JOURNALS NEWS

IUCr Main Editor appointments

Acta Crystallographica Section E: Crystallographic Communications appoints Elena Boldyreva and Chiara Massera



Elena Boldyreva received her PhD in Physical Chemistry in 1988 and Dr Sci. in Solid State Chemistry in 2000 from the Institute of Solid State Chemistry and Mechanochemistry, Russian Academy of Sciences (Novosibirsk). She is now a Chief Researcher at this Institute and the Head of the Division of Solid State Chemistry of Novosibirsk State U. Her research interests include reactivity of solids, mechanochemistry, photo- and thermo-mechanical effects, non-ambient crystallography and spectroscopy, molecular and inorganic materials, polymorphism, crystallisation, phase transitions, dissolution of molecular solids, metastable and amorphous states of molecular solids, physical pharmacy, drug research and development. Elena has held many senior committee positions, including being an elected member of the Executive Committee of the IUCr (2008-2014). From 2008 to 2017 she was a co-editor of *Acta Cryst. B*. From 2012 to 2014 she was a member of the Presidential Council of Science and Education of Russia and since 2014 has been a member of the Scientific Advisory Council of the Russian Ministry of Science and Education. She has received many national and international awards, the latest being an Honorary Doctorate from the U. of Edinburgh in 2016.



Chiara Massera obtained her PhD in Chemistry in 2001 from the U. of Parma, Italy, where she is currently Associate Professor. Her research projects focus on the crystallographic analysis of supramolecular complexes and coordination compounds, with the aim of studying molecular recognition phenomena and of elucidating structure-function correlations. She is a member of the teaching commission of the Italian Crystallographic Association, and promoter and vice-chair of GIG3, the General Interest Group on Education in Crystallography of the ECA.

Acta Crystallographica Section F: Structural Biology Communications appoints Mark van Raaij



Mark van Raaij studied Chemistry at the U. of Leiden, the Netherlands, and obtained a PhD in Biology from Cambridge U., UK, working at the MRC Laboratory of Molecular Biology with John Walker on biochemical and structural studies of inhibitors of mitochondrial F1-ATPase. After that he pursued postdoctoral research with Stephen Cusack at the EMBL Grenoble outstation, France, where he solved

high-resolution crystallographic structures of the human adenovirus fibre protein and its receptor. As an independent scientist, first at the U. of Leiden and then at the U. of Santiago de Compostela, Spain, he continued work on viral proteins, solving structures of reovirus proteins, adenovirus proteins and proteins of bacteriophage T4. Currently Mark is a group leader at the Centro Nacional de Biotecnologia in Madrid, Spain, where his group specialises in macromolecular crystallography, concentrating on bacteriophage and adenovirus receptor-binding proteins.

Journal of Applied Crystallography appoints Garry McIntyre



Garry McIntyre is currently Research Leader at the Australian Centre for Neutron Scattering, one of the landmark infrastructures run by the Australian Nuclear Science and Technology Organisation (ANSTO), which is host to OPAL, one of the youngest research reactors worldwide. He is also Visiting Professor in the Dept. of Chemistry at Durham U., UK. His primary role at ANSTO is management of the scientists responsible for the operation of the neutron-beam instruments and supporting X-ray instruments, neutron polarisation capability, and computer modelling. Garry's research interests focus on neutron scattering techniques, especially single-crystal diffractometry and polarised-neutron techniques, diffraction physics, charge and spin density in molecular compounds, structural chemistry and cultural heritage.

The IUCr would like to take this opportunity to thank all those scientists who have expressed an interest in joining the IUCr Journals editorial board.

IUCR JOURNALS NEWS

Come and meet us in Hyderabad



The 24th IUCr Congress and General Assembly will be taking place in Hyderabad, India, between August 21 and 28, 2017 (www.iucr2017.org/). This will be the first time that India has hosted the Congress so it will be a very important time in the Union's and India's history.

We are planning many activities in and around our stand so please do come and pay us multiple visits. During the entire Congress, delegates will be able to access our archive of journal articles free of charge via journals.iucr.org or the handy conference app.

If you have not yet seen the 6th edition of *International Tables Volume A: Space-group symmetry* (http://it.iucr.org/A/), edited by Mois I. Aroyo, drop by our booth to take a look. This new edition, an essential reference for any crystallographic or structural study, has been extensively updated and revised. See the review by Massimo Nespolo on pp. 22-23, which gives a good explanation of what has changed since the previous edition, such as the simplified layout of the space-group tables.

Still on the theme of books, we plan to host a Book-A-Day giveaway at the stand. Following up on the message from *IUCr Newsletter* editor Bill Duax (www.iucr.org/news/newsletter/volume-24/number4/packing-for-india), we would like to encourage you to squeeze a couple of your old or unwanted text books into your suitcase and bring them to the IUCr exhibition booth for us to donate to the next generation of crystallographers. If you like, add your name and short message of encouragement to the flyleaf.

We will organise a number of meet-the-editor sessions, which will take place either at our booth or in a nearby room. You will have the opportunity to talk with some of our main and co-editors about the benefits of publishing with IUCr Journals. The timetable will be available at the stand. If you have any specific questions ahead of the sessions, please send them to me at ja@iucr.org.

Face-to-face meetings are invaluable but you can also engage with the crystallographic community through our social media channels: Twitter (https://twitter.com/IUCr), Facebook (https://www.facebook.com/iucr.org) and LinkedIn (www.linkedin.com/company-beta/5334871/). In addition, we have a new blog called *Crystallites: News and opinion in crystallography* (blogs.iucr.org/crystallites/). The blog features some of the latest activities in the crystallographic community, presented to you in an easily digestible style and format. If you are interested in submitting a blog post, please get in touch with me at ja@iucr.org.

Last but not least, we will be launching the IUCr Associates Programme (www.iucr.org/people/associates) at IUCr2017. This exciting new individual membership programme aims to promote a sense of belonging for our many professional crystallographers, students and retired crystallographers, whilst enabling the IUCr to serve our community better and support a greater number of worthy activities. The programme offers a series of benefits and tools to help Associates network, share ideas and discover more about crystallography. Drop by our booth where you will be able to sign up at the special Congress rate and take away a handsome lapel pin and welcome pack.

We look forward to welcoming you at the 24th IUCr Congress and General Assembly in Hyderabad!

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

IUCR ACTIVITIES

Mike Dacombe retires as IUCr Executive Secretary



Mike joined the IUCr in 1975 as an Editorial Assistant, before moving on to be Technical Editor in 1986 and Executive Secretary in 1993. He has seen the IUCr Chester offices move from Whitefriars to Abbey Square, and then expand further to the current three offices. In the same period, the stable of IUCr Journals has increased from paper copies of *Acta Cryst. A* and *B* and *J. Appl. Cryst.* to the present suite of online publications.

Mike succeeded Jim King, who was the highly regarded first ever Executive Secretary of the IUCr. Not only did Mike provide a steady hand on the IUCr's tiller for the past 24 years, but he also oversaw the modernisation of the organisation in general and the Chester offices in particular. Few industries can have undergone as much turmoil in that period as scientific publishing has experienced, with the transformation from subscription-based printed journals to online-only offerings with increasing levels of open access, but Mike calmly navigated the IUCr safely through.

From the 16th Congress in Beijing through to the 24th Congress in Hyderabad, Mike has worked with nine different IUCr Presidents and four different General Secretaries and Treasurers. Each has benefitted greatly from Mike's stoic support and sound advice. Mike has attended a total of 11 Congresses. He has always been available to help with various issues - his cheerful and friendly personality has been warmly appreciated by those he met. Under his stewardship, the Chester offices have enjoyed a supportive environment where the staff have felt genuinely appreciated, and while we all wish him a long, happy and healthy retirement, he will be greatly missed by the colleagues who have been privileged to work with him.

...and is succeeded by Alex Ashcroft



Alex has a Chemistry degree and D.Phil. from Oxford U., where he was based in Tony Cheetham's group in the Chemical Crystallography Laboratory. Alex's D.Phil. was on catalysis, so despite doing powder XRD in Oxford, the Royal Institution and Daresbury, powder neutron diffraction at the Rutherford Laboratory and dabbling in electron microscopy and EXAFS, he doesn't claim to be a crystallographer but says he

does know some really good ones. He once made a cup of coffee for Dorothy Hodgkin. One of his D.Phil. examiners was **IUCrJ** Main Editor Richard Catlow, who complimented him on having the best spell-checked thesis he had ever seen. Those of you who have published in *Acta Cryst. A* or *International Tables* can probably guess the origin of this flawless presentation, and will deduce that Alex was an early beneficiary of the excellence typical of the Chester office's editorial staff.

After a year Post Doc at the U. of California Santa Barbara, Alex joined Unilever R&D in Port Sunlight, UK, where he worked for 23 years on a variety of projects, mostly in the oral care, deodorants and household cleaning areas. Alex's duties included leading research projects, developing strategies to grow science areas, setting up PhD studentships with university departments and even cleaning local consumers' bathrooms and kitchens in the name of science.

Alex is well aware that by following Mike, who has been such a stalwart of the IUCr, he has very high standards to live up to, but is really excited about having the opportunity to work for such a highly regarded scientific organisation. Reading about the history of the IUCr, and looking through the minutes from the Montreal Congress in preparation for his interview, Alex says he was hugely impressed by the sense of community, integrity and dedication to high-quality science that the IUCr embodies, and he is relishing the opportunity to support that as Executive Secretary. Alex will be in Hyderabad, wearing his Associate Member lapel pin with pride, so please introduce yourself if you see him. He can be contacted at execsec@iucr.org.

Celebrating 25 years at the IUCr



The IUCr prides itself not only on the expertise of its staff but also on their dedication. This year five members celebrate 25 years of service, and recently received geodes in a special event at the IUCr offices to mark the occasion. From l-r: Katie Moore (Editorial Systems Developer), Gillian Holmes (Managing Editor, *Acta Cryst. E* and *IUCrData*), Louise Jones (Managing Editor, *Acta Cryst. D* and *F*), Carol Cook (Administrative Assistant) and Sean Conway (Managing Editor, *Acta Cryst. C*).

IUCR ACTIVITIES

IUCr bursary case studies

In 2016 alone, the IUCr sponsored 40 international meetings and schools. Three recent recipients of IUCr Young Scientist Awards reveal below the importance of these travel grants to their research and experience.

Lanthanoid metal-organic frameworks



Metal-organic frameworks (MOFs) have been extensively studied with small organic molecules and transition metals, and in the past years more and more interest in developing MOFs with lanthanoids has emerged. Lanthanoids are a group of *f*-block metals with similar chemical behavior, and they tend to have larger coordination numbers and less strict bond directionality compared with *d*-block transition metals. As hard bases, lanthanoids tend to form coordination compounds with hard acids, and carboxylic acid derivatives are by far the most studied group of ligands. Practical applications for lanthanoid-MOFs (Ln-MOFs) have been studied, and these include, for example, small-molecule capture and storage, gas adsorption, catalysis and metal extraction.

In my PhD studies I have been concentrating on multipodal zwitterionic ligands, which possess carboxylate functionality and thus can be used in Ln-MOFs as organic linkers. The backbone of these linkers is an aromatic center joined by two or more methylene bridges to pyridinecarboxylic acids, which in turn have several substituent configurations available, leading to various isomers. Pyridinecarboxylic acid groups can have several different spatial orientations with respect to the aromatic center because of the freely rotating methylene bridges, and if the ligand has been synthesized from, say, nicotinic acid (3-pyridinecarboxylic acid), there are even more directions for the carboxylic acid to coordinate to, than in the case of isonicotinic acid (4-pyridinecarboxylic acid). One problem associated with high degrees of freedom in these Ln-MOF systems is that they tend to crystallize in several different crystal systems and have different types of disorder within the structure.

The bursary towards attending the 16th BCA/CCG Intensive Teaching School in X-ray Structure Analysis (Durham, UK; 25 March-2 April 2017; http://community.dur.ac.uk/durham.x-ray-school/index.html) was crucial for me to gain new insights in the fundamentals of X-ray crystallography. As my materials in question are intrinsically crystalline, X-ray crystallography is the most powerful way to gain information from MOFs. The contents of the course helped me to critically assess my own work up to this point in a new way, and I gained many new pieces of information to aid my further studies.

Antti Tiihonen, MSc, Department of Chemistry, U. of Jyväskylä, Finland

Structural and biological study of tin-based complexes against enzymes that propagate cancer



Cisplatin and its subsequent clinical success generated interest in researchers with regard to the use of metal complexes as anticancer drugs. Cisplatin still plays a major role in treating over 90% of testicular cancer cases and is now one of the most successful anticancer drugs available on the market. Cisplatin generally interacts with DNA by inducing programmed cell death (apoptosis). Although cisplatin is used in cancer treatment there are side effects such as anemia, diarrhea, alopecia, petechia, fatigue, nephrotoxicity, emetogenesis, ototoxicity and neurotoxicity. This then opened up research areas in synthesizing metal-based drugs, including developing tin-based anticancer drugs derived from dithiocarbazate Schiff bases.

I have embarked on the structural and biological study of tin-based complexes against four enzymes that propagate cancer: ribonucleotide reductase, thymidylate synthase, thymidylate phosphorylase and topoisomerase II. Sponsorship from the IUCr allowed me to attend the 16th BCA/CCG Intensive Teaching School in X-ray Structure Analysis at Durham U., UK. There, with help from tutors and lecturers, I learned much about the theory behind X-ray crystallography, which enabled me to solve single-crystal X-ray diffraction data while understanding the processes involved. Single-crystal X-ray diffraction analysis allows me to determine the real mode of coordination for docking analysis functions. In addition, I had the opportunity to meet and collaborate with front-line researchers in the field of crystallography from different universities. These connections have helped me to view my project from different perspectives and to gain more understanding on how to better apply single-crystal X-ray data to my own work.

Enis Nadia Md Yusof, Department of Chemistry, U. Putra Malaysia, Malaysia

Structure determination of the *Schistosoma mansoni* enzyme fumarate hydratase, a potential macromolecular target for new antiparasitic drug design



Schistosomiasis is a neglected tropical disease, caused by the parasite *Schistosoma*, which affects 230 million people worldwide, and is responsible for thousands of deaths every year. In the search for new targets against schistosomiasis, an important strategy involves the identification and characterization of essential enzymes from *Schistosoma*. The *S. mansoni* enzyme fumarate hydratase (SmFH) catalyzes the reversible hydration of fumarate to malate and is involved in aerobic processes to obtain energy in the parasite. Thus, an understanding of how the enzyme works allows its evaluation as a potential macromolecular target for new antiparasitic drug design.

I have been studying SmFH and, for a better understanding of the enzyme, have been trying a careful structural analysis. Several crystallization experiments were performed, and an X-ray diffraction data set

was collected at Synchrotron SOLEIL, France. However, some difficulties were found in the structure solution. RapiData 2017 (Stanford, CA, USA; April 16-22, 2017; http://smb.slac.stanford.edu/news/rapidata/rapidata-2017/) appeared as a great opportunity to improve my knowledge of data collection and processing. All the tutorials offered by the course made possible a better understanding of crystallization and X-ray data processing, and allowed contact with great researchers in the area. As Brazil is experiencing a major crisis, investment in research is very scarce, which makes it difficult for students to attend courses abroad. Thus, the award granted by the IUCr allowed me to have this experience, which will add so much knowledge in my research area.

Iara Aimé Cardoso, Master Student, U. of São Paulo, Brazil

IYCR LEGACY

Rigaku OpenLab Bolivia, September 12-16, 2016



Participants of the OpenLab, La Paz, Bolivia, September 12-16, 2016.

The IUCr-UNESCO Rigaku OpenLab took place at the Facultad de Ciencias Puras y Naturales of U. Mayor de San Andrés (UMSA) in La Paz, Bolivia, September 12-16, 2016. At 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 UMSA, La Paz, advanced the idea of organizing a crystallography event in Bolivia. They mentioned there had never been an event in crystallography in their country and that they would be very happy to work in the organization of such an event. The LACA General Assembly supported the proposal, in the collaborative spirit that permeates the LACA organization and fulfilling its mission to promote and expand crystallography in our region. Given the success of the IUCr-UNESCO OpenLabs program, it was considered appropriate to organize an OpenLab at UMSA, taking advantage of the instrumentation available. They have a Rigaku powder diffractometer (old but still in excellent working condition) and a new PANalytical XPERT diffractometer. Rigaku Latin America co-sponsored the OpenLab along with the Institut de Recherche pour le Développement (IRD) and the International Centre for Diffraction Data (ICDD). Several companies including Benton, Save SRL, ESLC SRL and Oberon SRL provided additional support.

The OpenLab was attended by about 100 young scientists and students from La Paz, Potosí and Cochabamba (Bolivia) and from Chile, El Salvador, México, Nicaragua and Perú.

Santiago García-Granda (U. Oviedo, Spain / IUCr Executive Committee), Michele Zema (U. Pavia, Italy / IUCr), Diego G. Lamas (U. San Martín, Argentina / Vice-President LACA), Miguel Delgado (U. de Los Andes, Venezuela / ICDD Regional Co-Chair) and Akihiko Iwata (Rigaku Latin America) constituted the International Advisory Committee. They worked closely with the Local Organizing Committee composed of María Eugenia García (Vice-Dean of Facultad de Ciencias Puras y Naturales), Luis Morales Escobar (Director of the Chemistry Program), Giovanna Almanza Vega, Victor Ismael Ramírez, Mario Blanco Cazas, Rigoberto Choque A. and Oswaldo Ramos (Chair). The wonderful and enthusiastic team of young scientists and students needs to be recognized for their hard work: Wilma Ticona Chambi and Naviana Leiva, Julián Ticona Chambi, Macguiver Pilco, Grace Villanueva, Leydi Salinas, Carolina Trigero, Neddy Alejo, Alison Parisaca and Samuel Lonza.

To provide additional help to the students with little crystallography background, a two-day mini course was held on September 8-9, taught by Miguel Delgado, Diego G. Lamas and Graciela Díaz de Delgado. For the OpenLab, José Antonio Henao (UIS, Colombia) and Akilesh Tripathy (Rigaku Americas) also participated as instructors. Santiago García-Granda could not participate as an instructor due to many commitments as part of his inauguration as Rector of U. de Oviedo in Spain (Congratulations, Santiago!).

Mario Blanco Cazas, Head of Instituto de Investigaciones Geológicas y del Medio Ambiente, and Ariana Zeballos were in charge of the practical sessions showing the students sample mounting and powder data collection. Inasmuch as Bolivia is a country with an extraordinary mineral diversity and a vibrant mining activity, the OpenLab was centered on powder diffraction. However several lectures dealt with single-crystal X-ray diffraction, and an event dedicated to structure determination and refinement from single-crystal data is being planned for 2017 to celebrate the 50th anniversary of the Chemistry Program at UMSA. Several formal and informal meetings were held during the week to start and strengthen collaborations between the institutions involved in this OpenLab.

On a personal note, all the instructors agree that this was one of the most memorable events in which we have ever participated. The warm reception with the attention provided by University officials and faculty members of the Facultad de Ciencias Puras y Naturales, the enthusiastic participation of all the attendees, and the help provided by the local students created a superb academic environment. At the closing ceremony, Luis Morales Escobar (Director of Chemistry Studies), Franz Cuevas Quiroz (Dean of Facultad de Ciencias Puras y Naturales) and Waldo Albarracin Sánchez (Rector of UMSA) highlighted the importance of the OpenLab and opened the doors of the institution to continue and strengthen collaborations, particularly in crystallography. We felt so welcome, and we hope to return to Bolivia soon for another academic (or other!) activity.

Excerpted from the article CristAL - Crystallography News from Latin America by Graciela Díaz de Delgado, ACA RefleXions, Spring 2017, pp. 7-9

IYCR LEGACY

OpenLab Senegal, November 20 - December 2, 2017

www.iycr2014.org/events/openlabs/iucr-iupap-ictp-openlab-senegal

The IUCr-IUPAP-ICTP OpenLab Senegal 'Laboratory and synchrotron X-ray crystallography: applications to emerging countries' will take place November 20 - December 2, 2017, in Ziguinchor, Senegal.

Crystallography is an interdisciplinary science that finds application in technological areas of strategic importance for emerging countries, such as cement, mining, electronic and pharmaceutical research. Special emphasis will be placed on the role of advanced synchrotron light sources.

Crystallography enables the inner properties of matter and accurate atomic structures of molecules, materials, proteins and any kind of compound to be accessed; without the knowledge of the structure, the functionality of a given material cannot be understood and therefore improved. Mining and cement companies use crystallography for quality and purity control and for research aimed at developing novel materials; the pharmaceutical industry uses crystallography to identify the correct polymorph and understand the functionality of new medicines. Today synchrotron light sources complement laboratory X-ray equipment and allow access to unprecedented capabilities. Students will be encouraged to test their understanding of crystallography using single-crystal and powder portable diffractometers, which will be installed on site for at least the duration of the school.

Directors: C. Lecomte (U. de Lorraine, France), M. Zema (IUCr and U. of Pavia, Italy), S. Onesti (Elettra Sincrotrone Trieste, Italy), M. Camara, (U. of Assane Seck, Ziguinchor, Senegal), P. Kenfack (U. of Dschang, Cameroon) and J. Niemela (ICTP, Trieste, Italy).

ICTP Scientific Contact: S. Scandolo, ICTP, Trieste, Italy.

Local Organizers: M. Camara, D. Kobor, C. Balde and A. Gassama (all from the U. of Assane Seck, Ziguinchor, Senegal).

Topics will include:

- X-ray and neutron diffraction physics
- powder and single-crystal methods
- physical properties of crystals
- symmetry and space groups
- structural refinement
- crystallographic databases
- applications to cement, mining, electronic and pharmaceutical industries
- nano-crystallography
- bio-crystallography
- quasicrystals
- synchrotron light sources

Partners:	LAAMP, ALBA, Laboratoire Léon Brillouin, AIC, AFC

Registrations are open at http://indico.ictp.it/event/8243/.

IUCR ACTIVITIES

IUCr2017 Special Activities Programme

For the first time at an IUCr Congress, a major programme of events has been timetabled to showcase the strategic community initiatives, outreach efforts and data and publishing activities of the IUCr and its partners. These are complementary to the traditional scientific sessions organised by the IUCr's scientific Commissions, but they demonstrate the much wider range of activities in which the Union is engaged.

Scientific data and information

KN-18. The science is in the data

Thursday, August 24, 18:00-19:00, Hall 6
John R. Helliwell



Understanding published research results should be through one's own eyes and thus include the opportunity to work with the raw diffraction data to check the various decisions made in the analyses by the original authors. Today preserving raw diffraction data is technically and organisationally viable at a growing number of data archives, both centralised and distributed, which are empowered to register data sets and obtain a preservation descriptor or 'digital object identifier'. Secondly, key policy makers are also looking to see more rapid science discovery for urgent societal problems, such as improved treatment of disease and mitigation of environmental pollution; facilitating early data sharing is a key part of their new 'Open Science' vision. A third role of preserving raw data is to provide understanding of where we fail in our analyses. Individual case studies of this will be provided. Finally, the education of the new generation of crystallographers and the continuing professional development of existing crystallographers should include the issue of raw data management and reuse.

W5. COMCIFS Dictionary Writing Workshop

Monday, August 21 , 09:00-16:00, MR 1.04
Chair: James Hester

The Dictionary Writing Workshop will provide participants with the skills to create high-quality dictionary definitions and complete data dictionaries suitable either for inclusion within the CIF/mmCIF framework

or as standalone dictionaries for use within other data frameworks, such as NeXus. Participants will be guided during practical sessions towards the goal of producing a complete dictionary or set of additional definitions in a scientific domain of interest to them.

Aims: at the end of the workshop, participants will be able to:

- Understand the role that dictionaries play in data specifications
- Understand how datanames are stored in a variety of data formats (including '3-column ASCII'/CIF/NeXus)
- Construct a high-quality dataname definition
- Construct a DDL2/m domain dictionary potentially building on previously existing dictionaries and/or prevously existing data standards

Participants wishing to construct a dictionary for a particular domain are encouraged to bring a wish list of the items for inclusion in the dictionary to the workshop, and will be guided throughout the workshop in constructing their particular dictionary.

Prerequisites: There are no specific requirements. In particular, no programming or CIF experience is assumed.

MS-053. The scientific value of raw data

Thursday, August 24, 14:55-17:30, MR 2.02
Chairs: Loes Kroon-Batenburg, Brian McMahon
Speakers: George Phillips, Marek Grabowski, James Parkhurst, Christopher Chantler, Andreas Foerster, Kamil Dziubek

The activities of the Diffraction Data Deposition Working Group have highlighted the growing importance of retaining at least some raw data sets. Long-term archival demands that data files are well characterised so that they can subsequently be interpreted and evaluated. Detailed metadata characterisation is important for this. Contributions will highlight the work in the past triennium of CODATA and DDDWG in working towards these objectives which will form one of the invited presentations.

MS-099. Crystallographic data and structure validation from data collection to publication - IUCr setting standards

Sunday, August 27, 10:30-13:05, MR 2.03-2.04
Chairs: Wladek Minor, Anthony Linden
Speakers: Anthony L. Spek, Loes Kroon-Batenburg, James Simpson, Jan Van De Streek, John Westbrook



The IUCr has always been inclusive in science coverage and ability to respond to new and emerging technologies, approaches and challenges, from synchrotrons in the latter quarter of the last century to FELs, cryo-EM and powerful pulsed neutron sources in this decade. New approaches and methods will continue to develop. The IUCr and its journals have always led the way in providing a rigour in data and structure validation for its publications, setting the standards for other leading journals. With an expanding range of commissions representing a whole range of techniques and data, it is timely to hold a microsymposium that brings the whole community together.

MS-107. Robust programming for CIF, NeXus, and related file structures

Sunday, August 27, 14:55-17:30, MR 2.02
Chair: John Bollinger
Speakers: James Hester, Brian McMahon, Robert Hanson, John Westbrook, John Bollinger, Herbert Bernstein

A new CIF syntax (CIF2) has recently been published, together with a high-quality, freely available C programming library for accessing CIF1 and CIF2 files. In parallel, the machine-readable language used in the CIF dictionaries has been upgraded, including the provision of machine-interpretable algorithms for specifying relationships between datanames.

Taken together, these features provide rich new opportunities for enhancing the behaviour and scope of CIF applications.

Education and training

MS-016. New approaches in crystallographic teaching

Tuesday, August 22, 14:55-17:30, MR 2.01
Chairs: Louise Dawe, Peter Moeck
Speakers: Robert Hanson, Gemma de la Flor Martin, Saulius Grazulis, Helen Maynard-Casely, Amy Sarjeant, Bill Duax



Crystallography is a rich and interdisciplinary science, although in the past 20 years, crystallography as a science has largely migrated from a research speciality to a technique employed by a broad user community. During this same period, which has coincided with the growth of the World Wide Web, the crystallographic community has come to rely increasingly on non-traditional curricular resources for instruction, such as web pages and, more recently, online courses. The new pedagogy made possible by Web developments can facilitate deeper understanding among those who use and consume

crystallographic information in related fields, and enable those teaching crystallography to transmit the fascination and excitement of the field necessary to attract a future generation of professional crystallographers.

From Editorial to special issue of Journal of Applied Crystallography on Crystallography education and training for the 21st century (October 2010).

MS-032. Crystallography courses around the world

Wednesday, August 23, 14:55-17:30, MR 1.05
Chairs: Annalisa Guerri, Juan Manuel Garcia Ruiz
Speakers: Amy Sargeant, Alessia Bacchi, Diego G. Lamas, Michele Zema, Fermín Otálora, Andreas Roodt, Ivana Kuta Smatanova, Dubravka Sisak Jung

Formal courses have all but disappeared from university course offerings, particularly in the United States, and in many European universities former departments of crystallography have been dedicated to other research fields. Crystallography is rarely covered in undergraduate textbooks. These realities have led to the growth of and dependence on independently funded workshops and summer schools in crystallography, as well as in related scientific areas (*e.g.* materials science) containing relevant aspects of crystallography. Notable examples are the well known and highly regarded Cold Spring Harbor X-ray Methods in Structural Biology course, held annually since 1988, and the European Crystallography Schools, now in their fourth edition.

Based on Editorial to special issue of Journal of Applied Crystallography on Crystallography education and training for the 21st century (October 2010).

MS-044. Structural databases as teaching tools - part A (macromolecules)

Thursday, August 24, 10:30-13:05, MR 2.02
Chairs: Joel Sussman, Christine Zardecki
Speakers: Jaime Prilusky, Shuchismita Dutta, Urmila Kulkarni-Kale, Matthew J. Conroy, Alexey Kikhney, Hirofumi Suzuki

The availability of three-dimensional macromolecular structures not only drives research and development worldwide, but also supports educational initiatives that impact students and researchers in different fields. This microsymposium will present a broad look at structures in education, including curriculum development, online encyclopedias that explore structure-function relationships, visualization tools, and other teaching tools.

MS-045. Structural databases as teaching tools - part B (organics, minerals)

Thursday, August 24, 10:30-13:05, MR 2.03-2.04
Chairs: Amy Sarjeant, Graciela Delgado
Speakers: Louise Dawe, Simon Coles, José Miguel Delgado, Edgar Eduardo Villalobos

Crystallographic databases provide a wealth of information on the solid-state structures and chemical properties exhibited by the molecules and compounds contained therein. Such collections of data can be

extremely powerful educational tools. By providing students with real-world experimental results and interactive three-dimensional representations of solid-state structures, these databases facilitate comprehension of difficult chemical concepts. This session will focus on pedagogical strategies that incorporate chemical crystallography databases in the classroom and laboratory setting to teach crystallography, chemistry and materials science.

MS-087. How does crystallography help you in your career?

Saturday, August 26, 14:55-17:30, MR 1.06
Chairs: Ashwini Nangia, Soorya N. Kabekkodu
Speakers: Sudhir Nambiar, Anant Paradkar, José Miguel Delgado, Martin Viertelhaus, Soorya N. Kabekkodu

The next steps after a PhD can often seem daunting and confusing for a young crystallographer. This microsymposium may alleviate that stress by offering some answers and guidance to young crystallographers as well as senior Post-docs about when and how to start looking for a job; how to sell a PhD's qualities and qualifications to employers; how to start a career in academia or in industry and what is the difference between them; how to find any other alternative jobs for a PhD; and real-life examples of the path of PhD graduates.

Outreach

MS-080. Emerging science in the emerging world

Saturday, August 26, 10:30-13:05, MR 2.02
Chairs: Claude Lecomte, Michele Zema
Speakers: Gihan Salah Kamel, Robert Kingsford-Adaboh, Altaf Hussain, Suzanna Ward, Aldo Craievich, Andrea Lausi, Marielle Yasmine Agbahoungbata, Sandro Scandolo, David Dodoo-Arhin, Patrice Kenfack Tsobnang, Rishad Kunafiev, Kim Ngun Bun, Dinesha Hansamali Perera, Tonle Kenfack Ignas



The IUCr is continuously reaching out to wider communities. In IYCr2014, it engaged in the launch of a new journal IUCrJ with its own name, brought nations together through crystallographic summit meetings in three continents and held a number of OpenLabs in emerging crystallographic countries all around the

globe. Many emerging countries have as yet rather small crystallographic communities. Internet access, new training and education efforts through schools/video lectures and remote access to research instruments and the opportunity to work on local developmental problems are spurring these young scientific communities to produce work of increasing quality.

This microsymposium will allow brief oral presentations of a number of research projects from representative countries covering the whole spectrum from Brazil to Bangladesh.

MS-113. Anticipating the harvest: post IYCr

Monday, August 28, 10:30-13:05, MR 1.05
Chairs: Juste Jean-Paul Ngome Abiaga, Michele Zema
Speakers: Juste Jean-Paul Ngome Abiaga, Daniel Nyanganyura, Areej Abuhammad, Claude Lecomte, Brian McMahon, Diego G. Lamas, Bujar Dida, Altaf Hussain



An important goal of IYCr2014 was prompting the crystallography community to look outwards and engage with other Scientific Unions, with bodies promoting the development of science, with new initiatives in curriculum development, and with schoolchildren and the general public. This session will describe ongoing programmes and invite ideas on ways in which the IUCr can contribute even more to the development of scientific education and research infrastructure. A number of strategic partnerships will be described, listing their achievements to date and their future prospects.

Art and cultural heritage

MS-071. Crystallographic patterns in art and cultural heritage

Friday, August 25, 14:55-17:30, MR 2.02
Chairs: Louise De Las Penas, Rima Ajlouni
Speakers: Youssef Aboufadil, Peter Moeck, Louise De Las Penas, Rima Ajlouni



These presentations explore crystallographic symmetries and quasi-periodic structures in art and artefacts, with examples drawn from traditional architectural and weaving practices, as well as cultural creations in the modern computer age.

MS-104. Synchrotron measurement in conservation and cultural heritage

Sunday, August 27, 14:55-17:30, MR 1.05
Chair: Eric Dooryhée
Speakers: Marine Cotte, Apurva Mehta, Bernadette Fruehmann, Alison Edwards

Synchrotron radiation continues to be an invaluable diagnostic tool in the analysis of artistic materials, from hard matter (pigments, glasses, ceramics) to soft matter (papyri, plastics) or any combination thereof (*e.g.* modelling materials, photographs). Analyses are usually carried out on tiny fragments from historical artworks and can be completed by the analysis of model samples, mimicking historical objects and effects of aging. Other advanced structural techniques such as neutron tomography are now coming to the fore, yielding insights for example into the deadening of guitar strings with age.

MS-114. Crystallography and cultural heritage: from microsampling to non-invasive techniques

Monday, August 28, 10:30-13:05, MR 1.06
Chairs: Manfred Schreiner, Serge Cohen
Speakers: Koen Henri Janssens, Wieslaw Lasocha, Gilberto Artioli, Marek Kotrly, Roman Senin, Bernadette Fruehmann, Rita Wiesinger, Alicja Rafalska-Lasocha, Simona Quartieri, Natalia Kolobylina

This session presents an overview of the research programmes being carried out in the interdisciplinary fields of art history, archaeology and conservation-restoration on one side and scientific disciplines on the other. In general, so-called non-invasive analytical techniques are required for the characterization of the materials used in art or archaeological objects. However, for detailed information about the original materials as well as their long-term stability (corrosion behavior), small samples are indispensable. In such cases, the various non-destructive techniques of XRD allow the study of the microstructure as well as the corrosion products formed during the centuries or even a millennia that an artwork was exposed to the ambient atmosphere or to the soil.

New directions

MS-021. Terminology issues in crystal engineering

Wednesday, August 23, 10:30-13:05, Hall 6
Chairs: Christer Aakeröy, Carolyn P. Brock
Speakers: Gautam R. Desiraju, Pierangelo Metrangolo, Jagadese J. Vittal, Len MacGillivray, Christer Aakeröy

A Dictionary project on crystal engineering nomenclature is proceeding under the aegis of IUCr and IUPAC, and sanctioned by ICSU. Terms in crystal engineering may be important in litigation concerning crystal forms of active pharmaceutical ingredients. IUCr approval for a term will carry weight in the courts. There are several terms where there has been a lot of heavy debate amongst influential scientists in this area. Individual talks on *e.g.* 'hydrogen bond', 'halogen bond', 'polymorph', 'pseudopolymorph' and 'cocrystal' from some of these scientists will lead to a popular, lively and indeed humorous session.

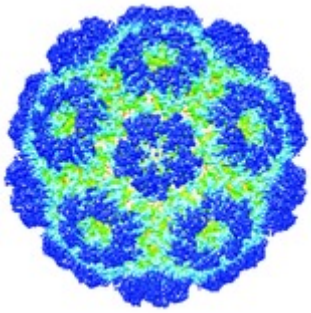
MS-095. Crystallography for space sciences



Sunday, August 27, 10:30-13:05, MR 1.05
Chairs: Hanna Dabkowska, Juan Manuel Garcia Ruiz
Speakers: David Blake, Tomoki Nakamura, Helen Maynard-Casely, Yuki Kimura, Giuditta Perversi

Building on the 'Crystallography for Space Sciences' school in Mexico, this will be an interesting session covering a relatively new field of active research, and strengthening ties with COSPAR.

MS-109. CryoEM: method of the decade



Monday, August 28, 10:30-13:05, Hall 4
Chairs: Richard Henderson, Samar Hasnain
Speakers: Yifan Cheng, Nikolaus Grigorieff, Bridget Carragher, Werner Kühlbrandt, Helen Saibil

Following the Gjonnes Medal award lectures given by Nigel Unwin and Richard Henderson, leaders of the field will celebrate the success of cryoEM. IUCrJ has made special efforts to welcome the cryoEM community and has appointed Richard Henderson, Werner Kühlbrandt and Sriram Subramanian to its editorial board. Similar actions are taking place on the IUCr's structural biology journals.

Details correct at time of going to press.

MEETING REPORT

13th International Conference on Quasicrystals (ICQ13)

Kathmandu, Nepal, September 2016

The 13th International Conference on Quasicrystals (ICQ13) was held in Kathmandu, Nepal, from September 18 to 23, 2016. The first event in this successful series of conferences on quasicrystals, the International Workshop on Aperiodic Crystals, was held in Les Houches, France, in 1986. This was followed by the International Workshop on Quasicrystals in Beijing, China, in 1987 and the International Meeting on Quasicrystals in Vista-Hermosa, Mexico, in 1989. Thereafter, a series of ICQs took place respectively in St Louis, MO, USA, in 1992 (ICQ4); Avignon, France, in 1995 (ICQ5); Tokyo, Japan, in 1997 (ICQ6); Stuttgart, Germany, in 1999 (ICQ7); Bangalore, India, in 2002 (ICQ8); Ames, IA, USA, in 2005 (ICQ9); Zürich, Switzerland, in 2008 (ICQ10); Sapporo, Japan, in 2011 (ICQ11) and Cracow, Poland, in 2013 (ICQ12).

The Opening Ceremony







ICQ13 covered a wide range of topics on quasicrystals: formation, growth and phase stability; structure and modeling; mathematics of quasiperiodic and aperiodic structures; transport, mechanical and magnetic properties; and finally, surfaces and overlayer structures. In addition, other aspects of materials science such as metamaterials, polymer science, metallic glasses and metallic alloys were discussed. The conference also reviewed the state-of-the-art of quasicrystal research and its future direction.

ICQ13 was attended by 113 participants (including 15 accompanying persons) from 22 countries, including 26 PhD or master students. There were 13 invited talks (including a public lecture by the 2011 Nobel Laureate in Chemistry, Dan Shechtman), 3 tutorial lectures, 50 contributed talks and 36 poster presentations. The conference was truly interdisciplinary - comprising theoretical and experimental physicists, chemists, materials scientists and mathematicians.









The proceedings of the conference have been published in the open-access Journal of Physics: Conference Series Volume 809 (2017) (http://iopscience.iop.org/issue/1742-6596/809/1). The papers have been reviewed in the regular refereeing process. Among the 35 proceedings received, 30 have been accepted for publication.



Meeting with the President of Nepal.

The conference itself was held at the Dhulikhel Lodge Resort. The public lecture was organised at the central campus of Trubhuvan U. in Kirtipur, hosted jointly by the Nepal Physical Society and the Central Department of Physics, while the tutorial lectures were held at Kathmandu U. These two events were open to local researchers and students. A special ceremony was organised for the inauguration of ICQ13, which was addressed and attended by the vice-chancellors of Tribhuvan U., Kathmandu U., Nepal Academy of Science and Technology (NAST), and representatives of various professional organisations, including the Nepal Government.

The Jean-Marie Dubois Award for Excellence in Quasicrystals (2016) was presented to Marek Mihalkovič for the theoretical work that has enabled and demonstrated the simulation of thermodynamic and dynamic properties of quasicrystals - based on realistic atomic-scale models and energetics. The Jean-Marie Dubois Award was established to recognize important, sustained research on any aspect of quasicrystals in the last 10-year period preceding the award. The prizes for best student presentation were awarded to Ito Natsu from Toyo U., Japan, for her paper titled 'Synthesis and magnetic properties of the Au-Al-Yb approximant' and Nicolas Macé from U. Paris-Saclay, France, for his paper titled 'Gap structure and topological indices on the Fibonacci quasicrystal'.

We gratefully acknowledge the generous financial support from the IUCr, the European Integrated Center for the Development of New Metallic Alloys and Compounds (C-MAC), the International Centre for Diffraction Data (ICDD), Rigaku Oxford Diffraction, Embassy of Israel Kathmandu, Deutsch-Nepalische Gesellschaft, TBI Group, Phul Kumari Mahato Memorial Trust, Nepal Science Foundation Trust, Holy-Cow, officials of Non-Resident Nepali Association (NRNA) and NRNA-Australia.



Participants at the 13th International Conference on Quasicrystals (ICQ13) in Kathmandu, Nepal, September 18-23, 2016.

We would like to express our sincere thanks to the members of the Organising Committee, Program Committee and International Advisory Board, invited speakers, session chairs, editorial board members and reviewers of the conference proceedings and all others for their support and involvement in the conference.

Last, but not least, we would like to thank the Local Organisation Committee of ICQ13 - chaired by Narayan Prasad Adhikari - for the efforts that made the conference so successful. We would also like to express our gratitude for the support we received from the U. Liverpool, UK, Tohoku U., Japan, and Tribhuvan U., Nepal.

We hope that the conference helped to promote the struggling tourism sector of Nepal after the country was hit by devastating earthquakes in 2015. We thank the Nepal Tourism Board, Atithi Devo Bhava, Chandragiri Cable Car and Cultural Bands for helping ICQ13 participants explore the culture, history and natural beauty of the Himalayan country Nepal during their stay.

The 14th International Conference on Quasicrystals (ICQ14) will be held May 26-31, 2019 in Bled, Slovenia.

Hem Raj Sharma and An Pang Tsai, Conference Chairs

MEETING REPORT

Second Meeting of the Latin American Crystallographic Association

Mérida, Yucatán, México, October 2016



Participants of the Second Meeting of the Latin American Crystallographic Association (LACA), Mérida, Yucatán, México, October 22-27, 2016.

A new meeting of the Latin American Crystallographic Association (LACA) took place in Mérida, Yucatán, México, October 22-27, 2016. This was LACA's second meeting after the organization was accepted as a Regional Associate of the IUCr by the General Assembly of the 23rd IUCr Congress celebrated in Montreal, Canada, in 2014. The II-LACA meeting was organized by Sociedad Mexicana de Cristalografía (SMCr) as part of the VI Mexican Synchrotron Light Users Meeting and the VIII National Congress of Crystallography of the Mexican Crystallographic Society.

The LACA organization was created at a meeting attended by representatives from Argentina, Brazil, México, Chile, Colombia, Cuba, Perú, Uruguay and Venezuela, held during the IX annual meeting of the Argentinean Crystallographic Association (AACr) in 2013 at U. Nacional de Córdoba (UNC), Córdoba, Argentina. The first formal meeting of LACA was held in São Paulo, Brazil, at the Institute of Physics of the U. de São Paulo, in September 2015, in conjunction with the XII meeting of the Brazilian Crystallographic Association (ABCr).

The scientific program of II-LACA included five plenary lectures, 20 invited lectures and close to 100 poster presentations by participants from Argentina, Bolivia, Brazil, Chile, Colombia, Costa Rica, México, Uruguay, Venezuela and from the USA, Spain and Belgium. Miguel José Yacamán from the Physics Department of U. of Texas at San Antonio delivered the first plenary lecture.

Other invited speakers included Marvin Hackert (U. Texas at Austin, President of the IUCr and Past President of the ACA), Santiago García Granda (U. Oviedo, Spain, member of the Executive Committee of the IUCr), Amy Sarjeant (CCDC, USA, Current President of the ACA), Gabriela Aurelio (CAB-CNEA, Argentina), Aldo Craievich (U. São Paulo, Brazil), Miguel Delgado and Graciela Delgado (U. Los Andes, Venezuela), Márcia Fantini (U. São Paulo, Brazil), Diego G. Lamas (U. San Martín, Argentina), Stavros Nicolopoulos (Nanomegas, Belgium), Bruce Noll (Bruker, USA), Oscar Piro (U. La Plata, Argentina) and Iris Torriani (U. Campinas, Brazil). Several distinguished Mexican scientists were also invited speakers, among them Otilio Acevedo Sandoval (UAEH, Hidalgo), Gerardo Aguirre (IT-Tijuana), Sylvain Bernés (IF-BUAP, Puebla), Luis Fuentes Cobas (CIMAV, Chihuahua), Mayra Cuéllar Cruz (U. de Guanajuato, León), Gonzalo González (IIM-UNAM, México City), Erick A. Juárez Arellano (U. del Papaloapan, Oaxaca), Rufino Lozano Santacruz (IG-UNAM, México City), Abel Moreno Cárcamo (IQ, UNAM, México City), María Elena Montero Cabrera (CIMAV, Chihuahua), Teresa Pi Puig (IG-UNAM, México City) and Guadalupe de la Rosa Alvarez (U. de Guanajuato, León).

In keeping with the tradition and format of the SMCr events, six workshops and courses on different crystallographic topics took place October 22-23 at the Mérida Unit of CINVESTAV. They were: 'Crystallography Databases: I. Introduction to CSD-Enterprise and II. The ICDD's Powder Diffraction File', a

workshop led by Amy Sarjeant and Paul Sanschagrin (CCDC), Thomas Blanton (ICDD), Graciela Díaz de Delgado and Miguel Delgado (ULA); 'Synchrotron Crystallography', coordinated by Abel Moreno Cárcamo (IQ, UNAM, México City); 'Physical Properties of Crystals', taught by Jacques Soullard Saintrais (IF-UNAM, México City); a 'Crystal Growth' course run by Héctor Riveros Rotge (IF-UNAM, México City); and 'Basic Crystallography' and 'Roentgen Crystallography' courses, for which the instructors were Alfredo G□ómez Rodríguez (IF-UNAM, México City) and Rubén Alfredo Toscano (IQ-UNAM, México City), respectively. Graduate students and young scientists participated in these courses.

Three poster sessions were held in the exhibition hall, along with an equipment and software display from manufacturers including Bruker (Bruker Mexicana, S.A.), Micra-Nanotecnología/Nanomegas, PANalytical (PANalytical México), Rigaku (Martek, S.A.), Stoe-Inel (Spectramex, S.A.), Thermo Scientific (Falcón/División Analítica), Alta Tecnología de Laboratorios, S.A., and the International Centre for Diffraction Data (ICDD). In each poster session, the two best posters presented by students were selected. A certificate and a piece of Mexican artisanry were presented to each winner at the farewell dinner. The IUCr and ICDD provided funds to cover the travel and accommodation expenses for about 20 students.

Patricia Quintana Owen (CINVESTAV-Unidad Mérida, IPN) and Rudy Almicar Trejo Tzab (U. Autónoma de Yucatán) for the Local Committee, the National Committee headed by José Reyes Gasga (IF-UNAM), Lauro Bucio Galindo (IF-UNAM), Jesús Ángel Arenas Alatorre (IF-UNAM) and Gustavo Tavizón Alvarado (FQ-UNAM), and the support team headed by Gabriela García Rosales, Secretary of SMCr, did a superb job in the organization of all the aspects of these events.

The General Assembly of LACA met during the event to discuss the status and progress of the organization and to elect a new Executive Board. The members elected are Diego G. Lamas (President, Argentina), José Reyes-Gasga (Vice-President, México), Graciela Díaz de Delgado (Secretary, Venezuela) and Iris Torriani (Treasurer, Brazil). An Adjunct Secretary of the board (José Vega Baudrit, Costa Rica) was elected after consulting the national crystallographic organizations.

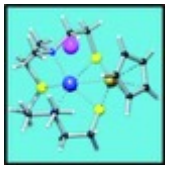
Since the 24th Congress and General Assembly of the IUCr will take place in Hyderabad, India, in 2017, the next meeting of LACA is scheduled for 2018 in Valparaíso, Chile, organized by Mauricio Fuentealba (Pontificia U. Católica de Valparaíso, Chile). The venue for the 2019 LACA is under consideration. Colombia is a strong candidate, with José Antonio Henao as the organizer.

Excerpted from the article CristAL Crystallography News from Latin America by Graciela Díaz de Delgado, ACA RefleXions, Spring 2017, pp. 7-9

MEETING REPORT

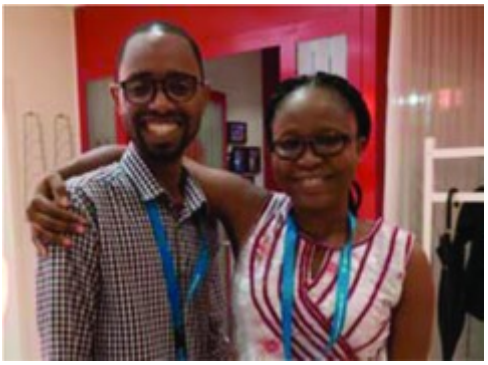
The Zürich School of Crystallography - Bring your Own Crystals

Zürich, Switzerland, June 2017



The 7th Zürich School of Crystallography was held June 11-22, 2017, within the Department of Chemistry at the U. of Zürich (UZH). The 20 participants comprised 1 BSc, 1 MSc and 11 PhD students, 2 postdocs, 2 junior and 3 senior academics. They came from 16 countries: Benin, China, Croatia, Finland, Germany, India, Italy, Kazakhstan, Lithuania, Mexico, Russia, Saudi Arabia, Senegal, Switzerland, Thailand and the UK. We had our usual popular 2:1 student:tutor ratio.

All of the participants were very enthusiastic and maintained their eagerness and dedication throughout the School. Everyone mixed well and chatted eagerly together and with the tutors over the meals and during the breaks. Some were just getting their feet wet in the field of crystallography, while others were more experienced, but all came away having learned something new and feeling better equipped to tackle structure determination on their own.













We were very impressed by two young scientists from Africa (Benin & Senegal), who were not only talented and keen to learn, but also eager to take their knowledge home in order to spread the word about crystallography in their region. These participants came highly recommended by Claude Lecomte and significant bursary support, donated by the IUCr, CCDC and UNESCO, was provided in order to facilitate their attendance.

The central goal of the School is to equip each participant with enough knowledge of the theory and practice of X-ray diffraction and single-crystal small-molecule structure determination so that they can competently determine their own structures when they return to their home laboratory. With this in mind, the practical sessions and example structures are designed to allow the participants to see behind the button-pushing, to learn about the actual procedures going on when various operations are performed, and to interpret whether or not the results obtained are appropriate. We successfully used the *Olex2* software once again this year and found it to be quite suitable in the School environment. The ever expanding range of special tools and options in the program for easily handling special modelling issues, such as disorder, is very useful. The daily schedule alternated lecture blocks and practical work so that the participants could readily associate the theory with the practical aspects. The practical work

included access to five diffractometers at the UZH and ETH Zürich campuses and a fully equipped computer classroom. The diffractometers included the modern Bruker Photon 100 and the newest Rigaku Oxford Diffraction Synergy instruments which are impressive in terms of speed, the availability of two radiation wavelengths and detector sensitivity.

The participants then worked on a data set collected from one of the samples they had provided. The ease of use of *Olex2* allows us to demonstrate more aspects of structure solution and refinement in a shorter time. On the final day, each participant sat a two-hour written exam either to obtain ECTS credit points or to self-test their knowledge. Each day concluded with a short discussion where participants can express their feelings about their experience that day.

This year we shortened the School by two days by dropping the scientific excursion and the ten minute participant presentations. We had been concerned that the participants were worrying too much about preparing their presentations from midway through the School, rather than concentrating on the material we were trying to teach. While giving a short presentation is good experience, we think that it is not essential for the aim of the School. A side benefit of the shorter School is the reduced subsistence costs. We concluded that this change was beneficial and will repeat the shorter format for the next School planned for June 2019.

The questionnaire filled in by the participants provided overwhelmingly positive feedback. The perennial criticism is the intensity of the School. Participants often wish for more breaks so they can digest the content better. To do so would add accommodation costs and require more time from our team of dedicated tutors, so we feel people have to accept that it is an intense block course, unlike a semester course. Each participant received a certificate and a copy of 'Crystal Structure Refinement, A Crystallographer's Guide to *SHELXL*' by Peter Müller, kindly donated by the IUCr and OUP. The personal impressions of one of the participants are given below.



Participants at the 7th Zürich School of Crystallography held in Zürich, Switzerland, June 11-22, 2017. We are very grateful for the generosity of the sponsors and supporters: Department of Chemistry of the U. of Zürich, Swiss Society of Crystallography, Cambridge Crystallographic Data Centre, European Crystallographic Association, International Union of Crystallography, Oxford University Press, Rigaku Oxford Diffraction, Dectris Ltd, Oxford Cryosystems, Hotel Coronado in Zürich, the Chemistry Platform of the Swiss Academy of Sciences, and MiTeGen.

Tony Linden and Hans-Beat Bürgi, School Directors

The Zürich School of Crystallography 2017 - Report from a participant

The Zuürich crystallography school exceeded all of my expectations in terms of the quality of tutors, lectures, layout and venue. I was very impressed with the university, hotel and the convenience of the hotel being just a short walk through the park, which provided a nice place to relax in when we were able to.

Having a background in powder diffraction, I had previously not been happy with my grasp of some of the concepts of crystallography. These very difficult concepts were explained clearly and in several ways to us by the tutors. I feel so lucky to have been given the opportunity to learn from such experienced crystallographers, and having one tutor per pair of participants was incredibly beneficial to us. They all went above and beyond, very eager to answer questions at any time and spend time with participants - even late in the evening!

Since crystallography is used in so many areas of science, I was concerned about having many topics that weren't relevant. This was not the case and I ended up really learning a lot from the less relevant talks. My other main concern was about the intensity of the course, of which I was warned, however with so many breaks throughout the day and a carefully planned schedule alternating between lectures and practical sessions this wasn't a problem. The organisers clearly spent a lot of time working out the best way to arrange everything, and this made a huge difference.

The practical sessions were invaluable, especially being able to measure our own crystals on the instruments we use in our home institutions and then actually analyse this data. All the practical exercises were incredibly useful and taught us how to handle a variety of different challenges that we are likely to face. It was so enjoyable to interact with the tutors and other participants, I appreciated having a mixture of people from such different backgrounds to learn from and socialise with. Zürich is a beautiful place and we were lucky to have a day off to explore the city.

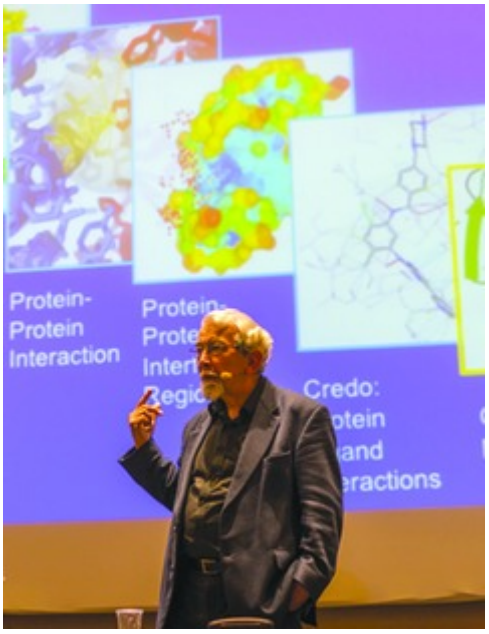
From this course I feel like I have gained knowledge of the theory of crystallography as well as all the practical aspects I need to go forward, including how to measure and solve crystal structures, which I would not have had the opportunity to learn elsewhere. This is vital for my current position as well as future career, as being taught correctly and thoroughly now will enable me to use this and pass on this knowledge in the future.

The course also gave me a greater appreciation of crystallography than I had previously, and has inspired me to consider new career paths within this area. I highly recommend this course for anyone wanting to gain a proper understanding of crystallography and learn from the best of the best!

Emily Reynolds, University of Oxford, UK

AWARDS AND PRIZES

Tom Blundell awarded the 2017 Ewald Prize



Tom Blundell, Director of the Erice International School of Crystallography, describing advances in his laboratory's programme in drug discovery at the 2014 School on Crystallography in Structure-Based Drug Design. Photo by Jeff Blaney.



(l-r) Tom Blundell, Eddy Arnold and Michael Rossmann (1996 Ewald Prize winner) at the Erice International School of Crystallography in 2008.



Tom Blundell dances with his wife, Lynn, at the ECA Meeting in 2003 in Durban, South Africa. Photo by Eddy Arnold.



(l-r) Tom Blundell, Samar Hasnain and Louise Johnson at the 2011 Dedication of the Barkla X-ray Laboratory of Biophysics at the University of Liverpool.



Eddy Arnold, Tom Blundell and Paola Spadon in Erice, Sicily, cutting a cake commemorating the 40th Anniversary of the International School of Crystallography in 2014.
Tom Blundell has been awarded the 2017 Ewald Prize, recognizing his very broad contributions to the field of crystallography. Tom will receive the award at the IUCr triennial congress in Hyderabad on August 21, and will give a lecture following the award presentation. His Ewald lecture is marked by the publication of a feature article entitled 'Protein crystallography and drug discovery: recollections of knowledge exchange between academia and industry' in IUCrJ, 4, 308321 (2017).

Professor Sir Tom Blundell has been one of the worldwide leaders in crystallographic innovation, especially at the interface with life sciences, starting with his work on determining the structure of insulin with Dorothy Hodgkin. Tom has determined an exceptionally broad array of medically critical human-protein structures, has championed methods enabling drug design and discovery through structural optimization, crystallographic fragment screening, and computational modelling, and has been a leader in advanced crystallography education on the international scale.

Tom began his brilliant career in macromolecular crystallography as a postdoctoral associate with the 1964 Nobel Prize winner Dorothy Crowfoot Hodgkin at Oxford U., UK, and was a member of the team that solved the structure of insulin, the first three-dimensional structure of a protein hormone. Tom has established the molecular structures and mechanisms of a remarkable array of medically significant human proteins, including polypeptide hormones (insulin, glucagon, pancreatic polypeptide and oxytocin), growth factors (NGF, FGF, HGF/SF), DNA repair factors (RAD51/BRCA, DNA-PKcs, PAXX), lens crystallins proteins, and aspartic proteases (renins, HIV protease), among many others, often in complex with receptors or small-molecule ligands. His group's highly creative work on building advanced computational tools for structural bioinformatics (such as *Composer*, *Modeller*, *Fugue*, *SDM* and *mCSM*) and chemoinformatics (*CREDO*, *CHOPIN*) has enabled structure-informed design of small-molecule drugs and engineered macromolecules. He has pioneered the use of crystallography in fragment-based drug discovery, both in academia and through the co-founding of Astex, moving many candidate drugs into clinical trials.

Tom has been heavily involved in education, first teaching in Brasenose and Linacre Colleges in Oxford U. until 1973, before moving to Sussex briefly to work in Biological Sciences and then between 1976 and 1996 as Bernal Professor of Crystallography at Birkbeck, where he developed a major multidisciplinary crystallographic team researching on a range of themes, from materials to macromolecules, with extensive teaching programmes. In 1996 Tom moved to the Sir William Dunn Chair of Biochemistry in Cambridge, where crystallography remains a central experimental theme in understanding complex multicomponent cell regulatory systems. Tom has been the Director of the International School of Crystallography at Erice since 1980 when Dorothy Hodgkin stepped down as the director after a four-year stint. Tom's commitment to crystallographic education is demonstrated by his uninterrupted engagement as the Erice School director for nearly 40 years, contributing to the education of thousands of crystallographers through the yearly courses on advanced topics in crystallography.

Tom has also managed to find time to be an elected Labour Councillor in charge of city planning in Oxford, an advisor to Prime Minister Margaret Thatcher, a Chief Executive of UK research councils, including founding CEO and Chair of the Biotechnology and Biological Sciences Research Council, Chairman for six years of the Royal Commission on the Environment, and President of the UK Science Council. Tom's scientific achievements and services to science have been recognized through many awards and prizes including Fellowship of the Royal Society (1984), FEBS Krebs Medal (1987), the Royal Society's Bernal Medal (1998) and a Knighthood in 1997. His international stature is evidenced by the many high honors he has received. His honorary doctorates from 16 universities include one from the University of Liverpool where he, together with Dame Louise Johnson, opened the Barkla X-ray Laboratory of Biophysics in July 2011. Tom's book co-authored with Louise, *Protein Crystallography*, remains the best treatment of the subject on many fronts.

Tom's son, Ricky, a computer scientist, and his wife, Raffy, have produced two wonderful grandchildren, Giorgio and Leandro. Tom and his wife/long-time co-worker, Dr Bancinyane Lynn Sibanda Blundell, originally from Zimbabwe, have two beautiful daughters: Kelesi, now a lawyer, and Lisa, a medical doctor, who share their parents' passion for world travel.

Eddy Arnold and Samar Hasnain, also see ACA RefleXions, Spring 2017

BOOK REVIEW

International Tables for Crystallography, Volume A, Space-group symmetry. 6th edition

Edited by Mois I. Aroyo. Wiley, 2016. Pp. xxi + 873.
Price GBP 295.00, EUR 354.00 (hardcover). ISBN 978-0-470-97423-0.



Volume A of *International Tables for Crystallography* approaches its 100th birthday. In fact, although it first appeared under this title only in 1935, its predecessor is the book by Wyckoff (1922), which already contained lists of general and special equivalent positions (later to be called Wyckoff positions) and, in its second edition (Wyckoff, 1930), also three-dimensional drawings of the symmetry elements within the (conventional) unit cells of most of the space-group types.

This brand-new edition of Volume A looks smaller than the previous one, despite the almost identical number of pages (873 *versus* 911); this has been achieved by using a glossy paper which is thinner but no less robust than that for the previous edition. The corresponding decrease in weight is a side effect that will certainly be appreciated by the reader. The sixth edition presents many changes, and many improvements, with respect to the fifth edition (denoted *ITA*5 in the following), which is now 15 years old (although minor corrections have been published in the meantime). One of the most significant improvements is the introductory material in Part 1, where, using the matrix formalism, the authors have made a remarkable effort to offer a homogeneous text of educational nature explaining the different kinds of symmetry information found in the tables.

The daily user of crystallographic techniques is certainly most familiar with (and interested in) the space-group tables. We therefore start our analysis with the changes in this part of the volume. The most evident difference is in the cubic space-group types, where the diagrams of the general positions have been completely redrawn using *VESTA* (Momma & Izumi, 2011) and are now readable and understandable. For the holohedral groups, the general-position diagrams are now also shown in perspective projection (in the online edition these diagrams are shown for all cubic groups). Another change is the disappearance of the lists of maximal subgroups and minimal supergroups; these lists were incomplete and therefore potentially misleading for the inexperienced user. The complete information is today available in Volume A1 (Wondratschek & Müller, 2010) so there is no reason to keep a partial, highly incomplete version in Volume A. In *ITA*5, each space-group type was presented over two pages (with a few exceptions for some hexagonal and cubic cases, which spanned over three pages): the diagrams and the information about the origin, asymmetric unit and symmetry operations on the left, the rest on the right. In the new edition, the removal of the incomplete group-subgroup information has enabled some groups to be presented on only one page.

More fundamental and profound changes in this new edition concern the theoretical chapters, which seem to be insufficiently known to and read by 'daily' crystallographers. As a matter of fact, the volumes in the series *International Tables for Crystallography* provide much more than tables and diagrams: they are the authoritative reference for each and every aspect of our discipline and contain the precise and exact definitions of every term and concept, accompanied by a wide range of examples. In *ITA*5, a few sections required some special effort by the reader, especially the newcomer to the field; this has been largely taken into account in the new edition, thanks also to new authors joining the team. The material has been considerably reorganized and some parts of the text have been completely rewritten, making them definitely more approachable while keeping the rigour that is mandatory in a reference text. We therefore proceed in our critique by making comparisons with *ITA*5.

The sixth edition has been reorganized into three parts: (1) *Introduction to space-group symmetry*; (2) *The space-group tables*; and (3) *Advanced topics on space-group symmetry*. Although at first sight this may seem to closely follow the structure of *ITA*5, with just some merging into a single part of what were separate parts, in fact some of the topics that were previously *after* the space-group tables, and thus implicitly considered to be 'advanced topics', now come *before* and have been largely rewritten. This is the case for Part 8 of *ITA*5 (*Introduction to space-group symmetry*), where basic definitions as well as fundamental concepts like crystal classes, crystal families, crystal systems and lattice systems, Wyckoff positions, crystallographic orbits, generators and normalizers are introduced. These topics now span Chapters 1.3 and 1.4, and have been extensively rewritten in a more reader-friendly way.

Part 1 bears the title *Introduction to space-group symmetry* and is divided into seven chapters. The first chapter, *A general introduction to groups*, is a new and most welcome addition. Authored by B. Souvignier, a rare example of a mathematician who is capable of conciliating the necessary rigour with a language close to that used by the daily crystallographer, this chapter concentrates in ten pages the basic definitions of groups, subgroups, cosets, homo- and isomorphisms and related concepts. It stands as the foundation of the whole construction that follows and should be digested by everybody who wants to go beyond the surface. Chapter 1.2 is devoted to the introduction and definition of symmetry operations and their matrix representation, symmetry elements and geometric elements. We find here part of the contents of Chapter 8.1 and Part 11 of *ITA*5, largely rewritten to give a more consistent and easy-to-follow presentation. The choice of moving this content to before, rather than after, the space-group tables is definitely wise.

Chapter 1.3 is *A general introduction to space groups*. Starting from the concepts of lattices and unit cells, it introduces the definitions of point and space groups as well as their classification into classes, systems and families. This content has been moved from Part 8 in *ITA*5 and rewritten, lifting what several readers experienced as a fog; now there is really no further excuse to mistake trigonal, rhombohedral and hexagonal (just to give an example): everything is crystal (*sic*!) clear.

Chapter 1.4 is devoted to a detailed presentation and explanation of space-group symbols, operations (including the Seitz symbols that were not used in *ITA*5, although they were already used in Volume E), the construction and interpretation of space-group diagrams, the choice of the generators, Wyckoff positions, Wyckoff sets and crystallographic orbits, and is completed by a few pages on sections and projections of space groups. Parts of the content of this chapter were previously scattered across different sections of *ITA*5 (*e.g.* Part 11) but most of the text is new or completely rewritten. This chapter is an absolute must-read for everybody who wants to be able to extract the wealth of information contained in the space-group tables. The text, accompanied by a number of examples (as is the case for all the chapters), is remarkably well written and easy to follow.

Chapter 1.5 deals with the transformation of coordinate systems. The first part of this chapter corresponds to the fifth chapter (*Transformations in crystallography*) of *ITA*5, with some additions, redrawn figures and new examples. The second part, about transformations of space-group descriptions, is brand new and is certainly of great help to the reader who is too often at risk of losing their way when

staring at non-conventional symbols. The third part of the chapter contains the synoptic tables of plane and space groups. With respect to Part 4 of *ITA*5, where the same tables were presented, we note two differences: (1) a completely rewritten and enlarged theoretical introduction, and (2) a more consistent notation for the extended symbols of space groups. In fact, while the short and full Hermann-Mauguin symbols of space groups present the symmetry *elements* along each symmetry direction, the extended symbols give the symmetry *operations*. For space groups containing the double glide plane (symbol *e*) the extended symbols should give the two glides (operations) instead of writing the glide plane (element) twice, as was the case in *ITA*5. This inconsistency has now been fixed. The tables are still partly incomplete, because for monoclinic groups the settings corresponding to a non-conventional unit cell with double volume (*S* instead of *P*; *F* instead of *C*) are absent. These are, however, present in the literature (Nespolo & Aroyo, 2016) and may perhaps be included in a future revision.

Chapter 1.6 is devoted to methods of space-group determination. We find the tables presenting the reflection conditions compatible with the various types of space groups (Part 3 in *ITA*5), now preceded by a detailed theoretical introduction about the information that can be obtained from diffraction data (this part makes a useful link with Volume B) and followed by guidelines for space-group determination in macromolecular crystallography, from powder diffraction and from electron microscopy. A wealth of information has been added with respect to *ITA*5. It is regrettable, however, that the extinction symbol has been removed. Apart from the bad choice of name, which is reminiscent of the incorrect yet often used term 'systematic extinctions', this symbol is widely used, for example in electron crystallography and in the analysis of the diffraction patterns of twins. The information needed to build the symbol is all present, but the handy and useful symbol is gone. We hope that it will be reinstated in the first reprint, whenever it comes out.

Chapter 1.7 is a short introduction to Volumes A1 and E, and is a very welcome addition that should help the reader to understand that Volume A, although extremely rich in information, is not the end of the story. Examples of group-subgroup relations, derivative structures, phase transitions, Bärnighausen trees, subperiodic groups and domain walls are presented. After reading this appetizer, the reader will certainly rush to discover a whole world beneath the usual three-periodic landscape of stand-alone structures. This chapter also supersedes Part 13 of *ITA*5 (*Isomorphic subgroups of space groups*).

Part 2, as we have mentioned, contains the well known tables of space groups. The theoretical introduction that came at the very beginning of *ITA*5 is now right before the tables, a much more reasonable choice especially for the occasional user.

Part 3 (*Advanced topics on space-group symmetry*) is divided into six chapters and includes the revised content of Parts 9, 10, 14 and 15 of *ITA*5 (the content of Parts 11 and 13 having been moved to Part 1). The text has been revised, corrected, updated and in some parts rewritten with new and extended content.

Chapter 3.1 is devoted to crystal lattices. With respect to the homonymous Part 9 of *ITA*5 we notice: (1) a significantly modified table (Table 3.1.2.3) of Delaunay classification, now with the corresponding projections along symmetry directions and Dirichlet (Voronoi) domains in the unit cell; (2) a detailed example of Delaunay reduction; and (3) an extended description of the metric restrictions imposed by symmetry, with emphasis on the limiting cases.

Chapter 3.2 deals with point groups and crystal classes, and is an extensively rewritten text with respect to Part 10 of *ITA*5. The 47 crystal and point forms are now presented not only in a table but also with the corresponding drawings (the change in the name of point form No. 7, from 'quad' to 'rectangular prism', is appreciated). A major update consists of a new section on molecular symmetry (Section 3.2.4), accompanied by the corresponding Wyckoff positions for point groups; chemists will certainly appreciate this addition.

Chapter 3.3 explains the space-group symbols and their use. It corresponds to Part 12 of *ITA*5 with a few updates. Chapter 3.4 is devoted to lattice complexes and is a significant update of Part 14 of *ITA*5. In particular, efforts have been made to clarify the relations and differences between lattice complexes, point configurations and crystallographic orbits. Their kinship often hides the differences and these concepts have often been the cause of some headache for the less-experienced reader. With this revised text, new light should now be shed on this landscape.

Chapter 3.5 inherits the text about normalizers that occupied Part 15 of *ITA*5, with the addition of a third category of normalizers (besides Euclidean and affine): the chirality-preserving Euclidean normalizers, *i.e.* the Euclidean normalizers of Sohncke types of space groups. In the literature we keep on seeing widespread confusion between the chirality of crystal structures (which is possible in any of the 65 Sohncke types of space groups) and that of groups (which concerns the 22 types forming 11 enantiomorphic pairs). A simple way to avoid this confusion is to look at the Euclidean normalizer: the condition for a group to be chiral is that it possesses only a chirality-preserving type of Euclidean normalizer.

The last chapter, 3.6, is brand new and provides an introduction to magnetic subperiodic groups and space groups. The tables of magnetic groups are available in electronic format (Litvin, 2013) and could never be printed as they are too extensive; this chapter gives guidelines on how to read and understand them.

In conclusion, the updates and improvements in this new edition of Volume A are too numerous and important to describe all of them in full detail. Special care has been taken to get a result approachable by the good-willed beginner, while nevertheless keeping the necessary rigour. No doubt every investigator working with condensed matter will greatly benefit by having a copy of this new edition handy on their shelf.

*Massimo Nespolo, from Acta Cryst. (2017). A**73**, 274-276*
https://doi.org/10.1107/S2053273317005526

References

Litvin, D. B. (2013). *Magnetic Group Tables. 1-, 2- and 3-Dimensional Magnetic Subperiodic Groups and Space Groups*. Chester: International Union of Crystallography. Freely available from www.iucr.org/publ/978-0-9553602-2-0.

Momma, K. & Izumi, F. (2011). *J. Appl. Cryst.* **44**, 1272-1276.

Nespolo, M. & Aroyo, M. I. (2016). *Acta Cryst.* A**72**, 523-538.

Wondratschek, H. & Müller, U. (2010). *International Tables for Crystallography*, Vol. A1, *Symmetry Relations Between Space Groups*, 2nd ed. Chichester: Wiley.

Wyckoff, R. W. G. (1922). *The Analytical Expression of the Results of the Theory of Space-Groups*. Washington: Carnegie Institution.

Wyckoff, R. W. G. (1930). *The Analytical Expression of the Results of the Theory of Space Groups*, 2nd ed. Washington: Carnegie Institution.