The First Pan-African Conference on Crystallography
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Greetings. As many of us are about to end another busy semester, we realize that summer is almost here, and August and IUCr XXIV are just a few months away.

I want to call special attention to a couple of articles in this issue of the IUCr Newsletter. I highly recommend the Cover Story on The First Pan-African Conference on Crystallography by Bill Duax starting on Page 9. The conference was held in Dschang, Cameroon last October where a mix of scientists, students and policy makers from 35 countries discussed ways that crystallography can be a vehicle for promoting science in Africa. Be sure to read the article all the way to the end. In addition to providing a nice summary of the scientific programme, Bill gives an insightful look at what he describes as “the most educational, exciting, and enjoyable meeting” of his life!

The other article is “Lighting the LAAMP” on Page 6. The IUCr had partnered with IUPAP to submit a proposal to the 2016-2019 ICSU Grants Programme. Just as my copy was being sent in for the last Newsletter, we received the very good news that this joint proposal was one of three funded by ICSU for this period. Congratulations to Michele Zema who led the IUCr efforts and our thanks to IUPAP and the many organizations (UNESCO, TWAS, etc.) and large scale facilities that supported this joint effort. The acronym LAAMP (Lightsources for Africa, the Americas and the Middle East Project) has been chosen for the initiative. The grant is for 300,000 euros over three years. In addition to this grant providing support for new initiatives, the scope of the proposal will help support a number of OpenLabs.

Speaking of ICSU, the fate of this organization is uncertain as active discussions are underway about a possible merger of ICSU with ISSC (International Social Science Council). A committee is working on how to address the concerns expressed by many of the International Unions about handling dues, identifying official national representation, etc. I invite your comments (positive or negative) about the merger. ICSU will meet in Taiwan later this fall to vote on the proposal.

The financial health of the IUCr continues to be a major concern. In March the Finance Committee, led by Malcolm Cooper, met in Leuven. The IUCr experienced another substantial deficit for 2016 and a shortfall is predicted again for 2017. The Finance Committee worked hard to identify savings and new income streams which could address these deficits and return the Union to a sound financial footing without seriously damaging its operations. The Finance Committee has recommended 8 measures that should ameliorate the situation within 12-18 months. Examples of items that will result in savings include making changes in the production of the IUCr Newsletter, reducing the Calendar Committee budget but compensating in part by shifting some of the funding of educational schools from the Calendar Committee to being supported by the Education and Outreach Fund. Examples of new income streams are implementing the Associates scheme, increasing open access charges, and recognizing that the new ICSU grant can support some OpenLabs. These recommendations have been reviewed and approved as necessary by the IUCr Executive Committee.

The IUCr Associates Programme will launch officially at the Congress in Hyderabad. The programme offers a series of benefits and tools to help you network, share ideas and discover more about crystallography. The benefits of joining include a 20% discount on the open-access fee for publishing an article in an IUCr journal, the ability to download 6 free articles from Crystallography Journals Online, a 50% discount for individuals purchasing the print version of International Tables for Crystallography, tools for professional networking, and many more. Joining the IUCr Associates Programme also supports many of IUCr’s charitable
activities. If you have registered for the Congress or visited the IUCr website, you have had the opportunity to indicate interest in the “pre-launch” pricing discount of 20% off of the Associates Programme joining fee (USD 160 or USD 48 for students and retired scientists), which gives you access to all the benefits for a period of 3 years. If you have any questions about the Associates Programme, please contact us at associates@iucr.org.

As noted earlier, the IUCr Outreach and Education Fund has been established to enable the continuation of many of the initiatives successfully launched during the International Year of Crystallography in 2014 and to pursue the objectives stated in the declaration “Crystallography for the Next Generation.” Namely, these goals are to increase awareness of crystallography, to build capacity in the developing regions of the world, and to forge collaborations with governmental, scientific and educational institutions and organizations aimed at facilitating strategic projects for the development of crystallography in all parts of the world. Requests for IUCr sponsorship through the IUCr Outreach and Education Fund must be submitted to the IUCr no later than 3 months before the event and should include a description of the event, tentative programme, and a provisional budget. All requests will be evaluated by the Oversight Committee for the IUCr Outreach and Education Fund. See the IUCr web site for additional details.

The only Regional Associate conference this year will be the ACA meeting in New Orleans, May 26–30. The theme of this year’s ACA Transactions Symposium is Cryo-Electron Microscopy. Of the four workshops offered on May 26, “Research Data Management”, organized by John Helliwell, Brian McMahon and Tom Terwilliger, is part of the IUCr’s Diffraction Data Deposition Working Group efforts focused on the issues of raw diffraction data preservation.

Of course, the major event for the summer is IUCr XXIV Congress in Hyderabad from August 21–28. The International Programme Committee and the Commission representatives have put together an outstanding programme along with additional events offered as part of a “parallel programme” with titles like “Salt of the Earth” and “Symmetry in India” (Page 22). Gau-
IUCr Crystallites blog

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

February 2017 saw the launch of the new IUCr blog, IUCr Crystallites (http://blogs.iucr.org/crystallites). The blog features news and opinion in crystallography and related disciplines.

It is our opportunity to bring you, in an easily digestible format, a snapshot of the rich variety of research, experts and resources available to researchers in the field, and let you know how work in this area is enabling others and having an effect on society.

Even though the IUCr is a relatively small Union, we support many good causes. In 2016 alone we provided travel bursaries to allow students and young scientists to attend 40 conferences and workshops spread over 25 countries. We also provided grants to more than 20 professors to travel to developing regions so they could help students, research groups and institutions develop capacity in crystallography. Because of this fantastic commitment to our community and your tireless support of our work, we are now witnessing an unprecedented number of new countries seeking membership of the Union during the 2017 IUCr Congress and General Assembly. You’ll see news about our outreach and capacity-building activities in the blog, so please bookmark http://blogs.iucr.org/crystallites and share any comments you may have about our work on the site.

Our blog will feature selected IUCr journal papers shortened into easy-to-read summaries for you to catch up on before reading the underlying article more leisurely. These summaries will also appear on other news and information sites across the web such as RekAlert! run by AAAS, so do look out for us during your browsing.

I hope you have heard about our new IUCr Associates Programme (www.iucr.org/people/associates). This is a new venture for us, which will bring you closer to our journals and charitable work; we know you will enjoy being part of this exciting initiative. Associates’ thoughts and views will be shared through IUCr Crystallites, improving our reach and relevance in the wider community. To register your interest and to ensure you are in line for a 20% discount on registration, please fill in your details at http://www.iucr.org/people/associates/congress-special-offer. We look forward to welcoming you.

We hope you enjoy IUCr Crystallites and await your comments.

IUCr webinar series

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

You may remember reading in a previous column of mine about the launch of a series of educational webinars to help support authors’ articles published in our journals. We now have three webinars currently nearing completion. These webinars will air over the coming months and will allow attendees the opportunity to learn or brush-up skills in particular areas of crystallography. Each event will last between 35 and 45 minutes with some time at the end for questions and answers. Attendees tuning in live will have the opportunity to ask questions of the speaker by typing their comments into the webinar interface and the speaker will then answer live for the entire audience to hear. A listen-on-demand recording of the event will also be made available for those not able to attend the live event.

In no particular order the three events to launch this series will be as follows:

- Naomi Chayen of Imperial College, London, UK, talks about smart materials for protein crystallisation [Khurshid et al. (2015), Acta Cryst. D71, 534–540; http://doi.org/b45w]. Paul asks the questions, “Are we accepting all the interpretations that arise from our present description of X-ray diffraction? Is it reasonable that all crystals have to be “ideally imperfect” to determine their structure? Bragg’s law cannot avoid dynamical effects, and therefore the measured intensity is not equal to the square of the structure factor unless the crystal is assumed to be “ideally imperfect”. If polycrystalline diffraction is formed from crystals satisfying Bragg’s law, why is the background so high compared with single-crystal profiles? Are more crystals required in polycrystalline diffraction to study complex structures with large unit cells to ensure all the peaks are captured? If the variation of intensity around the diffraction rings from polycrystalline samples is associated with a large range of crystal sizes, why does the data from a standard reference material of similar size crystals still reveal this variation? Are we not just modifying our sample description and instrument performance so that the current theory fits the data?” By attending this webinar you will hear directly from Paul on how he explains his new theory.

- Fabrice Gorrec, MRC, Laboratory of Molecular Biology, Cambridge, UK, considers the advances in macromolecular X-ray crystallography and the complexity of this ever-evolving field in a presentation titled “Formulation of the MOR- PHEUS protein crystallisation screens” [Gorrec (2015), Acta Cryst. F71, 831–837; http://doi.org/b45w]. Over the last four decades, different strategies to formulate crystallisation screens have been established. In addition to altering the main parameters of crystallisation, other aspects have been considered, notably the need to produce/refine conditions, the cryoprotection of crystals and the phasing of crystallographic data. For this, many reagents have been investigated and integrated into crystallisation conditions. Experienced researchers from related fields, students and non-experts alike will find Fabrice’s presentation essential as it provides both theoretical and experimental evidence-based aspects of macromolecular X-ray crystallography.

In each of these events we hope that attendees leave with some useful hints and tips ready to apply to their day-to-day research. The opportunity to interact with our authors could help in connecting with other experts in the field, ready and able to help you in your daily work.

In addition to this fascinating programme, we are working on another series of IUCr educational webinars that will cover – in a more pedagogic style – different aspects of symmetry, diffraction techniques, structural science and crystallography. More on this project in a later column.
New additional Main Editors

Acta Cryst. B (http://journals.iucr.org/b) is pleased to announce the appointment of a new additional Main Editor, Ashwini Kumar Nangia. Nangia, who is based at the School of Chemistry, U. of Hyderabad, India, established his research group working on the synthesis of natural products and enzyme inhibitors, and continued research in this field until 1995. He then shifted focus to supramolecular chemistry and then crystal engineering in the second half of the 1990s. He established an active research programme in the emerging topics of host–guest complex formation, and March 2017 issues of Acta Cryst. D (http://journals.iucr.org/d/issues/2017/02/00/ and http://journals.iucr.org/d/issues/2017/03/00/). Guest Editors Charles Ballard, Judit Debreczeni and Paul Emley hope the concepts and tools described in these open-access issues will contribute to further improvements in generating protein–ligand complexes and the quality of the resulting structures.

Advanced neutron scattering instrumentation: call for papers

The Journal of Applied Crystallography (http://journals.iucr.org/j/) invites papers on advanced neutron scattering instrumentation to appear in a special issue planned for April 2018, which will coincide with the journal’s 50th anniversary. The volume will be edited by Guest Editors Dimitri Argyriou and Andrew Allen, together with several Guest Co-editors. The deadline for paper submission is September 1, 2017. Please go to http://doi.org/b6d9 for more information and submission instructions.
inclusion compounds, hydrogen bonding, inter-halogen interactions, polymorphism and co-crystals, and made seminal contributions over the next decade. From 2005 to the current time, his research group continues to direct efforts on solid-state pharmaceutical co-crystals, polymorphs and eutectics with the idea of drug translation to make improved medicines. A member of the IUCr Commission on Structural Chemistry, Nangia took over as the 11th Director of CSIR-National Chemical Laboratory (CSIR-NCL), Pune, India, in February 2016 (www.iucr.org/news/newsletter/volume-24/number1/nangia-at-ncl).

Acta Cryst. C (http://journals.iucr.org/c) welcomes two new Section Editors, Larry Falvello (pictured top left, beside Managing Editor Sean Conway at the ACS Fall Meeting in Boston in 2015) and Jonathan White. Falvello is Professor of Inorganic Chemistry at the U. of Zaragoza, Spain, where he is also a member of the Aragón Materials Science Institute. Falvello’s research programme in the physical properties and transformations of molecular solids combines the synthesis of new coordination compounds of transition metals and lanthanoids, using ligands rich in functional groups, with their structural characterization and studies of their physical properties and possible transformations. White is Professor of Chemistry at the U. of Melbourne School of Chemistry, Australia. His wide research programme includes structural organic chemistry, where he has applied the structure correlation principle to a number of organic chemical reactions and rearrangements. White is also particularly interested in the use of accurate low-temperature X-ray determinations of model organic compounds to investigate donor–acceptor interactions between a variety of functional groups in both organic and organometallic compounds.
Lighting the LAAMP

The IUPAP-IUCr project “Utilisation of Light Source and Crystallographic Sciences to Facilitate the Enhancement of Knowledge and Improve the Economic and Social Conditions in Targeted Regions of the World” has been approved and funded under the 2016–2019 ICSU Grants Programme. The ICSU Grants Programme is a competitive, peer-reviewed programme that supports innovative collaborative scientific initiatives of relevance to science and society. The programme seeks to facilitate active collaboration between Scientific Unions and other members of the ICSU community (for example ICSU Regional Offices, Interdisciplinary Bodies, Joint Initiatives, Networks, etc.) by addressing long-standing priorities for ICSU members in developing science education, outreach and public engagement activities, and to mobilise resources for international scientific collaboration (www.icsu.org/what-we-do/projects-activities/icsu-grants-programme/?icsudocid=grants-2016-2019).

The IUPAP-IUCr proposal, prepared by Sekazi Mtingwa and Sandro Scandolo for IUPAP and Michele Zema for the IUCr, and supported by as many as 25 institutions (including UNESCO, ICSU-ROA, ICSU-ROLAC, ICTP, TWAS, IUMRS and several large-scale facilities), received maximum grades in all of its aspects: relevance to the thematic topics, innovation, scientific quality, cost effectiveness and proposed participants.

Through this project, now known as LAAMP (Lightsources for Africa, the Americas and Middle East Project; https://www.iucr.org/outreach/laamp), ICSU will partner with IUPAP and IUCr to enhance Advanced Light Source (AdLS) and crystallographic science in Africa, the Middle East, Mexico and Caribbean. AdLSs have revolutionized research in many science and technology disciplines, leading to a proliferation of facilities worldwide (the website lightsources.org has links to some 47 facilities), received maximum grades in all of its aspects: relevance to the thematic topics, innovation, scientific quality, cost effectiveness and proposed participants.

To start the process of growing and enhancing AdLS and crystallographic science in those regions, LAAMP will undertake the following tasks: (1) develop a Strategic Plan for each region to grow and enhance its AdLS and crystallography user communities; (2) establish a Colloquium Programme for each region to recruit new AdLS and crystallography users; (3) publish an Information Brochure that describes AdLSs, crystallography and the many fields that they impact; (4) facilitate researchers’ visits to AdLS and crystallography facilities; and (5) convene a meeting at UNESCO to present the regions’ Strategic Plans and define the charge for more detailed Business Plans that include feasibility studies of constructing AdLSs in regions where they do not yet exist. By enhancing AdLS and crystallographic sciences, the regions’ peoples will benefit from research that will tackle devastating viruses such as Zika, Ebola and HIV; the development of sustainable sources of clean energy; and investigations into archaeological and paleontological treasures. Thus, a major outcome of this project will be acceptance by governments that AdLSs and crystallography will bring major advances in their countries’ socio-economic development.

Calls for applications

LAAMP is inviting applications from Faculty–Student Teams to spend two months at participating AdLSs during the 2017–2019 triennium. The faculty should be employed at a university in Africa, the Caribbean, Mexico or the Middle East and accompanied by his/her PhD student. LAAMP will provide 2000 Euros per person to cover transportation. Any excess will be applied to accommodation/subsistence. The remainder of accommodation/subsistence should be negotiated with the host AdLS and other sources of support. After the visit, the team should provide a description of the research conducted, including any resultant publications, and an evaluation of the non-scientific aspects of the visit, including positive experiences as well as ways that the visit could be enhanced in the future. The first call closed in April 2017 and those teams will start their training soon. The second call is expected to open before the end of 2017; please visit www.iucr.org/outreach/laamp regularly for more information.

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In the company of his parents and younger sister, Prithvi Rajan receives his silver medal certificate (under-11 category) from his teacher, R. Karthik (right; IISC, Bangalore, India). Prithvi was trained in crystallisation by his mother.

**IUCr worldwide crystal growing competition**

**Winners of the 2016 competition**

The IUCr Crystal growing competition is open to all schoolchildren up to the age of 18, and aims to introduce students to the exciting, challenging and sometimes frustrating world of growing crystals. Following the great success of the IYCr2014 and 2015 competitions, schoolchildren were invited to take part in the 2016 edition and convey their experiences of growing crystals through a video. An international panel of judges has evaluated the entries based on creativity, aesthetic value, description of working plan and experimental work, clarity of explanations, scientific background and safety. The details of the winning teams can be seen in the table below; all will receive a ‘Young crystal growers’ certificate and a medal. We congratulate the laureates, and hope you will enjoy watching the winning videos at www.iycr2014.org/participate/competition-winners/2016-winners.

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**Launch of the 2017 competition**

The 2017 competition has now been launched. For rules and guidance, please see www.iycr2014.org/participate/crystal-growing-competition-2017. The closing date for submissions is **November 19, 2017**. Please note that videos submitted to local competitions during 2017 may be also submitted to the IUCr competition.
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- Focussing monochromatic radiation, $K_\alpha$, stripping not required
- Range of Bragg angles 100° 2-theta, 20001 steps @ 0.005°, read out time 4 sec
- Laser scans signals @ 16 Bit A/D resolution. Linear dynamic range up to 200,000 counts
- Creates all common ASCII file types ready for data evaluation like Rietveld-Refinement
- Low-temperature attachment: Closed cycle He-refrigerator, 10 to 320 K
- Hi-temperature attachment: Diode laser heater, 300 to 1800 K
- Hi-pressure attachment: Diamond anvil cell, upto 70 GPa

www.xhuber.com
The First Pan-African Conference on Crystallography was held in Dschang, Cameroon (PCCr1) in October of 2016 with the theme “Crystallography for Sustainable Development in Africa.” The conference was organized by the Cameroonian Crystallography Association (CCrA), the Ministry of Higher Education of Cameroon, the U. of Dschang (UDs), the United Nations Educational, Scientific and Cultural Organization (UNESCO), the International Council for Science (ICSU) and the IUCr. PCCr1 is part of an IUCr effort to bring the science of crystallography to developing countries, where the powerful technique can contribute to sustaining the intellectual property rights, economic growth, and human welfare of the country.

The program included round table discussions devoted to “Crystallography as a vehicle to promote science in Africa and beyond” and “Equipment for African laboratories and the African light source, AiLS.” The program included a exhibition of commercial instruments and innovative solutions from sponsors. An X2S Bruker single-crystal diffractometer, installed at meeting site, allow researchers from Camaroon and neighboring countries to conduct XRD single-crystal measurements during months following the meeting. The meeting brought together researchers, students, government representatives and policymakers from more than 35 countries. Patrice Kenfack Tsobnang, Valerie Richalet, the organizing team, all the partners, and sponsors are to be commended for creating an extraordinarily rich, educational, productive and rewarding event.

The opening ceremony included welcome addresses by the Vice-chancellor of UDs and representatives of sponsoring organizations. Gautam Desiraju, Immediate Past President of the IUCr, gave an opening keynote address entitled “From molecule to crystal.” The four days of the meeting covered most applications of crystallography. Summaries of those sessions follow.

Crystal engineering and structural chemistry (function through design)

A session on supramolecular synthons and their influence on material properties began with a keynote lecture given by Alessia Bacchi (Italy) entitled “Designing MOFs that breathe aromas.” A series of Metal Organic Frameworks (MOFs) containing decorated pyridyl ligands were used to selectively capture liquid active pharmaceutical ingredients (APIs) which have prominent aromas. Eugenol (oil of cloves), propofol (an anaesthetic) and carvacrol (the aroma of oregano) were stabilized by interactions with host MOFs. Clement Tella (Nigeria) presented an overview of the use of mechanochemical methods to prepare co-crystals and complexes in bulk. If materials are to be used in large scale devices it is imperative to develop methods to produce complexes on a larger scale than is possible from simple crystallisation. The reduction in solvent waste fulfills the need to do useful chemistry more efficiently and cost-effectively. Loyic Ledreau presented the latest innovations in X-ray diffraction equipment, by highlighting developments made by Bruker AXS GmbH (Germany). Gift Mehllana (Zimbabwe) highlighted strategies for the design of porous materials for catalytic hydrogenation of carbon dioxide. The latter process is potentially of importance to Africa where increasing industrialization is beginning to have a significant impact on the levels of carbon dioxide and other pollutants in the atmosphere. Delia Haynes (South Africa) described the use of dithiadiazolyl radicals as building blocks for organic magnets. Dimerization of the radicals can be controlled using co-crystallization and inclusion in porous compounds enhances their properties. Materials of this type form topologically complex structures. Lars Öhrström (Sweden) spoke of the use of network topology analysis to provide insight into such structures. Jule Abodou Tenon (Côte d’Ivoire) and Claude Lecomte (France) brought the session to an end with two excellent talks describing the use of charge density studies to give insight into spin-crossover complexes and other structures. The session gave a sense of work being done by and in collaboration with African scientists from across the continent.

Much of the research presented touched on important aspects of science required for African development; from the production of novel materials for the beneficiation of natural resources to the remediation of pollution caused by industrial processes.

Susan Bourne, Chair
Inorganic materials and industry minerals

The African continent is rich in raw materials critical to modern civilization including minerals, metals, diamonds and phosphates. However, large parts of the value added manufacturing chains for these materials are currently situated outside Africa. For a sustainable economic development of the continent, larger parts of these chains must be relocated to Africa, and the cross-border cooperation improved. This is where crystallography and the crystallographic community can be of help. This session combined many aspects of the study of structures, size effects, functionalities and applications of inorganic materials. The keynote lecture “Ordered inorganic materials as templates for advanced functional nanostructures” delivered by Robert Mokaya (UK), revealed how to create new functional materials on the nanometer scale by manipulating suitable precursor structures. Michele Zema, (Italy) described very intricate ordering phenomena in “Coltan: a mineral family with unusual crystal chemistry.” Donald Tschuifon’s (Cameroon) described the “Growth of ZnO nanotube arrays by hydrothermal methods on ZnO film coated Si substrates.” Lahcen El Ammari (Morocco) gave a broad overview of the structures of phosphates and vanadates. Wulf Depmeier (Germany) reviewed the amusing scientific history of a potentially economically important Li-mineral (jadariite) and then went on to describe the structure of denisovite: A fibrous, nano-crystalline, polytypic, disordered mineral, that he studied by electron crystallography and X-ray powder diffraction.” Jerome Muswema (DR Congo) discussed Gamma rays induced synthesis of supermagnetic Fe3O4 nanoparticles.” Márcia Carvalho de Abreu Fantini (Brazil), President of the Latin American Crystallography Association described “Mesoporous zirconia based materials for catalysis and SOFCs.”

Wulf Depmeier and Lahcen El Ammari, Co-chairs

Crystallography for life sciences

Co-chair Alejandro Bushiazzo (Uruguay) began the session on “Crystallography for life sciences” with a comprehensive history of the field from Dorothy Hodgkins insulin through viruses, with emphasis on molecular interactions dependent on sequence and fold and the evolution of conformational change in kinases. He noted that early ideas about one gene - one protein and one sequence - one structure were oversimplifications and that amyloids reveal that even a single sequence can have different 3D structures. Heini Dir (South Africa) described multifunctional superfamily of proteins as molecular machines and stressed how much can be learned by examining a structure under dozens of conditions. He discussed his determination of the first protein structure completed by an African Crystallographer. Elsie Yekwa (France) gave an excellent presentation of her studies of inhibitors of African arenavirus nucleases. She cloned, expressed and determined the structures of four proteins, and identified metal ions critical to the structure of a drug target. Co-chair Mino Caira (South Africa) described drug design using crystal structures of drugs and their protein targets. He discussed relative stabilities and solubility of polymorphs of a drug candidate and how to design drugs that are the most potent, selective, and soluble. Cyclodextrins have been used to deliver drugs and hormones, including steroids, and Caira determined the structure of estradiol in a cyclodextrin. Bryan Sewell (South Africa) spoke of molecular evolution of amidases and industrial applications for nitrate production. One of his students from Kenya soaked 100 compounds into an amidase. His results raise questions about a popular theory about the design of antimalarial drugs. Eric Chabriere (France) has determined the structure of a thermo stable protein from Vesuvio hot springs that has two catalytic activities and degrade insecticides and nerve gas. Details of the two mechanisms and the basis for stability revealed by X-ray analysis are being used to engineer more potent agents to decontaminate nerve gas and insecticides. Adwami Adeyeye (South Africa) addressed tuberculosis resistance due to cell wall mycolic acid and structure determinations of proteins in the mycolic acid synthesis pathway. Richard Garratt (Brazil) discussed his studies of monomeric and polymeric human septin filaments that interact with the membrane and remodel it. The only reported crystal structure of a polymeric form is that of a hexamer composed of three types of monomers, but the active form seems to be an octamer of the four putative different monomers. Garratt has found that homo dimers of one type seem critical to extended filament production.

Co-chair Suzanna Ward surveyed the size, growth and content of the Cambridge Structural Database (CSD). On the morning of Oct 8, 2016 it had 853,000 structures, has been growing by 60,000 per year and 1002 were added on its biggest day. Of these, 60% are metal organic and 75% have aromatic rings. The top 200 pharmaceuticals are present and accounted for. Ward noted the existence of thorough reviews concerning the use of the data to understand the structural basis for the chemistry, properties, and functional potential of molecules. She
also described the predictive power of patterns derived from the data. CSD user Z.D. Yav (DR Congo) discussed selenium’s potential as a hydrogen bond acceptor based upon CSD data and \textit{ab initio} calculations. Pinak Chakrabarti (India) has analyzed a pattern of specific NH…N interactions in adjacent peptides in the Protein Data Bank (PDB) and detected a secondary structure in which parallel $\beta$ strands having these intramolecular NH…N interactions are linked together by intra $\beta$ strand hydrogen bonds in a C5-fused ring motif that Chakrabarti terms topi. He suggests that topi may be conformational features as important as $\alpha$ helix and $\beta$ strand and he finds them within 10 residues of ligand binding sites. Patrice Kenfack (Cameroon) describes a structure of a hydrated catananes having Co and Cr ions and a novel dodecameric water ring. Amy Sarjeant (USA) gave a clear, lively, and entertaining presentation about some of the more unusual structures in the CSD. She was personally involved in solving the first neon containing structure to the CCD. Only a few elements are not yet represented and radioactivity may prevent them from ever being crystallized. Matteo Leoni (Italy) described the content and use of the ICCD Powder Diffraction File, arguably the most powerful database available for comprehensive material identification. He also discussed the advances in Rietveld technique for detailed quantitative characterization of structure, microstructure and phase. Oliver Smarts (UK) reviewed enhancements of PDB programs for presentation and analysis of PDB structures. One useful feature was a simultaneous illustration of three types of protein representation (amino acid sequence, 3-D ribbon drawing, and a map of $\alpha$ and $\beta$ segments) on which the positions of individual amino acids can be highlighted. He also showed how CSD results could be used to improve resolution of small molecules in PDB structures.

**Inorganic materials and mining**

This topic was of immediate relevance to middle Africa at this time. The repair and replacement of the decomposing roads throughout the country could benefit from new technologies and materials that are becoming available but not widely or well known in most African Countries.

Co-chair Gilberto Artioli (Italy) reviewed traditional cement composition and production and discussed alternate materials that are more ecologically friendly (use less water to produce and release less CO$_2$ upon decomposition). He contrasts the molecular and crystal structures of cement and new materials. He illustrated the value of using tomography to follow the nucleation of phases in cement. Herbert Poellman (Germany) described new techniques to reduce CO$_2$ in cement production and reviewed the structures, reactions, and CO$_2$ release properties of different components. Kolawole A. Olanade (Nigeria) forcefully asserted that world consumption of concrete and cement is second to water, that less than 40% of roads in Africa are paved and that Africa must use eco-friendly methods and materials and “act local and think global” as it builds its roads. He advocated adoption of the methods and materials described by Poellman. He listed impediments to a better life in Africa, ways to overcome those barriers, and quoted William Clinton, “Advancing equal opportunity and economic empowerment is both morally right and good economics, because discrimination, poverty and ignorance restrict growth, while investments in education, infrastructure, scientific and technological research increase it, creating more good jobs and new wealth for all of us.” Sidione Bonou (Benin) reported that because African women eat clays when pregnant, the composition and decomposition products of the clays are being analyzed by crystallographic techniques to detect potential toxins. The list of the dozens of compounds detected in power diffraction patterns of fecal matter of clay eaters was stunning. Co-chair Rene Guinebretiere (France) discussed phase transitions and strain in zirconium containing industrial refractory blocks and learning more about material properties with the help of advances in techniques for gathering and interpreting reliable data. Roussin Lontio (Cameroon), discussed using metal oxide containing gas sensors to detect air pollution due to gases. He discussed different ways to prepare metal oxide sensors (hydro thermal, Sol-gel, electrochemical, precipitation, \textit{etc.}). His focus narrowed to Ni-Zn mixed metal oxides as gas sensors with semi conductive properties. They have found increased conductance with increased Zn content in NiO. David DoDoo-Arhin (Ghana) described the electronic properties and potential use for solar energy generation and storage of newly synthesized Copper Oxides nanomaterials. The effect of high energy milling, XRD, SEM, TEM, UV-Vis, and FTIR were tested. Marielle Aghahounghata (Benin) is studying TiO$_2$ catalysts to combat waste water pollution, to purify water supplies and to improve catalytic properties with doping.
Crystal engineering, structural chemistry, function through design

Robert Kingsford-Adaboh (Ghana) described isolation, purification, synthesis, X-ray structure characterization, and biological testing of natural products having potential antimicrobial and antioxidant properties. The talk was illustrated with unpleasant pictures of infected skin. Other talks in the session concerned Schiff Base complexes of transition metals (Aliou Barry, Mauritania), quantum information processing with crystal engineering (Cornelius Fai, Camaroon), NMR studies of hybrid nano materials (Dominic Schaniel, France), silver deficient coordination polymers hosting water in a one dimensional proton channel (Justin Nenwa, Cameroon), hybrid amino acids and amines (Nourredine Benali-Cherif, Algeria), and features of Rigakus new XtaLAB Synergy (Tadiusz Skarzynski, Poland). The final talk in the session by Christian Lehman (Germany) was a well illustrated summary of charge density studies and their relationship to crystal engineering with specific focus on halogen-halogen bonds and the photorefractive effect.

Large facilities for emerging countries

Andrew Thompson (France) described the beamlines available for X-ray crystallographic studies at the French national synchrotron facility (SOLEIL). Plans for an African Light Source (AFLS) were described by Andreas Roodt (South Africa). Yvan Georges Ngassa (France) described the use of precision electron diffraction tomography and dynamic calculations to study cation distribution in spinels of importance to understanding their chemical reactivity in the field of geoscience. Arij Abuhamed (Jordan) discussed important features of Jordan relevant to its hosting a synchrotron facility (SESAME) that will serve the countries of the middle east. In Jordan 50% of the population is under 24, and 95% is under 55. Jordan’s main industry is education (50% of that is medical education). Because Asia, Europe, and Africa are connected physically at Jordan and because people from all countries of the world are welcome in Jordan it is an especially appropriate site for a synchrotron facility. Arij hopes that the first protein structure completed in Jordan will come from her lab. Florence Porcher (France) talked about neutron diffraction projects and what constitutes a suitable neutron diffraction study. She presented a survey of all neutron Diffraction Instruments and their distinguishing features.

In a closing plenary lecture, “What is a crystal?”, Ron Lifschitz discussed the evolution of the definition of a crystal from early definitions based on external appearance, surfaces and geometric features, through definitions based on the composition of the building blocks internal to a crystal and the symmetry relationships relating those building blocks. This more detailed definition arose when crystals were shown to diffract X-rays and generate complex symmetric patterns. Diffraction seemed to require long range order and certain types of symmetry that excluded 5-fold symmetry. When 5-fold symmetry was detected in diffraction patterns the definition of a crystal had to be further refined. The definition may continue to evolve. Fortunately, flawed definitions of what a crystal is did not prevent the determination of hundreds of thousand of structures that have improved the daily life of real (not theoretical) people over the course of the past 100 years.
An African Education

When elected President of the IUCr, I stated that I thought the future growth of crystallography would be in Asia, Latin America and Africa. I have attended 15 IUCr Congresses, 14 meetings of the Asian Crystallographic Association, 20 European Crystallographic Meetings, 45 meetings of the American Crystallographic Association, and dozens of other crystallographic meetings in countries that are members of the IUCr. I have witnessed the formation of the Latin American Crystallographic Association. As incredibly rewarding as these experiences have been, I have to say that the First Pan African Crystallographic Meeting in Cameroon, Africa in October, 2016 was the most educational, exciting, and enjoyable meeting of my life. I would like to describe some of my experiences in Cameroon.

After arriving in Cameroon, I collected my luggage and joined other crystallographers for a two hour shuttle ride on a road crowded with automobiles, trucks, motorcycles, and road construction vehicles. There were six or seven lanes to the road, all of which were under repair, and drivers were encouraged to drive in either direction in all seven lanes. The road had once been cement, but after years of heavy traffic, intense rain, and little or no maintenance it was now a dirt road with occasional huge chunks of cement here and there that drivers attempted to dodge by moving into other lanes. Each of four shuttles dropped its passengers at one of four hotels. Desk clerks took our passports in order to assign us rooms. We were told we should be in the lobby in the morning ready for a six hour bus ride to the meeting site, the University Conference Center in Dschang.

I started the next day by dropping my backpack onto my left foot smashing two toes. The pain was intense. I was able to read one email before losing Wi-Fi. I went to the lobby at 7:50 a.m. to find it empty. Everyone had been taken at 7:00 a.m. to another hotel for breakfast. I was taken to that hotel. There was chaos in the small lobby where the luggage of 100 crystallographers was piled in a huge heap. Porters were hauling the luggage to two buses that were parked in the street. The meeting staff were unrolling large banners proclaiming “1st Pan African Crystallographic Conference” and taping them to the sides of the busses. We were advised to take water. I had no cash. A German theoretician gave me a 500 Whatzit coin (I never did learn the name of the currency). I got a big bottle of water and got 200 Whatzits in change.

We finally set out at 9:00 a.m. The road was the worst I had ever ridden upon in my life. Because of deep ruts and large pools of water of uncertain depth, vehicles drove not in the road but on either side of it. The constant jolting and jarring had my joints in rebellion with one another. After three hours we had a bathroom stop in a bucolic setting, surrounded by lush fields of coffee, banana, coconut, pineapple, and palm plants. With so many plants it was hard to choose one to whiz upon. The men followed red dirt trails into the dense foliage. Women had a greater challenge. The tour guide said it was better to pee in the bush than in the shack at the rest stops. He said that they were unsanitary. After three more hours on the bus we reached the university conference center and registered. We were taken to hotels to sort out the luggage and the Musée Des Civilisations, a museum of Cameroonian history.

I had been aware that mankind “came out of Africa” but the visit to the museum illustrated exactly how it happened. Although the museum included local artifacts from the Stone Age, the earliest people known to have inhabited what is now Cameroon were of the Sao civilization that came to the region in the sixth century BC. The museum presented the cultures of four or five kingdoms that evolved. Each kingdom had its own culture (polygamous or monogamous) and distinctly different life styles that persist to this day. The style of housing and roofs (pointed or flat, thatched, straw or wood) depended upon altitude (in the mountains or near the sea) and what building materials were near at hand. The cultures of the distinct kingdoms are present 2,500 years later. I had never appreciated the fact that the sexually explicit sculptures and carvings of early African tribes reveal an openness concerning the human body that was healthy and realistic. The visit to the museum was worth the trip to Cameroon.

One evening I had dinner at an all African table rather than an all white table. I talked with a sixth generation Cameroonian. He could trace his family back to one of the original kingdoms and described the form of polygamy that some of his ancestors practiced. Men of that kingdom could have just two wives and three houses. The man lived in a house with the sons of both wives and each wife lived in a different house with her daughters.

Over two thirds of the 400 attendees at the Congress came from 20 African nations. They were the most colorfully dressed collection of scientists I had ever seen in any of the countries I have been lucky enough to
visit. They give new meaning to the phrase “People of Color”. I began taking pictures of many the most colorfully dressed attendees. On the opening day, Francis Merlin Tchieno Metalagauia, the young man who ran the registration desk, wore the most amazing multi colored, intricately patterned matching shirt and pants I had ever seen. I told him I wanted one like it. He sent for his tailor who took my measurements. I told Francis how much I was learning at the meeting and about my African-American son Stephen and my three grandsons. I told him that I would like my son and grandsons to visit their roots in Africa.

My hotel room had no internet, no hot water, no fresh towels, no shower curtain, a large barrel of fresh water, and an amazing collection of insects that were an entomologist’s dream. It was wonderful. The conference center was appointed with a spacious auditorium and ample break time facilities. However the internet and PA system needed work. Talks were periodically interrupted by power failures. When the lights would come back on the projector would need to be restarted before the speaker could continue.

On the last morning of the meeting hot water miraculously arrived in my bathroom. But there was still no Wi-Fi and the local bank did not exchange dollars. After the closing session, another six-hour bus ride with two bathroom stops, one bottle of pop and a bag lunch brought us to a bona fide Holiday Inn. The Holiday Inn had a life size statue of an Angel Gabriel out front, a life size portrait of the Sacred Heart of Jesus in the lobby and a crucifix over the door. A pile of 70 keys and 70 registration forms were on a table in a gazebo and we were instructed to take any one and register ourselves on the forms. The amenities of my room were no hot water, no drinking water, a broken air conditioner, and Wi-Fi that I could not connect to no matter how many passwords I was given by the desk clerk. But there was a working TV in my room that had eight religious stations in English. Guests are encouraged to pray for miracles (such as restoration of air conditioning) or offer the inconveniences up for the blessing. Guests are encouraged to pray for miracles (such as restoration of air conditioning) or offer the inconveniences up for the blessing (such as restoration of air conditioning) or offer the inconveniences up for the blessing. Guests are encouraged to pray for miracles (such as restoration of air conditioning) or offer the inconveniences up for the blessing. Guests are encouraged to pray for miracles (such as restoration of air conditioning) or offer the inconveniences up for the blessing (such as restoration of air conditioning) or offer the inconveniences up for the blessing. Guests are encouraged to pray for miracles (such as restoration of air conditioning) or offer the inconveniences up for the blessing.

A 40 minute ride brought us to the base of Mount Cameroon and we climbed to observation shelters at the top overlooking the Atlantic. Then we were taken to the seashore where some people went into the water. One of them was Alwyn Bernard Dippinaar, a young protein crystallographer from South Africa that I had had dinner with on the first night. Before leaving the Holiday Inn we posed together with the Angel Gabriel. Cima and Mongi Debabbi who led the singing of Italian songs on the excursion bus, with Alissa Bacci as a backup singer in Verdi’s “Chorus of the Hebrew Slaves.”

To pass the time I suggested that we sing songs from different countries. I explained that it was a crystallographic tradition to sing national songs at international meetings. The tradition had begun at NATO conferences in Erice, Italy. One of the organizers of the Erice Conferences, Lodovico Riva di Sanseverino, had collected the songs of over 50 Nations into a song book. To get the ball rolling, I sang the bawdy English bar room ballad “Her Mother Never Told Her.” This got laughter from those who understood English. I threatened to sing again unless some else did. Mongi Debabbi from Tunisia sang an Italian song. The song had many verses and a simple chorus and soon everyone was singing along. Then Mongi’s wife, Cima Elia Maria, began to sing the Verdi Chorus of the Hebrew Slaves from Nabbucco and other Italians including Alissia Bacci joined her. Cima sang the entire aria beautifully and received resounding applause. Then the Cameroonian stood and sang the National Anthem of Cameroon with their hands over their hearts. It was wonderful. Ludovico would have been pleased.

Holy Holiday Inn!!
that were put down by the British military. The botanical gardens were started when Germans began a rubber industry and set up a social club. After the Germans left, the British took over the port, the gardens and the Club. This began the anglophile era of Limbe and the introduction of Christianity. The club is now a restaurant called “The Hot Spot”. The medicinal garden consisted of a diverse collection of trees including coffee, cinnamon, cocoa and rattan. We learned how chewing the barks and sucking the saps of specific trees cured specific illnesses. We were taken into the orchid greenhouse. It has probably been 20 years since an orchid has bloomed in the orchid house, but there are acres of beautiful flowers and trees in the pristine jungle surrounding it. Suddenly a downpour of rain began. It rains in Limbe every day all year round. We loaded the bus for the ride to the airport through the traffic jam/road construction/motorcycle clogged/and cement dust filled air.

Months later a package with two Cameroonian outfits arrived in time for me to wear them at our family Christmas gathering and the annual musical review of the 130 year old Saturn Club of Buffalo. Since then a dozen friends from the Saturn Club and my sons and grand sons have ordered outfits and are now decked out in Cameroonian high fashion.

Hot Topics in Contemporary Crystallography 2

Poreč, Croatia, April, 2017

htcc2017.org; www.facebook.com/HTCC2017

by Aleksandar Višnjevac

The Second Hot Topics in Contemporary Crystallography Workshop (HTCC2017) organized by the Croatian Association of Crystallographers was held in Poreč, Croatia, April 22–26, 2017. The workshop was designed to highlight achievements in experimental methods and theoretical approaches in crystallography, that have brought the discipline to the frontiers of structure-activity studies and natural sciences in general. The program covered three “hot topics”: (i ) dynamical crystallography [HT1], (ii ) crystallography under non-ambient conditions [HT2], and (iii ) charge density studies [HT3].

Lectures were presented by nine distinguished crystallographers: S. Hasnain,(Barkla X-ray Laboratory of Biophysics and Editor-in-Chief of the IUCr journals , UK) [Introduction]; H. Chapman,( CFEL DESY; U. of Hamburg, Germany) [HT1]; I. Schlichting, (Max Planck Inst. for Med. Res., Germany) [HT1], D. Š. Jung, (Dectris Ltd, Switzerland) [Detectors]; S. Parsons, (Centre for Science at Extreme Conditions, U. of Edinburgh, UK)[HT2]; M. Adam, (Bruker AXS Inc., Germany) [HT2]; P. Macchi, (U. of Bern, Switzerland) [HT3]; C. Jelsch, (CRM2, CNRS, U. de Lorraine, Nancy, France) [HT3]; and K. Molčanov, (Ruder Bošković Institute, Zagreb, Croatia [HT3].

The organizing committee was chaired by A. Višnjevac, president of the Croatian Association of Crystallographers,and the program coordinator was B. Kojić-Prodić. HTCC2017 was attended by 20 students, 9 lecturers, 7 organizers and 2 accompanying persons from 13 countries. A. Bacchi, president of the European Crystallographic Association (ECA), addressed the audience at the opening ceremony. The ECA generously supported the organization of the meeting and bursaries for students. The workshop was sponsored by Bruker AXS Inc. as main sponsor, as well as by Dectris and MiTeGen. The Croatian Association of Crystallographers has already begun to plan the third workshop in the series.
Crystallographic Society of Japan annual meeting

Mito, Japan, November 2016
www.crsj.jp/activity/annualMeetings/nenkai2016/

by Takashi OHHARA

The 2016 annual meeting and the general assembly of the Crystallographic Society of Japan (CrSJ2016) was held November 17–18 at the Ibaraki Prefectural Cultural Center in Mito. Over 351 crystallographers participated. The meeting featured 52 oral and 125 poster presentations covering all aspects of crystallography, three award lectures, three microsymposia, a special lecture promoting gender equality, two luncheon seminars, and industrial exhibitions from 16 companies/organizations. The microsymposia were titled “New Materials and Their Crystallography Promising for Sustainable Development of Society”, “Crystal Chemistry of Functional Materials Based on Proton, Ion-Migration”, and “Recent Advances in X-ray and Neutron Protein Crystallography” and a total of 14 invited talks were given.

At the CrSJ Awards Ceremony, the S. Nishikawa Award was presented to N. Kamiya (Osaka City U.) and J.-R. Shen (Okayama U.), the Research Award was given to Y. Kubota (Osaka Pref. U.) and G. Kurisu (Osaka U.). At the general assembly, an Honorary Membership was awarded to O. Nittono (Fukushima city educational facility “Komukomu”) and Y. Noda (Tohoku U.).

The Young Crystallographer’s Meeting 2016, a satellite meeting of the CrSJ 2016, was held on November 16 at the Tokai Industry and Information Plaza in Tokai (10 km north from Mito) and 40 researchers/students participated. This meeting is held every year to make an opportunity for young researchers and graduate students to communicate and network with each other, especially beyond the barriers between physics, chemistry and biology, in an informal environment. This year, three lectures by two graduate students, K. Terao (Tsukuba U.) and H. Sugiyama (Tokyo Inst. Tech.) and a post-doctoral researcher, A. Shinoda (KEK) were given and a banquet was held after the lectures. In addition, a tour of J-PARC MLF, a neutron and muon experimental facility at Tokai, was held before the lectures as a special event of the meeting. The participants looked at four neutron diffractometers in the MLF.

The recipients of the Honorary Membership and the 2016 CrSJ Awards with the President of CrSJ (from left): Sasaki (President), Nittono, Noda, Kamiya, Shen, Kubota and Kurisu.

Five young scientists were honored with the Poster Awards. They are S. Shimono (Osaka Pref. U.), R. Tanaka (Rikkyo U.), T. Yamano (U. Tokyo), K. Fukuda (U. Tokyo) and M. Yamada (U. Tokyo).

The poster Awardees and the President of CrSJ (from left): Yamada, Fukuda, Yamano, Tanaka, Shimono and Sasaki (President).

The poster Awardees and the President of CrSJ (from left): Yamada, Fukuda, Yamano, Tanaka, Shimono and Sasaki (President).

A full program of the meeting can be viewed at the CrSJ website www.crsj.jp/activity/annualMeetings/nenkai2016/. The chair of the organization committee was T. Tamada (QST) and the program committee was chaired by M. Unno (Ibaraki U.).

The 2017 annual meeting will be held November 23–24, 2017 at JMS Aster Plaza, Hiroshima. The chair of the organization committee is Y. Kuroiwa (Hiroshima U.) and the program committee is chaired by C. Moriyoshi (Hiroshima U.).
Summer of crystallography in Croatia

Bol, Croatia, September 2016
http://cscm24.xyz

BY MARIO CETINA, STANKO POPOVIĆ AND ANTON MENEN

The 24th Croatian-Slovenian Crystallographic Meeting (CSCM24) was held in September of 2016 at Bol on the island of Brač in the Adriatic Sea. Together with the 3rd European Crystallographic School that followed, it was a great summer of crystallography in Croatia.

The meeting was jointly organized by the Croatian Crystallographic Association (CCA) and the Slovenian Crystallographic Society (SCS), under the auspices of the Croatian Academy of Sciences and Arts. The Chair of the Organizing Committee was Mario Cetina (CCA). The Chairs of the Meeting were Stanko Popović (CCA) and Anton Meden (SCS). Overall, 98 scientists participated in the meeting coming from Croatia (59), Slovenia (12), Austria, Germany, Italy, Korea, Poland, Serbia, South Africa, Switzerland and the UK.

Five plenary and eighty short oral contributions were presented. The plenary lectures included: “Handling crystal pathologies in macromolecular crystallography” (M. Jaskolski, Poland); “Flexibility, Dynamics and Chemical Reactions in Solids: Molecular Crystals to Framework Materials” (L. Brammer, UK); “Direct imaging and quantification of crystal structures at the atomic level using C, corrected scanning transmission electron microscope” (G. Dražić, Slovenia); “Crystallography and Society: outcomes of IYCr2014” (M. Zema, UK); “Thermosalient crystals- acrobatics on the nanoscale” (Ž. Skoko, Croatia).

Short oral contributions dealt with modern development of crystallography and closely related fields and gave students an excellent opportunity to gain experience presenting to a large scientific audience.

As there was no registration fee for this meeting, the Organizing Committee is thankful for financial support of the sponsors: PANalytical I Renacon (The Netherlands I Croatia), Rigaku (UK), Bruker I Aparatura (Germany, Austria, Croatia), Doulgas Instruments (UK), Stoe (Germany), Dectris (Switzerland), PLIVA Croatia Ltd., Croatian National Tourist Board, Bluesun Hotels (Croatia). All information about the meeting can be found at http://cscm24.xyz.

An excursion to Pučišća included visits to a stone carving school, a wine cellar, and Vidova Gora Peak, the highest peak on the island.

Comments from the plenary lecturers

M. Jaskolski: The Island of Brač and Bol have left unforgettable impressions and memories.

L. Brammer: I am impressed with the very nice work being done in Croatia, The meeting format provides excellent opportunities for students to get experience in giving presentations to a larger scientific audience. The meeting certainly had the familiar, welcoming feeling that I find is present at most crystallographic meetings.

G. Dražić: I learned many new things and surely I will attend the future meetings.

M. Zema: I enjoyed the atmosphere, the presence of so many young and promising crystallographers and all discussions and conversations. Not to mention the beautiful scenery of Croatia and Bol in particular!

The 25th SCCM will be held in Ljubljana, Slovenia, June 15–17, 2017, http://slocro25.fkkt.uni-lj.si/
Howard Flack (1943–2017)

Howard Flack died February 2, 2017 from pneumonia. Howard's PhD project, Studies of disorder in anthrone and in mixed crystals of anthrone–anthraquinone, exposed him to the need for a deep understanding of the diffraction process and its mathematical treatment. The introduction to his 1970 paper Calculation of dimensions of ordered regions in triclinic and monoclinic pseudosymmetric crystals from the intensity of diffuse scattering reveals a train of thought that was to reemerge a decade later in his work on absolute structure determination, and his desire to provide a detailed mathematical explanation of physical processes.

After gaining his PhD, Howard worked at the Cavendish Laboratory in Cambridge (UK) where he met Evelyne, a visiting Swiss girl whom he would marry. In 1972 Howard became an assistant to Erwin Parthé in the Laboratoire de Cristallographie at the U. of Geneva, Switzerland. Parthé's interdisciplinary Crystallography Laboratory was a central facility serving the Faculty of Science of the university. A year later, an Institute of Crystallography was created at the U. of Lausanne, and the U. of Neuchâtel and Basel developed structure determination services. Howard collaborated with all these start-ups and was involved in their success. For many years, the X-RAY76 program system was developed jointly at Geneva and Lausanne. Howard contributed code to X-RAY76 until its demise in the 1990s. He remained in Geneva until his retirement. He was part of the technical staff, but his brilliance, wit, courage, and generous unselfish services to the Swiss and international crystallographic communities outshone his professional position.

From 1981 to 1990 he was secretary of the Swiss Society of Crystallography. His work with Parthé on highly absorbing crystals of SmAu5 (μr = 5.9) made him realize that the approximations made in the absorption corrections of North et al. and Kopfmann & Huber were inappropriate. The problem was resolved by representing the absorption profile as a Fourier series, an idea which has since been developed to use spherical harmonics. This and all subsequent non-analytical absorption corrections essentially reduce the sample to a sphere, which will have an effect which cannot be corrected for experimentally. Alternative suggestions for dealing with this residual error are given in his paper Automatic absorption correction using intensity measurements from azimuthal scans. The computations were implemented in the computer program CAMEL JOCKEY, an early example of his anarchic sense of humour. The absorption algorithm was extended and appeared as the program CAMEL JOCKEY WITH THREE HUMPS, also compatible with the X-RAY76 software system.

Howard continued to have a deep interest in the problems associated with obtaining the best quality experimental data, especially as a result of his growing interest in the determination of absolute structure by X-ray diffraction. Prior to Rogers’ introduction of his η refinement, absolute structure estimation had depended on the careful examination of a small number of carefully measured reflections. Rogers’ idea, related to earlier attempts to experimentally determine anomalous (resonant) scattering factors, introduced a refinable parameter into the main structure refinement. Howard realized that the η parameter became singular midway between its extreme theoretical values, and that the problem could be better posed by regarding the sample as a twin containing x and 1 – x twin fractions of the two enantiomers (with x a refinable parameter) in an analogous way to his 1970 treatment of disorder. This elegant solution to the problem of absolute structure determination proved to be enormously popular, with the twin fraction x quickly being called the Flack parameter.

Howard was now even more in demand as a speaker and authority on absolute structure determination. He particularly enjoyed being with students and would take every opportunity to get them to talk about their own work. He was somewhat disappointed that his work on chirality overshadowed his other contributions including publications On the definition and practical use of crystal-based azimuthal angles and Merohedral twin interpretation spreadsheet, including command lines for SHELXL, and his papers on the intensity statistics of Friedel pairs.

Howard saw, very early on, the contribution modern computer-based communication systems could make to the dissemination of crystallography. His contributions to the digital publication of IUCr material, to the structured archiving of data and to the crystallographic community are detailed at www.iucr.org/people/crystallographers/flack_ep.

Howard’s knowledge of the early crystallographic literature led him to reinvestigate old problems. His 2015 paper on the Patterson function returns to the use of the resonant difference Patterson function, something he had briefly visited in Practical applications of averages and differences of Friedel opposites (2011). In that paper he wrote ‘The Fourier transform of D has never been used in structure solution but a simulation by Woolfson (International Tables for Crystallography, Vol. B, Reciprocal Space, ch. 2.3, pp. 235–263) confirms that it has interesting properties.’ Naturally, Howard could not leave anything with ‘interesting properties’ alone for long.

Howard was in the middle of active collaborations when he fell ill, but he was determined not to let his condition interfere with his dreams. Just a few weeks before he died, he had drastically reorganized a draft manuscript and changed the prosaic title to ‘HUG and SQUEEZE’ etc. One could not help remembering the CAMEL JOCKEY, with or without the humps.

With Howard, we have not only lost an influential scientist and teacher, we have also lost a widely interested and cultured person. He was well read and familiar with, for example, Tristram Shandy as well as with the lore of Middle-earth. He loved music, opera and concerts. With Evelyne he assembled and restored an impressive collection of vintage toy trains and railway accessories produced by the British firm Hornby between 1920 and 1963. He was a good downhill skier and horseback rider. And he was a wonderful companion with a fresh humour, funny and fair. He is survived by Evelyne, his son Patrick and his daughter Christine.
Raúl A. Mariezcurrena (1939–2016)

BY LEOPOLDO SUESCUN

On November 26, 2016, after a short disease, Raúl Mariezcurrena passed away at his birth city, Montevideo. A Professor Emeritus of Crystallography at the Facultad de Química, U. de la República, Uruguay, Raúl started his training in Crystallography and X-ray diffraction under Adolfo Amit (1925-2007) at Facultad de Química, also receiving some training from Stephenson Caticha-Ellis (1930-2002) at Facultad de Ingeniería (before he left the country for Brazil in the late 60’s). Thanks to a scholarship supported by UNESCO he spent a year between 1972-1973 at the Inorganic Chemistry Dept. of Aarhus U. in Denmark, where he was trained in single crystal structural analysis by Svend Erik Rasmussen producing his first publications (Mariez-currena et al., 1972; Mariezcurrena & Rasmussen, 1973). Back in Uruguay he kept the Crystallography Laboratory at work during the Military ruling (1973–1984), a period where research was disregarded as an important university activity in Uruguay. After recovery of normal activities, he trained six Master students and one PhD student in crystallography. He was a frequent participant in the Ibero-American Crystallography Meetings and organized the XIII Meeting and III School of the Iberoamerican Group of Crystallography in Montevideo in 1994 where young Uruguayan colleagues had the chance to meet top crystallographers in the region and 1984 Nobel Prize winners J. Karle and H. Hauptman, among other prestigious crystallographers such as Ray Young.

Raúl was an excellent lecturer, teaching classical physics at secondary and university level all along his career. His early retirement from the Professor position in 2002 did not prevent him from teaching some crystallography at the Teaching-training Pedagogical Inst. in Uruguay until 2012 when he finally retired from all teaching activities. Even though retired, Raúl participated in the inauguration of the IUCr/UNESCO OpenLab sponsored by Bruker in Montevideo in July 2014, one of the most important activities of the International Year of Crystallography in Uruguay.

Raúl will be remembered for his teaching skills, his enthusiasm when he was in front of a fresh hkl file ready to solve a structure but mainly for keeping crystallography alive in Uruguay during hard times, teaching Weissenberg and Buerger camera use (only available instruments in the lab) till the early 90’s, catching the interest of students that are now Professors in the current group of the Crystallography, Solid State and Materials Chemistry Laboratory (Cryssmat-Lab)/Cátedra de Física at Facultad de Química, U. de la República in Montevideo.

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News from the French Crystallography Association (AFC):
2016 events

BY PHILIPPE GUIONNEAU

The French Crystallography Association (AFC) held elections for its council in December 2016 using an electronic vote open to all AFC members. The elected council is composed of a mixture of both new and more experienced members. In February 2017, internal elections decided the new president and vice-president. All the details are available on the AFC website at www.afc.asso.fr/, a site that offers a dynamic presentation of crystallography news, including hot scientific results, job announcements, bursaries, PhD prizes and conference reports. Concerning the latter, the AFC participated in many events in 2016. In particular, the AFC provided financial support to the annual Structural Biology school that takes place in May on Ile d’Oléron (an island off the Atlantic coast of France) and is organized by the professional Rénafobis network. In 2016, the AFC also awarded bursaries to young researchers wishing to participate in the Pan African Conference on Crystallography - PCCr1 organized in Cameroon. Testimonies on these events and others can be found on the AFC website (in French), as well as comments on the two main events (co-)organized by the AFC in 2016: the AFC2016 conference and the GT-Bio colloquium described below.

The biennial conference, AFC2016, was held in Marseille, in the south of France, July 4–7, 2016. 260 participants enjoyed sunny weather, good science and lively discussions. A very rich program was organized with 3 plenary conferences and 17 symposia, covering all the disciplines related to crystallography. A special session on crystal growth was dedicated to Raymond Kern, a renowned crystallographer from Marseille. Two round-tables were organized that focused on respectively large-scale facilities (X-rays and neutrons) and on scientific edition (with the presence of Samar Hasnain, Editor-in-Chief of IUCr Journals). Three PhD prizes were awarded in Biology, Chemistry and Physics. Many young scientists were present and enjoyed the conference as well as the “Meet the experts” session. The congress was also the opportunity to hold the general assembly of the association. Overall, AFC2016 was a great success and showed the vitality of the French Crystallography community. More information on the conference is available at http://afc2016.im2np.fr/.

The 10th edition of the GT-Bio colloquium (2016-2017) entitled ‘Structural Biology meets Biophysics’ was organized in partnership with the French Biophysics Society (SFB). It was held in Obernai, near Strasbourg, in the Alsace region (northeast of France), December 13–16, 2016. Since 1993, the GT-Bio meetings have been bringing together AFC members interested in Structural Biology. For the 10th edition, 175 participants attended 9 sessions (nucleus and nucleic acids, biophysics and modelling, new technologies, membrane biophysics, cell signaling, hot structures, drug discovery, biological systems dynamics, host-pathogen interactions) with a total of 60 talks and 6 poster sessions. The abstract booklet is available for download at www.afc.asso.fr/images/actes/2016-GTBio-Obernai-LR.pdf. A touching tribute was dedicated to Vittorio Luzzati. More information is available on the conference website at http://sfb-gtbio2016.u-strasbg.fr/.

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Participants of the GT-Bio colloquium 2016 enjoying the sunny, but probably cooler, winter of the north-east of France.

Participants at the French Crystallography Association meeting (AFC2016).
Women in Science

by William L. Duax

The Royal Netherlands Academy of Arts and Sciences will hold special elections in 2017 and 2018 to recruit 16 additional female scholars and scientists. Ten will be added in 2017 and six in 2018. Currently only 13% (72) of the Academies 556 members are female. The Academy will proceed at the same time with its traditional election of 16 more members. It is unlikely that any women will be elected in the “traditional” election. Even if all 26 newly elected members in 2017 were women, female membership in the academy would only increase to 17%.

The appalling remarks made by the current US president disparaging women in vulgar terms and dismissing climate change as a Chinese plot prompted the formation of a Women’s Science group in the USA that had 10,500 adherents within weeks. The group hopes to develop into a global network for research support and to inspire young women to pursue science.

In 1985 the ACA found that the gender balance of its officers did not match that of its membership. To gain balance two highly qualified women were run against each other for the office of president a few times in the next several years until such a ploy proved unnecessary. Members found that not only were women fine scientists, they were superior organizers, planners and workers. In 2017, 23% of ACA members were female and 27% of the attendees at the annual meeting in Denver were female. It is not easy to find or gather data on the gender distribution of crystallographers in the countries throughout the world. The list of attendees at the 23rd Congress and General Assembly of the IUCr in Montreal in 2014 included at least 23% women. I would welcome input on the gender distribution in different countries that might have a bearing on the future of crystallography. After its most recent election four of the officers of the ACA council are women, President Amy Sargent, Vice President Lisa Keefe, Secretary Diana Tomchick, and Treasurer Sue Byram.

The IUCr has complex procedures governing the election of members of the Executive Committee (EC) that are designed in part to preserve global and international representation. This is appropriate and laudable. In view of the fact that the composition of the EC has never had female representation commensurate with the percentage of women in crystallography in many countries of the world, perhaps the delegates to the congress could develop a policy that would assure gender balance on the EC, its delegations and its commissions. See Pages 2 and 16 for more data.

For the past three years there has been only one woman on the 10 member EC. There is a real possibility that soon there will be no women on the EC. IUCr program committees, commission members, invited speakers, and session chairs often fail to have compositions reflecting the percent of women active in the field. The delegates to the general assembly elect members of the EC. While delegations from many countries have no women members, others have a more equitable composition. Although well-qualified women (in terms of scientific accomplishments and service to crystallography) have been nominated for membership in the past they were eliminated in early rounds of balloting. For the good of the IUCr perhaps the women delegates to the next general assembly should form a woman’s caucus before voting begins and adopt a strategy for electing women to membership in the next EC.

Collaboration between CCDC and PANalytical opens new possibilities for (metal) organic crystallographers

PANalytical and the Cambridge Crystallographic Data Centre (CCDC) have agreed that users of the Cambridge Structural Database (CSD) can now utilize this database in PANalytical’s HighScore software suite for the analysis of powder diffraction patterns without additional costs. This new feature is the result of the close collaboration between the renowned Cambridge Crystallographic Data Centre and PANalytical, a leading supplier of analytical X-ray instrumentation and software.

The Cambridge Structural Database (CSD) is a highly curated and comprehensive resource that is essential to scientists around the world. Established in 1965, the CSD is the world’s repository for small-molecule organic and metal-organic crystal structures. Containing over 875,000 entries from X-ray and neutron diffraction analyses, this unique database of accurate 3D structures has become an essential resource to scientists around the world.

The HighScore software offers X-ray diffraction data treatments, phase identifications, reporting and profile fits. The (semi-) automatic handling of many datasets by configurable batches and similarity analysis are distinguishing features. The CSD is the most recent reference database added to HighScore. The Plus option adds phase fits (Rietveld, Pawley, LeBail and more), standardless quantifications with crystal structures and scripting to the basic HighScore package.

The main benefits for joint users of the CSD and HighScore (Plus) are:
- Use of the CSD database for the identification of (mixtures of) organic materials, as sole data source or in combination with other databases
- Direct availability of crystal structure information for identified phases, allowing subsequent structure refinement or quantitative analysis without the need of manually importing this data

These benefits are now available in the recent release of version 4.6 of the HighScore software suite. The combination of HighScore with the CSD database extends phase identifications, structure fits and applications to pharmaceutical, organic and metal-organic structures.

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Parallel programme
A line-up of fascinating, fresh and fun events has been planned to run in parallel with the traditional scientific sessions. Many of these events — discussions and roundtables on education, outreach and capacity building; seminars on general interest topics; contests for research grants for youngsters; an operational XRD lab; and exhibitions — stem from projects initiated and collaborations formed during IYCr2014.

Mega Structure Build
The world’s largest crystal structure model, which has been entered in the Guinness Book of Records, is being brought in from Vienna. The creator, Robert Krickl, will personally inaugurate the exhibition and help explain the model.

MicROCKScopica
Organizer: IUCr Commission on Art and Cultural Heritage
Award-winning photomicrographs of rocks and crystals by Bernardo Cesare (petrologist at U. Padua, Italy) will be on display throughout the Congress.

Rigaku XtaLab
Tutors and operators: Rigaku technical staff
A real X-ray diffraction lab will be in operation for participants to collect their own data.

Salt of the Earth
Chair: Gautam R. Desiraju
Various aspects of this unique compound, sodium chloride, that is so important in crystallography and elsewhere, will be covered in this 150-min session.

Academia/Industry/Govt Collaborations in Solid State Pharma
This session will highlight academia/industry/government interactions in the area of solid state pharma and novel crystal forms for innovator and generic companies.

Towards a global community: IUCr Associates Programme
Chair: Jonathan Agbenyega (IUCr)
The IUCr Associates Programme will launch officially during the Congress. By becoming an Associate, you will be supporting the IUCr in its many charitable activities and receive a variety of benefits.

Symmetry in Indian Art
In this session, eminent artist and calligrapher Poosapati Parameshwar Raju, who specialises in grids and space division for design, will describe his unique style, process and concepts.

Kick-off meeting of LAAMP, an IUPAP–IUCr Project within the 2016–2019 ICSU Grant Programme
Chairs: Sandro Scandoio (IUPAP) and Michele Zema (IUCr)
The Light sources for Africa, the Americas and the Middle East Project (LAAMP), which will enhance advanced light source and crystallographic sciences in these three regions, will be launched.

Crystallography in emerging nations I: BRICS countries
Chair: Andreas Roodt
This session will focus on the role played by the five BRICS countries (Brazil, India, Russia, China and South Africa) in the context of scientific research and technological development, and present general activities and initiatives on networking. It will also aim to increase collaboration, stimulate mutual discussions among young colleagues and discuss funding opportunities available.

Crystallography in emerging nations II: Africa
Chair: Michele Zema (IUCr)
This session will present projects and activities for a sustainable development of education and research infrastructures in Africa. It will highlight possible synergies among scientific unions and other bodies, like UNESCO and ICSU, to facilitate this process.

Crystallography in emerging nations III: LACA
Chairs: Diego G. Lamas and José Reyes
To maintain the momentum generated by the foundation of the Latin American Crystallographic Association (LACA) and its admission as a Regional Associate of the IUCr in 2014, in this session, the current situation of crystallography in the region will be revised with emphasis on equipment, human resources, synchrotron and neutron facilities, basic and advanced courses, and databases.

Commemorative symposium in honour of Howard Flack
Chairs: William Clegg and Gervais Chapuis
Howard’s legacy to the crystallographic community, both in terms of his scientific contributions and his pioneering activities in electronic publishing, will be celebrated.

Dragons’ Den
Young researchers with a maximum age of 35 and no permanent academic position, regularly registered at IUCr2017, will present and defend their idea for a scientific project in front of a selection panel. Awards will be announced at the end of the session.

These details were correct at the time this Newsletter went to press (April 2017); please see the final programme for up-to-date information.
2017 Workshop and Clinic Schedule

Fundamentals of X-ray Powder Diffraction: June 5–9
For the novice with some XRD knowledge or for the experienced with an interest in the theory behind XRD, this clinic offers a strong base for increased lab performance. The clinic covers instrumentation, specimen preparation, data acquisition and qualitative phase analysis through live demonstrations.

Advanced Methods in X-ray Powder Diffraction: June 12–16
For the experienced XRD scientist, this session offers enhanced analysis skills through intense problem solving, as well as an introduction to the Rietveld Method. The course emphasizes computer-based methods of data collection and interpretation, both for qualitative and quantitative phase analysis.

Rietveld Refinement & Indexing Workshop 1 & 2: September 25–29
Powder pattern indexing and Rietveld structural refinement techniques are complementary and are often used to completely describe the structure of a material. Successful indexing of a powder pattern is considered strong evidence for phase purity. Indexing is considered a prelude to determining the crystal structure, and permits phase identification by lattice matching techniques. This workshop introduces the theory and formalisms of various indexing methods and structural refinement techniques along with quantitative analysis. One unique aspect of this workshop is the extensive use of computer laboratory problem solving and exercises that teach method development in a hands-on environment.

Visit www.icdd.com/education, for more information and pre-requisites for the advanced Rietveld course.

Packing for India
by William L. Duax
Plan to take 20 lbs of crystallographic text books that you haven’t opened in five years to the IUCr Congress in Hyderabad. Your old books will be welcomed and eagerly read by the next generation of crystallographers who look to the IUCr for guidance and support.

As CEO of the American Crystallographic Association and Editor of the IUCr newsletter I have been asked many times to find a new home for collections of crystallographic texts at the time of a crystallographer’s retirement or death.

Shipping costs made it difficult to send collections of books to countries that could most benefit from them. Whenever I have brought copies of ACA transactions and IUCr Newsletters to an IUCr meeting and made them available to attendees they have been gratefully welcomed.

I urge you to bring 20 lbs or more of books on crystallography or science to Hyderabad and place them on a table at the IUCr booth. You will have made a valuable contribution to the future of crystallography and your name on the fly page will let the recipient know you care.

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A selection of future meetings. A more complete list is available at www.iucr.org. Corrections and new listings are invited by the Editor.

**JULY 2017**


**AUGUST 2017**


**OCTOBER 2017**


**NOVEMBER 2017**


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**AWARDS, NEWS AND NOTICES**

**International Center for Diffraction Data news**

**Executive Director announced**

Tom Blanton has been named as new Executive Director at the the International Centre for Diffraction Data (ICDD)™. Tom is a long-time ICDD member, an ICDD Distinguished Fellow, and past Director and Chairman of the Board of Directors. He joined the ICDD staff in 2013 as Publication Manager, and was later promoted to Principal Scientist and Database Manager. Prior to joining the ICDD staff, Tom graduated from Emory U. in Atlanta, Georgia and was a member of the research staff at Eastman Kodak Company in Rochester, NY, USA. While at Kodak, he served a dual role as an Analytical Scientist and Materials Characterization Scientist, reaching the position of Senior Principal Scientist. During his tenure at Eastman Kodak, Tom assumed a leadership role where he supervised an X-ray Spectroscopy laboratory and invented, developed, and commercialized materials. He is the co-inventor for 46 USA and 60 international patents, author or co-author of 180+ external publications including four book chapters; and author or co-author on over 275 external presentations. Tom’s extensive background in X-ray diffraction, his broad and varied knowledge of ICDD, its products and services, along with his experience in management and R&D for product development, will facilitate his successful transition to his new role as ICDD’s Executive Director.

**2017 Ludo Frevel Crystallography scholarship recipients**

The ICDD Ludo Frevel Crystallography Scholarship Committee has selected ten recipients for the 2017 Scholarship Program. These recipients were selected, on a competitive basis, from forty-three commendable applications received by the ICDD Scholarship Committee.

**Ivana Brekalo** (USA), “Solid State Synthesis and Templation of Metal Organic Frameworks”;

**Haoyan Diao** (USA), “In-situ Neutron Studies of the Atomic Distributions and Dislocation Evolutions in the Alcofreni High-Entropy Alloy System”;

**Debasmita Dwibedi** (India), Synergetic Approaches Using Diffraction Tools in Probing the Structure-Property Correlation in Novel Sodium Battery Materials;


**Stanislav Fedotov** (Russia), “Interrelation Between Crystal Structure and Electrochemical Properties in Cathode Materials for Rechargeable Batteries”;

**Igor Huskic** (Australia), “The Role of Octahedral Rotations and Distortions in Flexoelectric Phenomena”;

**Kipil Lim** (USA), “Study of the Battery Materials Through Operando X-ray Analysis”;

**Christopher Mizzi** (USA), “Organic-Inorganic Coupling and Disorder in Hybrid Perovskite Halide Semiconductors”;

**Patrick Tung** (Australia), “Diffuse Scattering: The Role of Local Disorder in Environmentally-Friendly Piezoelectric Na0.5Bi0.5TiO3-x%BaTiO3”;

**Yujun Xie** (USA), “Subcritical Nuclei-Coupled Crystal Growth in Metallic Glasses.”

The ICDD will present each of these students with a check in the amount of $2,500 to assist in the continuation of studies in their selected fields of crystallographic research. The ICDD has awarded 191 scholarships since 1991, totaling over $454,750. Scholarship awards are made possible by donations from both individuals and corporations. One hundred percent of all donations to the scholarship fund are applied to student funding, as defined by the program’s charter.

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**Volume 24, Number 4 • 2016**

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