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INTERNATIONAL UNION OF Crystallography

NEWSLETTER

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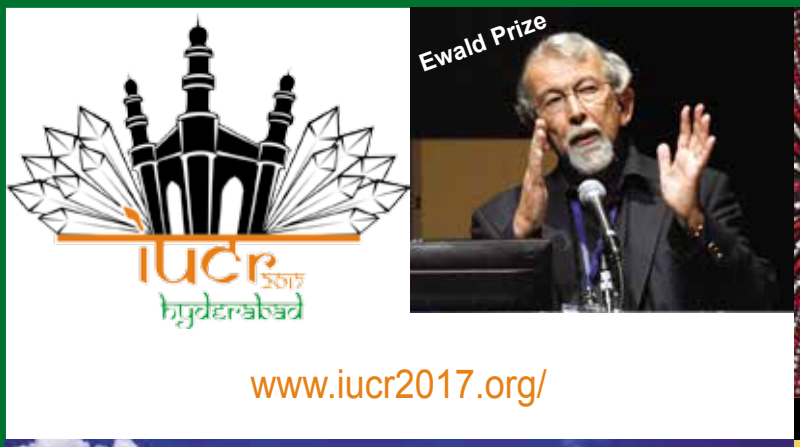

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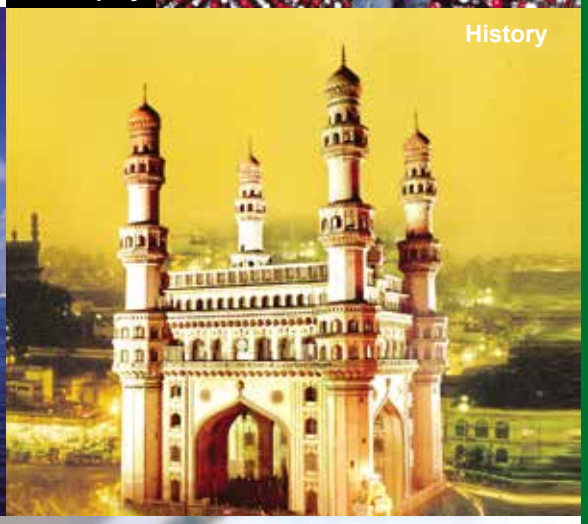

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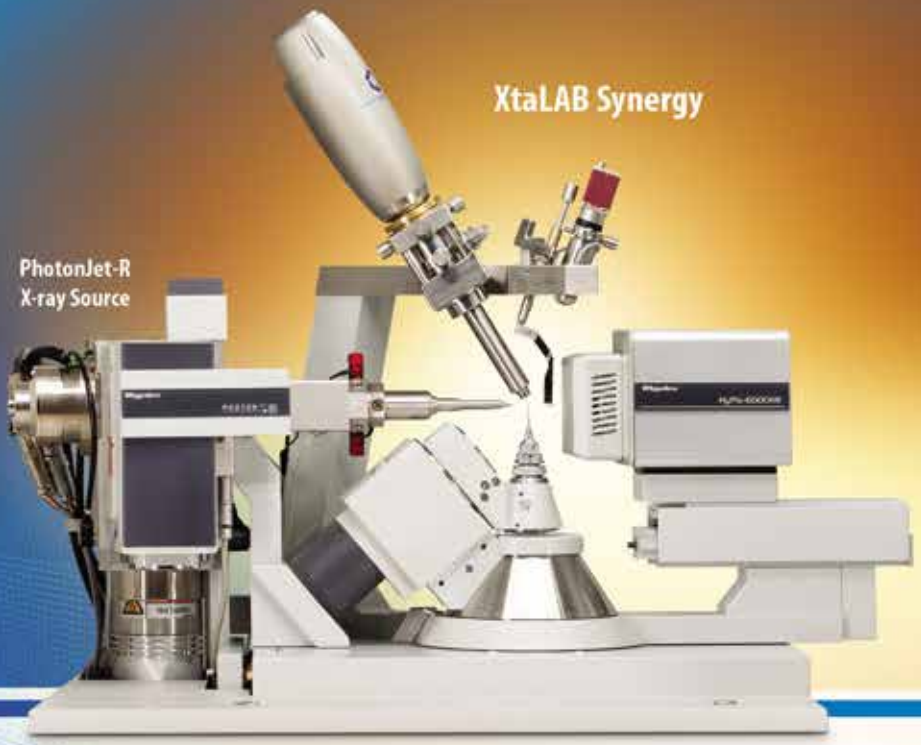

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On the Cover: See Page 22

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Marvin L. Hackert

Best wishes to all for the New Year! We witnessed a lot of change around the world in 2016, but now look forward with excitement to 2017 and the opportunities that lie ahead. Already in January we have had some highs and lows. One high was the recognition and announcement that the eleventh Ewald Prize will be awarded to Sir Tom Blundell (Cambridge, UK) for his work as one of the worldwide leaders in crystallographic innovation, starting with the structure of insulin with Dorothy Hodgkin, championing methods enabling drug design, fragment screening, and computational modelling. I am happy to report that Tom will be in Hyderabad to accept the award and present his lecture on August 21. Another bright spot was that a beam circulated for the first time in the pioneering SESAME synchrotron on January 11, 2017. SESAME is the first light-source laboratory in the Middle East, established under the auspices of UNESCO before becoming a fully independent intergovernmental organization in 2004 (see Page 20).

In contrast to those highs, many of our community were subjected to a fairly sophisticated scam by someone targeting the general goodwill and trust of crystallographers and their willingness to help others in trouble. The culprit sent emails pretending to be me using a gmail account that looked similar to my utexas email account, naming prominent crystallographers who were supposedly stranded in an airport and needing help. The names, airport and currency requested changed as the scam worked its way around the world. Be assured that neither I nor any member of the EC will ask you for funds like that.

One of the most impactful issues facing the IUCr in 2017 will be to find a new Executive Secretary. The IUCr has been fortunate having Mike Dacombe manage the day-to-day operations for many years, but he has announced plans to retire after our XXIV IUCr Congress later this year. The IUCr office in Chester employs 25 staff, chiefly in its publishing operations. The successful candidate is expected to direct the financial and administrative affairs of the Union, which has 50 Adhering Bodies and 23 Commissions, as well as having responsibility for the staff. The Executive Secretary also works closely with our General Secretary (Luc Van Meervelt) and the Executive Committee.

Of course the most anticipated event of 2017 will be the XXIV IUCr Congress and General Assembly in Hyderabad from August 21–28 (see Page 23). Registration is now open and the abstract deadline is February 28. The International Programme Committee and the Commission representatives have put together an outstanding programme and Gautam Desiraju and his colleagues have worked on local arrangements, including an extensive web site for registration and useful information on visas, etc. I have registered and encourage you to register early as well. In addition to looking forward to an excellent scientific programme, we will elect new members to the EC and all our Commissions. I have mentioned this frequently, but I cannot emphasize too much how important it is for the future health of our organization that we recognize the need for diverse representation in all phases of the IUCr – that starts with the nomination of delegates, and nominations for officers and Commission members to be voted on in Hyderabad. Last fall the IUCr emailed instructions to Chairs of all our Commissions requesting recommendations for the membership and Chair of each Commission and all National Committees for nominations to the EC.

At the present we have the following nominations for the EC:

- President: *S. Banerjee* (India), *W. Depmeier* (Germany), *A.M. Glazer* (UK), *S. Lidin* (Sweden)
- General Secretary and Treasurer: *L. Van Meervelt* (Belgium)
- Vice-President: *H. Dabkowska* (Canada), *M.R.N. Murthy* (India)

continued on Page 3

The International Union of Crystallography Newsletter is distributed by print to 585 libraries and various crystallographic meetings and electronically to 12,000 crystallographers and other interested individuals in 102 countries. The IUCr also runs Crystallography Online, available at www.iucr.org, as a complement to the IUCr print newsletter. Feature articles, meeting announcements and reports, information on research or other items of potential interest to crystallographers should be submitted to the editor at any time. Submission of text and images by electronic mail is requested. Items will be selected for publication on the basis of suitability, content, style, timeliness and appeal. The editor reserves the right to edit. Address changes or corrections and requests to be added to the mailing list can be made at www.iucr.org/news/newsletter.

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- Ordinary members of EC: *D.G. Billing* (South Africa), *G. Diaz de Delgado* (Venezuela), *P. Grochulski* (Canada), *K.A. Kantardjieff* (USA), *P. Karthe* (India), *K. Lawniczak-Jablonska* (Poland), *J.L. Martin* (Australia), *S. Ravy* (France), *M. Takata* (Japan), *A.E. Voloshin* (Russia), *M.S. Weiss* (Germany).

As a reminder, the election to the EC shall be arranged in such a way that there will not be more than two Officers from any one country and that amongst the six ordinary members there will be at least one Officer from a country of each of the three geographical regions (i) Europe and Africa, (ii) the Americas and (iii) Asia/Oceania. Of the current ordinary members on the EC, the terms of the two representatives from Asia/Oceania (Mitchell Guss, Australia and Masaki Takata, Japan) and the lone representative from the Americas (Hanna Dabkowska, Canada) will expire. Masaki is eligible for re-election and Hanna has been nominated for Vice-President. As nominations currently stand, for ordinary members the Assembly will first be asked to elect one of the three nominees from Asia/Oceania and one of three nominees from the Americas before filling the remaining vacancies on the EC. We also have country applications from Albania/Kosovo, Tunisia, Singapore and Bangladesh to join our IUCr family. Additional nominations are still possible, but our goal is to post all the nominations in advance of the Congress so that the delegates know who the nominees are well in advance. We have therefore asked to have the full slate of recommendations to the Executive Secretary by May 1, 2017.

In Denver last summer the IUCr EC approved a modified version of the proposed voluntary IUCr Associates Programme. The intent is to have the Programme in place before the IUCr Congress in Hyderabad. The Chester office is working on ways to articulate the structure and benefits of the Programme. We also discussed ways that the Chester office can provide a broader range of services economically to assist our country members and Regional Associates. The IUCr already provides web services for some country and Regional Associate groups and recently signed an agreement with the ACA to archive searchable abstracts. Once the Associates Programme is fully implemented, the IUCr will have additional expertise and capabilities in house to offer additional services.

Last fall I had the privilege of attending the second meeting of LACA in Merida, Mexico, and the pleasure of being part of the opening welcome ceremony and also to speak about the IUCr and how the IUCr supports crystallography around the world. It was a great meeting with an impressive number of young scientists in attendance.

The only Regional Associate conference this year will be the ACA meeting in New Orleans, May 26–30 (see Page 23). 2016 Nobel Laureate, Sir James Fraser Stoddart, is scheduled to give a plenary lecture at the Opening Ceremony. The theme of this year's ACA Transactions Symposium is Cryo Electron Microscopy. Of the four workshops 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. Information on the awards being presented at the meeting can be found on Pages 20–21.

I mentioned last time that our umbrella organization ICSU (International Council for Science) has been in discussions with ISSC (International Social Science Council) about a possible merger of the two organizations. An extraordinary General Assembly of ISSC and ICSU was held in Oslo on October 24, 2016. The IUCr was fortunate that former General Secretary Sven Lidin agreed to be our IUCr delegate in Oslo. 76% of the ICSU members and 87% of the ISSC members voted in favor of a merger, in principle, of the two organizations. Many of the International Unions represented expressed concerns about handling dues, identifying official national representation, the fate of ICSU Commissions, and how to include medicine and engineering in the discussion of global concerns, etc.

Thank you for your continued support of our collective mission to support and advance crystallography around the world. Please do not hesitate to contact me or any member of the EC with your suggestions for how the IUCr can work more effectively to serve you.

Marvin L. Hackert (m.hackert@austin.utexas.edu)

Second LACA conference in Merida, Yucatan, Mexico in October 2016.

IUCr Associates Programme

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

The IUCr Associates Programme (www.iucr.org/people/associates) will launch officially during the 2017 IUCr Congress and General Assembly in Hyderabad (www.iucr2017.org/). There will be an opportunity to sign up to the programme during the Congress registration process. To register your interest, please visit www.iucr.org/people/associates/congress-special-offer.

By joining the Associates Programme you can play a much stronger role in the IUCr and its many activities. As you know, the IUCr is involved in numerous charitable activities including

- supporting students to attend meetings around the world; the IUCr sponsors symposia and workshops on topics relevant to crystallography, enabling young scientists to travel and attend meetings where they may not have had sufficient funds to travel alone
- a Visiting Professor scheme, which provides support for some of the costs of having internationally recognised scientists as lecturers for short courses at workshops or schools organised in developing countries
- building crystallography capacity in Africa and other parts of the world; for instance, the first Pan African Conference on Crystallography (www.iucr.org/outreach/icsu2015/pccr1) was held recently at the U. of Dschang, Cameroon, with support from UNESCO.

What is the Associates Programme?

The Associates Programme offers a series of benefits and tools to help you network, share ideas and discover new knowledge.

The subscription rate will be for a three-year period with a fee of USD 200. A reduced rate of USD 60 will be available for students, retired scientists and those from developing countries.

The benefits will include (but will not be limited to) the following:

Discounts

- Six free articles on **Crystallography Journals Online**
- 20% discount on the open-access fee for the publication of one article in an IUCr Journal of your choice, for example **IUCrJ**, which has an impact factor of 5.3
- 20% discount on *A Little Dictionary of Crystallography*
- 50% discount for individuals purchasing the print version of *International Tables*

Professional networking opportunities

- Access to information on regional meetings, webinars and videos
- Access to the IUCr LinkedIn discussion group
- Jobs board
- *World Directory of Crystallographers* (find an expert)

IUCr community participation

- Opportunities to participate in the IUCr Outreach and Education programme, which has been established to enable the continuation of many of the initiatives successfully launched during the International Year of Crystallography in 2014.♦

Impact and influence of crystallography across the sciences

by Samar Hasnain, Editor-in-Chief, IUCr Journals

The first diffraction experiment on a single crystal of copper sulfate by Max von Laue in 1912 and subsequent interpretation by Lawrence Bragg gave birth to the field of crystallography.

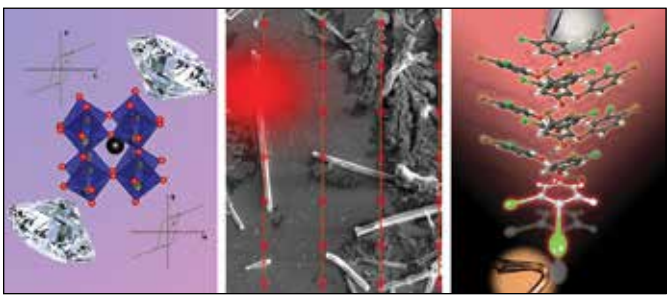
How does one assess the impact of a discipline such as crystallography, particularly when it spans the sciences and requires a cultural change in the way of thinking and looking at a problem?

Crystallography, whether using electrons, neutrons or X-rays, has transformed the way we look at a problem and the level at which we wish to glean the composition of a material and its internal arrangement. Whether it is something as simple as table salt or as complex as the ribosome, crystallography has provided an insight that no other approach could demonstrate.

One hundred years after the first Nobel Prize in crystallography to Laue in 1914, crystallography still features in current awards. The 2013, 2012 and 2011 Chemistry awards went to scientists who continue to demonstrate the multidisciplinary outreach of crystallography. We congratulate all these winners and indeed the 2016 Nobel Prize winners in Physiology and Medicine (Yoshinori Ohsumi, for his discoveries of mechanisms for autophagy) and Chemistry (Jean-Pierre Sauvage, Sir J. Fraser Stoddart and Bernard L. Feringa for the design and synthesis of molecular machines). We are pleased to note that Ohsumi, Stoddart and Feringa have published some 40 papers in IUCr Journals (http://journals.iucr.org/) during the period 1986–2014 (www.iucr.org/news/notices/announcements/nobel_2016).

To acknowledge the impact and influence crystallography still continues to play, the IUCr launched a cross discipline open-access journal **IUCrJ** (www.iucrj.org/) in 2014. The journal received its first impact factor of 5.3 in 2016. This impact factor results from our authors having the trust and confidence to submit some of their best work to the journal.

Along with many existing communities already publishing in **IUCrJ**, we wish to encourage the cryo-EM community to make **IUCrJ** their natural home. The importance of cryo-EM for structural science has been obvious to the IUCr for many years (www.iucr.org/news/notices/announcements/cryoem_at_iucrj_a_new_era) and will be an important feature of the next IUCr Congress in Hyderabad (www.iucr2017.org/), where as well as the IUCr Gjonnes Medal keynote lectures [from Richard Henderson (www.youtube.com/watch?v=jLxKf-lUGf0&feature=youtu.be) and Nigel Unwin], there will be an additional keynote [from Sriram Subramanian (www.youtube.com/watch?v=ExuvWDdf2zs&feature=youtu.be)] and three microsymposia each with six talks. Like the Congress, **IUCrJ** aims to take the lead in reporting important advances in cryo-EM methods as well as significant science results from the application of cryo-EM.



We encourage you all to consider **IUCrJ** alongside other notable journals such as *PNAS*, *JACS*, *Nature Communications* and *Nature Materials*. The journal provides readers with an opportunity to see some excellent science in the chemical, materials and biological fields while keeping up with significant advances in instrumentation, methods and approaches. We aim to continue this unique combination of structural sciences in one place while welcoming new areas like the chemistry and materials science pertaining to two-dimensional crystals such as graphene. ♦

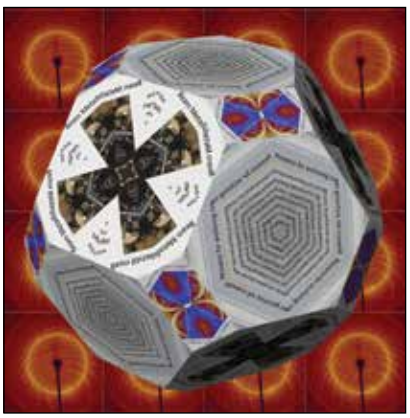
This is an extract from an Editorial published in **IUCrJ** *(https://doi.org/10.1107/S2052252516017012).*

Research news

Why keep the raw data?

The increasingly popular subject of raw diffraction data deposition is examined in a Topical Review in **IUCrJ** [Kroon-Batenburg, Helliwell, McMahon & Terwilliger (2017). *IUCrJ*, **4**, 87–99; https://doi.org/10.1107/S2052252516018315]. Building on the 2015 workshop organised by the IUCr Diffraction Data Deposition Working Group (DDDWG), the authors bring the story up to date with accounts of new subject-specific and institutional data repositories, and of growing policy pressures on research data management such as the European Open Science initiative.

The article is, however, more than just a workshop report or a survey of evolving policy. It seeks to inform the cost-benefit arguments over diffraction data deposition with examples from real front-line research. For example, Kroon-Batenburg and Helliwell have collaborated on studies of protein binding of the chemotherapeutic agent cisplatin, and have made all their 34 raw data sets available through the U. of Manchester Data Library. Some of these datasets have been reanalysed and resulted in fresh understanding of cisplatin–lysozyme models.



The prospect of extracting further information from archived primary data sets in this way (either by the insights of fresh pairs of eyes or through subsequent improvements in software analysis) has implications for structural databases, facilitating the idea of continuous improvement of studies, such as for macromolecular structure models (long championed by Terwilliger).

It is not only in the field of macromolecular structure determination that these considerations are important. One of the greatest challenges to reusing any raw data is the need for complete metadata associated with any raw data set, to allow its subsequent interpretation and full evaluation.

Various IUCr Commissions are actively publishing their summaries of the essential metadata that need to be captured alongside all experimental data sets. These initiatives and their relationship to the IUCr's standard for data characterization (CIF, the Crystallographic Information Framework) are reviewed

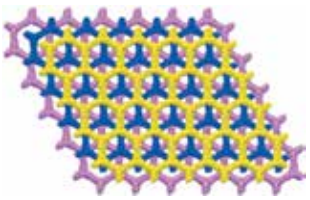
within the article. Again, practical pointers are given to essential metadata that need to be captured alongside diffraction data sets.

While there are encouraging signs that the scientific community is taking more informed interest in data management and its scientific potential, fresh challenges are being thrown up by the latest generation of instrumentation, capable of generating vast amounts of data at an incredible rate. It may not be possible to archive or even thoroughly analyse all the data that is being produced. However, this article will help to supply a deep understanding of the reasons why society should invest effort and resources into extracting the greatest value possible from the data deluge, in crystallography as in any science.

Further reading: a Scientific Commentary on the above article and a related Editorial have been published in the same issue of **IUCrJ** [Grabowski & Minor (2017). *IUCrJ*, **4**, 3–4; https://doi.org/10.1107/S2052252516020364 and Baker (2017). *IUCrJ*, **4**, 1–2; https://doi.org/10.1107/S2052252516020340, respectively].

A step to understanding polymorphs

In a paper published in *Acta Cryst. B* [(2016). **72**, 807–821; https://doi.org/10.1107/S2052520616017297], Carol Brock of the U. of Kentucky looks at some of the organizing principles behind crystal structures with high Z', where Z' is loosely the number of symmetry-independent molecules in the asymmetric unit. This study lies at the very heart of understanding and being able to control properties of molecular structures. Pharma and agrichem industries attach great importance to understanding crystal structure. The solid form impinges directly on properties such as solubility, bioavailability, processing characteristics, bulk density, dissolution rate, permeability, surface electrostatic charge and so on, so it is imperative to have a clear understanding of the molecular-level make-up of a material and how this affects its properties. This study illustrates that the high Z' phenomenon, like polymorphism itself, has many root causes but careful study of each structure allows the identification of organization principles in most cases.



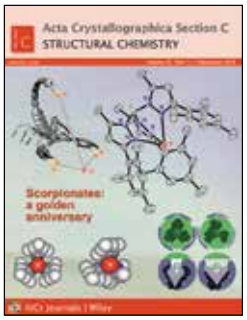
Crystal structure of the Z' = 56 polymorph of 1,3,5-tris(4-carboxyphenyl)-benzene (overhead view of the hexagonal sheets, shifted in respect to each other); reproduced with permission from C.A. Zentner *et al.* (2015). *Chem. Commun.* **51**, 11642–11645 © Royal Society of Chemistry.

Brock leaves the door open for future research saying "very few structures are so complex that it is difficult to understand how the crystals could have formed". This comprehensive survey, in conjunction with a groundswell of work by a number of groups on this increasingly intriguing problem over the past 20 years, shows that there is no one-size-fits-all explanation and that the details of each structure are uniquely tied to the chemical details of the molecules that comprise it. The search goes on, but perhaps we are now at least beginning to know how to formulate the question. ♦

*Taken from a Scientific Commentary by Jonathan W. Steed [Acta Cryst. (2016). B**72**, 805–806; https://doi.org/10.1107/S2052520616018734].*

Special issues

Scorpionate chemistry at the 50th anniversary



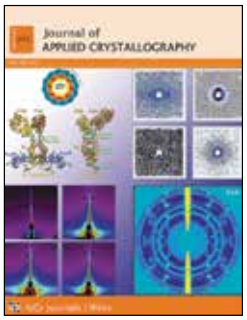
The year 2016 marked the 50th anniversary of the discovery of scorpionates, a class of compound with proven versatility afforded by the ease of tuning the steric bulk and electronic properties at the metal coordination site. In a seminal report by Trofimenko, a new class of chelating polypyrazolylborate ligands, trispyrazolylborates (Tp), was created by reaction of potassium borohydride with three equivalents of pyrazole. The resulting anion was then observed to coordinate to a large range of divalent metal ions.

Before 1966 there were only a few examples of polysubstituted boron compounds with B–N bonds, with all of them behaving as noncoordinated spectator anions. In a 1993 review, Trofimenko notes the multidentate features of Tp and states, "Nature provides the closest analogy to these features in the scorpion. This creature grabs its prey with two identical claws and then may proceed to sting it with the sharp point of the curving tail. Therefore, I found it appropriate to coin the term scorpionate ligands".

In 2013, the first special issue for *Acta Cryst. C* (http://journals.iucr.org/c/) was published featuring scorpionates (http://journals.iucr.org/c/issues/2013/09/00/). After just three years, the continued productivity of the field has made it necessary to publish a follow-up special issue featuring a further 16 cutting-edge papers on scorpionate chemistry (http://journals.iucr.org/c/issues/2016/11/00/). This clearly shows that the chemistry is as vibrant and relevant today as it was 50 years ago.

Kiyoshi Fujisawa and Glenn P.A. Yap, Guest Editors

Small-angle scattering



The 16th International Conference on Small-Angle Scattering (SAS2015) was held in Berlin, Germany, in September 2015. A fully open-access virtual special edition of the *Journal of Applied Crystallography* publishes work that provides insights into ongoing developments in the field of small-angle neutron and X-ray scattering (SANS and SAXS) covering different areas of fundamental and applied research (http://journals.iucr.org/special_issues/2016/sas2015/).

Some of the highlights from the issue include a paper from Lehmkühler *et al.* (2016), which describes the use of X-ray cross correlation analysis applied to the investigation of colloidal crystals. For the case of poly(methyl methacrylate) colloids it is shown how information beyond the static structure factor can be deduced from coherent X-ray scattering experiments, for example, enabling assignment of a face-centred cubic structure to the crystal. In a different direction the work by Perkins *et al.* (2016) dwells on the current state of the atomistic modelling of scattering data and reviews the achievement of the Collaborative Computational Project for Small Angle Scattering (CCP-SAS).

Certainly these developments will be important for the future when increasingly complex systems will probably need to be characterised by SAS with atomistic resolution.

The topics contained in the special issue describe the particular directions in which SAS is developing at the moment and which will become increasingly important in the future. There will no doubt be further substantial advances of the SAS technique, itself, and its application to solve important scientific questions in diverse research areas.

This is a short extract taken from the Editorial by Guest Editors Michael Gradzielski and Andrew Allen.

X-ray radiation damage to biological macromolecules: further insights

There are eight papers on various aspects of radiation damage in the January 2017 issue of the *Journal of Synchrotron Radiation* (http://journals.iucr.org/s/issues/2017/01/00/), guest-edited by Elspeth Garman and Martin Weik. The studies reported on macromolecular crystallography (MX) and small-angle scattering (SAXS) experiments were presented at the 9th International Workshop on Radiation Damage to Biological Crystalline Samples, held at MAX IV in Lund in March 2016.

There have been concerted efforts over the last 15 years to understand the manifestations and origins of radiation damage suffered by protein crystals during MX experiments, and to establish mitigation strategies using various approaches. These have gradually resulted in a deeper understanding of the physical, chemical and structural factors affecting damage rates, and there is a growing literature that seeks to elucidate the pertinent parameters. As the range and scope of the investigations have broadened, so has our appreciation of the complexities of radiation damage phenomena, although a full knowledge of all processes involved has not yet been achieved. The need for this has, however, become more pressing, especially with the advent of X-ray free-electron lasers and new fourth-generation synchrotron sources such as MAX IV in Lund and NSLS II at Brookhaven now coming on-line with even higher flux densities than hitherto utilised. The high rate of damage inflicted by these X-ray beams has brought the issue of radiation damage during structural biology experiments into even sharper focus. Thus, an awareness of the effects of radiation damage both on diffraction and SAXS data, and on the macromolecular structures derived from them, will become increasingly important.

The papers in the special issue include a re-examination of structural damage to tyrosine residues; two papers on finding the optimum MX data collection strategy for phasing of structures, one using sulfur SAD data in the presence of damage and the other on anomalous phasing with mercury by serial synchrotron data collection; a comparison of helical and standard rotation methods from a radiation damage standpoint; two papers examining damage rates in SAXS experiments and scavengers that could be used to reduce these rates as well as presenting some new visualisation tools; an analysis of the conformational heterogeneity of side chains as a function of dose in room-temperature and cryo-crystallography; and an imaging study on the effects of X-ray irradiation on microcrystals.♦

New edition of Volume A of *International Tables for Crystallography*

The new sixth edition of Volume A, edited by M.I. Aroyo, is now available in print and online.

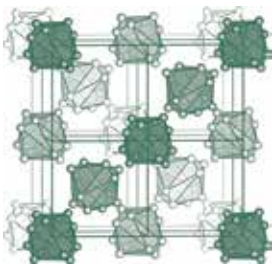
International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science. Volume A, *Space-group symmetry* (http://it.iucr.org/A/), is the flagship volume in the series, and contains diagrams and tables of data for the 17 plane groups, the 230 space groups and the 32 crystallographic point groups. This new edition has been extensively updated and revised.

Part 1 of the volume provides an introduction to space-group symmetry. It includes chapters on groups, crystallographic and space-group symmetry, descriptions of space groups, coordinate-system transformations and methods of space-group determination. The final chapter provides a useful introduction to topics treated in more depth in Volumes A1 (http://it.iucr.org/A1/) and E (http://it.iucr.org/E/) of the series. The chapters in this part have been written with teaching in mind, and will prove invaluable for undergraduates or graduates wishing to learn about symmetry in crystallography, while providing a clear introduction to the topic for researchers from other disciplines.

Part 2 of the volume presents the diagrams and tables of plane- and space-group data. The layout of the tables of data, the symbols used in the diagrams and the classification of the space groups are explained in a useful guide. Together these form an essential resource not only for professional crystallographers, but also for chemists, physicists, mineralogists, biologists and material scientists who employ crystallographic methods and who are concerned with the structure and the properties of crystalline materials.

Part 3 treats more advanced topics on space-group symmetry, and covers crystal lattices, point groups and crystal classes, space-group symbols and their use, lattice complexes, normalizers of space groups, and magnetic subperiodic groups and magnetic space groups.

There are eight new chapters in this edition of Volume A and five chapters have been revised. The layout of the space-group tables has been simplified as the sub- and supergroup data are now available in Volume A1, and there are new general-position diagrams for the cubic space groups. Additional diagrams showing tilted, perspective views of some of the more complex cubic space groups are also provided. For further details about the new edition, please visit http://it.iucr.org/Ac/newedition/. Purchase information, including a 50% discount on the print price for individuals, can be found at http://it.iucr.org/services/purchase/.



The IUCr would like to take this opportunity to thank Professor Aroyo and the authors of the individual chapters for their outstanding dedication and hard work in bringing this new edition to fruition.♦

The IUCr Journals Student Poster Prizes at the 5th International School of Crystallization (Granada, Spain; May/June 2016) were won by Elizabeth Horstman (left; U. of Illinois at Urbana-Champaign, USA) and Nuria Portoles Gil (right; Institut de Ciencia de Materials de Barcelona - CSIC, Spain). The winning posters were titled "Microfluidic Platforms for Pharmaceutical Crystallization" (EH) and "Supercritical CO_2 as a green solvent for the crystallization of 2D metal-organic frameworks".

The winners of the IUCr Journals Poster Prizes at ECM30 (Basel, Switzerland; August 2016) were Ali Abboud (U. Siegen, Germany; second from left; applied crystallography category), Boris-Marko Kukovec (U. Zagreb, Croatia; middle front; chemistry category) and Anna V. Lübben (Georg-August-U. Göttingen, Germany; structural biology category). The prizes and certificates were presented by IUCr Executive Committee member Radomir Kuzel (left).

Congratulations to all winners from IUCr Journals

From left, Sehrish Naz (Panjwani Centre, Karachi, Pakistan), Muhammad Tayyab (U. of Veterinary and Animal Sciences, Lahore, Pakistan) and Anil Yousuf (Forman Christian College, Lahore, Pakistan) stand beside their winning posters at the 2nd International Workshop on X-ray Crystallography in Structural Biology (Lahore, Pakistan; October 2016).

Maria Martinez-Molledo (centre) from EMBL, Hamburg, Germany, won the IUCr Journals Poster Prize at the Diffraction Data Collection Using Synchrotron Radiation Workshop (Berlin, Germany; June/July 2016) for her poster "Locking a proton-dependent oligopeptide transporter". Presenting the prize and certificate are local organiser and *Acta Cryst. F* editor Manfred Weiss (left) and poster-committee representative Shruthi Sridhar (U. of Oulu, Finland).

Tommi Kotila (left; U. of Helsinki Institute of Biotechnology, Finland) won the IUCr Journals Poster Prize at the DLS-CCP4 Data Collection and Structure Solution Workshop (Didcot, UK; December 2016) for his poster "Role of cyclase-associated protein in actin dynamics". The prize and certificate were awarded by workshop tutor and *Acta Cryst. D* co-editor Kay Diederichs.

Bruker OpenLab Albania, May 30 – June 3, 2016

by Bujar Dida, Dritan Siliqi and Michele Zema

The IUCr-UNESCO Bruker OpenLab Albania was held at the Polytechnic U. of Tirana (PUT) from May 30 to June 3, 2016. More than 90 participants attended the Opening Ceremony, which was held in the main auditorium of PUT and hosted by Andrea Maliqari, Rector of PUT, and Bujar Dida from the Faculty of Mathematical Engineering and Physical Engineering (FIMIF-PUT), Local Chair of the OpenLab, in the presence of invited attachés from the embassies of participating countries; delegates from the Ministry of Education and Sport and the U. of Tirana School of Medicine; and deans, professors, lecturers and students from public and private universities in Albania, Kosovo and Macedonia. Opening speeches were given by the just-elected Rector of PUT, Andrea Maliqari, and his predecessor, Jorgo Kacani. A special greeting was delivered via the internet by Alessia Bacchi, President of the European Crystallographic Association (ECA), and this was followed by welcome messages from Dritan Siliqi [Institute of Crystallography (IC)-CNR, Bari, Italy], co-Chair of the OpenLab, Bruce Noll (Bruker) and Michele Zema (IUCr), who also presented the Opening Lecture: "Crystallography and society: the contribution of the IUCr to the development of scientific education, research and infrastructure".

The five-day program at the FIMIF-PUT was attended by over 50 students and organized in lectures, tutorials and lab sessions. It covered the basics of crystallography and diffraction theory, as well as some advanced applications. An X2S portable single-crystal diffractometer was provided by Bruker for the lab sessions. In fact, the diffractometer is still operational at the FIMIF-PUT and other workshops and schools are being planned for 2017. The availability of this instrument is expected to also facilitate the development of research activities in crystallography in Albania and neighbouring countries.

The lectures were led by Gervais Chapuis (EPFL, Lausanne, Switzerland), assisted by Michele Zema, and covered the topics of "Symmetry in crystallography", "X-ray diffraction", "Structure solution", "Structure completion and refinement" and "Anisotropic tensor properties".

Tutorial and lab sessions on single-crystal X-ray diffraction, from crystal selection and mounting to data reduction and analysis, were held by Bruce Noll with the assistance of Michele Zema, by making use of Bruker instrumentation and software. The section on single-crystal diffraction was concluded by an interactive lecture with Q&A session by Michele Zema, who recapped all about single-crystal XRD analysis. Corrado Cuocci (IC-CNR, Bari, Italy), Dritan Siliqi and Francesco Capitelli (IC-CNR, Rome, Italy) were in charge of all the tutorials about the use and applications of X-ray powder diffraction, which covered the following topics: "Phase identification and qualitative phase analysis", "Structure determination" and "Crystallography for biology and medicine".

Gervais Chapuis lecturing at the IUCr-UNESCO Bruker OpenLab Albania.

The participants were able to mix during the lunch breaks and further social activities were encouraged in the late afternoons. Certificates were awarded to all participants at the closing ceremony by Bujar Dida, Dritan Siliqi, Michele Zema and Gervais Chapuis.

The participants were very enthusiastic about the OpenLab, which attracted much interest not only from Tirana's academic circles but also from the media. Michele Zema and Dritan Siliqi were invited to appear on a well-known talk show on national TV to explain the importance of crystallography and its wide range of practical applications.

(l-r) Michele Zema, talk-show host Rezear Xhaxhiu and Dritan Siliqi after the interview in the "NEWS 24" TV studio.

The IUCr-UNESCO Bruker OpenLab Albania also represented a fundamental step in the process for the establishment of the ***Association of Albanian Crystallographers*** (AAC), which has now formally been founded and includes crystallographers from both Albania and Kosovo. The OpenLab followed the success of events organized in Albania during IYCr2014, namely the International Conference "New Frontiers of Nanomaterial Technologies for Applications in Biology and Medicine" and the 1st Workshop on Crystallography, held in conjunction with the 20th Congress of the Carpathian-Balkan Geological Association. At that time, the local community of crystallographers, with Dritan Siliqi and Michele Zema as facilitators, formed the OPAL (Organiza-

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BRUKER

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Crystallography

Innovation with Integrity

Crystallographic Society of Japan 2015 Annual Meeting

Osaka, Japan, October 2015
www.crsj.jp/activity/annualMeetings/nenkai2015

by Tomoji Ozeki

Over 363 crystallographers participated in the 2015 annual meeting and the general assembly of CrSJ held at the Osaka Prefecture U., October 17–18. The meeting featured 50 oral and 129 poster presentations covering all aspects of crystallography, three award lectures, three microsymposia (a total of 14 invited talks), a special lecture promoting gender equality, two luncheon seminars, and industrial exhibitions from 13 companies/organizations.

At the CrSJ Awards Ceremony, the S. Nishikawa Award was presented to S. Iijima (Meijo U.), the Research Award was given to H. Ago (RIKEN), and the Young Crystallographer Award went to M. Suga (Okayama U.). At the general assembly, an Honorary Membership was awarded to M. Sakata (SPring-8).

The recipients of the Honorary Membership and the 2015 CrSJ Awards with the President of CrSJ (from left): M. Sakata, S. Iijima, Miki (President), H. Ago and M. Suga.

Five young scientists were honored with the Poster Awards. They are: D. Urushihara (Nagoya Inst. Tech.), M. Nishiyama (U. Hyogo), W. Shihoya (Nagoya U.), K. Hirabayashi (Osaka U.) and A. Tanaka (Osaka City U.).

The poster Awardees and the President of CrSJ (from left): Hirabayashi, Nishiyama, Miki (President), Tanaka and Shihoya.

A full program of the meeting can be viewed at the CrSJ website www.crsj.jp/activity/annualMeetings/nenkai2015/. The chair of the organization committee was Y. Kubota (Osaka Pref. U.) and the program committee was chaired by N. Kamiya (Osaka City U.).♦

7th European Charge Density Meeting (ECDM7)

Warsaw, Poland, June, 2016

by Krzysztof Woźniak, Chair and Paulina M. Dominiak, Vice Chair of ECDM7

The 7th European Charge Density Meeting was held from June 26 to July 1, 2016 at the Centre of New Technologies of the U. of Warsaw, Poland, and was attended by 114 participants from 20 countries including Germany, UK, France, Slovakia, Australia, Denmark, Russia, USA, Italy, Switzerland, Belgium, India, Brazil, Slovenia, Taiwan, Spain, Czech Republic and Poland. The meeting was organized by a Local Organising Committee chaired by Krzysztof Woźniak and Paulina M. Dominiak. Institutionally, ECDM7 was hosted by the U. of Warsaw (Dept. of Chemistry), the Polish Academy of Sciences (Crystallographic Committee) and the Polish Crystallographic Assn. The program included 22 invited lectures, 27 oral communications including ones selected from submitted abstracts and there were two poster sessions.

ECDM7 began with a session on the history of charge density investigations which included the lectures delivered by Mark Spackman ("A brief history of charge density analysis") and by Wolfgang Scherer who talked about "Past and recent developments of experimental charge density studies – a European perspective". Then, all participants enjoyed a Welcome Party for a couple of hours.

The Monday morning session was focused on potential errors in experimental and theoretical approaches with an excellent opening lecture by Julian Henn ("About Fit Quality Indicators") and oral communications by the present Laureate of the ECA M. Perutz Prize, Václav Petříček ("Diffraction data analysis in *Jana2006*"), and Regine Herbst-Irmer ("Empirical correction for resolution- and temperature-dependent errors caused by factors such as thermal diffuse scattering"). Then, Krzysztof Wozniak presented a lecture entitled: "A century after the Braggs: on precision and accuracy of X-ray results". The session was completed by Matthias Gutmann with his invited lecture on "Aspects of single crystal neutron diffraction". The other sessions included many excellent invited lectures, among others: "On hydrogen-atom treatment in high-quality single crystal structure analysis" by Birger Dittrich, "Is relativity the hammer in charge density of heavy elements and their compounds? How heavy is the hammer – how heavy is heavy metal?" by Lukasz Bucinsky, "A tale of two densities" by Dylan Jayatilaka,"Concerning measurement errors in synchrotron X-ray charge density studies" by John Helliwell (the 8th ECA Max Perutz Prize Laureate), "Insights into single molecule magnetism from charge and spin density studies" by Jacob Overgaard, "Reproducibility in biomedical sciences" by Wladek Minor, "Using QM methods to refine biological structure" by Kenneth M. Merz Jr., "GEM, a force field based on density fitting for scalable molecular dynamics simulations" by Jean-Philip Piquemal, "Information entropy towards atoms in molecules" by Patrick Bultinck, "On attraction of electrons" by Lucjan Piela, "Some emergent scalar and vector fields in Quantum Chemical Topology" by Angel Pendas, "When experimental charge and spin density data challenge *ab initio* and DFT calculations" by Claude Lecomte, "Locality of intermolecular interactions in organic crystals" by Tonglei Li.

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The last day of ECDM7 was devoted to cryo-electron microscopy. There were three excellent lectures delivered by Wolfgang Baumeister: "Electronic cryomicroscopy: from molecules to cells"; by Christopher J. Russo: "Approaching the physical limits of electron cryomicroscopy for structure determination" and by Philip Nakashima: "Towards the measurement of bonding in and around inhomogeneities in nano-composite materials".

The social program included sightseeing of Warsaw (Wednesday afternoon) and on Thursday evening a conference concert and dinner. The concert took place at one of the Warsaw theatres called in Polish "Kamienica" where, firstly, there was a performance of the Folk Song and Dance Ensemble of Warsaw U. named "Warszawianka" which presented its dance, vocal and instrumental repertoire. Then a conference dinner, during which Mark Spackman announced the winners of the best poster contest. As the best poster prizes were co-sponsored by IUCr, Sine Larsen presented a short presentation on the aims and activities of IUCr. The newly established Stewart Prize went to Anna A. Hoser, Ioana Sovago and Anders Ø. Madsen for the poster entitled: "Aspirin polymorphs revisited". The Best Poster Prize was awarded to Malte Fugel, Florian Kleemiß, Lorraine Andrade Malaspina and Rumpa Pal for their poster "Investigation of the hypervalency in polyoxoanions via theoretical and experimental charge density studies". The second Best Poster Prize was presented to Lennard Krause, Regine Herbst-Irmer and Dietmar Stalke for their poster "Validation of charge density refinement strategies". Finally, the Rigaku Oxford Diffraction Prize went to Anna Krawczuk and Piero Macchi for their poster "PolaBer - distributed atomic polarizabilities approach".

ECDM7 has clearly shown that modern crystallography goes far beyond routine applications. In fact there is plenty to be done in this field. Being concise, ECDM7 has stressed that there is plenty of room to improve the quality of the final crystallographic results when diffraction data collection is better planned, collected data are processed in a new way and data are refined using more advanced models of electron density than those routinely applied.

Thank you to all the sponsors including: the U. of Warsaw (in particular the Dept. of Chemistry), the Polish Academy of Sciences (Crystallographic Committee), the Polish Crystallographic Assn, the IUCr, the ECA, Rigaku Oxford Diffraction, Bruker, Oxford Cryosystem, STOE, AXO, DECTRIS and CENT, for all their support.

Now, we look forward to ECDM8 in Göttingen, Germany. ♦

(l to r) Christopher Russo lecturing on cryoelectron microscopy; the audience listening to Václav Petříček lecturing on *Jana2006*; "Many-body scientific interactions" during coffee breaks; and Mark Spackman looking for the best posters.

(l to r) Sight-seeing of Warsaw; King's Castle Square performance of the Warszawianka; laureates of the Best Poster Contest (from the left): representing Organisers, P. Dominiak, S. Larsen, and K. Wozniak, then the laureates: Anna Hoser, Anna Krawczuk, Malte Fugel and Lennard Krause with M. Spackman and M. Winter representing the Best Poster Committee.

ECDM7 conference photo in front of the CENT building in Warsaw. First row: K. Merz (USA), K. Woźniak (Poland) ECDM7 chairman, P. Dominiak (Poland) ECDM7 Vice-chairman, P. Becker (France) and M. Spackman (Australia).

Latin America MaThCryst workshop on nanocrystallography

Havana, Cuba, October, 2016
www.crystallography.fr/mathcryst/havana2016.php

by Ernesto Estévez Rams

The fifth biannual Latin America "International School on Fundamental Crystallography" was held at the U. of Havana from October 30 to November 5, 2016. The School was attended by 35 students from Cuba, Uruguay, Argentina, Costa Rica, Mexico, Puerto Rico, Brazil, Colombia, and Ecuador. The teaching staff included Mois Aroyo, Massimo Nespolo, Leopoldo Suescun, Raimundo Lora Serrano, Arbelio Pentón Madrigal and Ernesto Estévez Rams, four of whom are members of the IUCr MaThCryst commission. The program covered the fundamentals of the discipline including crystalline lattices, group theory, space groups, Fourier transform, reciprocal space, diffraction equations, and the use of the Bilbao Crystallographic Server. Students presented posters of their work and ample time was reserved for them to discuss their projects with the lecturers. The last day a workshop on nanocrystallography featured presentations by Serrano, Madrigal, Estévez and Cristy Azanza Ricardo.

The next school will be held in Colombia in 2018. ♦

ECM-30 Bringing the crystallographic flame to Basel, Switzerland

Basel, Switzerland, August 2016
http://ecm30.ecanews.org

BY Katharina M. Fromm and Jürg Schefer

The European Crystallographic Meeting 2016 (ECM-30) was held August 28 – September 2, 2016 in Basel, Switzerland. The opening ceremony was held in the congress center on Sunday, August 28. The 600 people in attendance were entertained with chemical experiments and intermezzi by the alp-horn trio Solodurum. The delegates were welcomed with talks from Katharina Fromm (meeting Chair), Mauro Dell'Ambrogio (Swiss State Secretary for Education, Research and Innovation), Hans-Peter Wessels (Government of the Canton of Basel-City), Joël Mesot (Director of the Paul Scherrer Inst.), Piero Macchi (President of the Swiss Society for Crystallography) and Alessia Bacchi (President of the ECA). Udo Heinemann (Vice-president of the ECA) presented the ECA 9th Max Perutz Prize of ECA to Václav Petříček (Prague, Czech Republic) for "his practical application of the theory of aperiodic and modulated structures in his computing system *JANA*". The reception that followed in the exhibit hall was generously sponsored by the City of Basel.

Katharina Fromm and Jürg Schefer opening the ECM-30.

ECA President Alessia Bacchi and Vice-president Udo Heinemann present the 9th Max Perutz Prize to Václav Petříček for his computing system *JANA*.

The 931 registrants from 47 countries included participants from Australia, Malaysia, Ecuador, Brazil, Mexico, Singapore, Canada, Taiwan, Hong Kong, Japan, USA and Korea. Close to one third of all participants were female, an upward trend which hopefully will continue in the future. 178 participants came from Switzerland, 166 from Germany, and 116 from the UK. The fact that 47 different countries were present shows that the mobility of scientists across borders is very important for our community.

Nobel laureates Ada Yonath (Jerusalem, Israel) and Jean-Marie Lehn (Strasbourg, Germany) gave fascinating plenary lectures framing the conference. ECM30 offered an excellent scientific program for physicists, chemists, biologists, mineralogists and, of course, crystallographers within 70 sessions, 300 oral presentations, 16 keynote lectures and two poster sessions based on more than 715 submitted abstracts.

For the first time, an ECM-science slam was organized, at which young scientists were asked to excite the audience with an entertaining 3 minute presentation of their work. The most successful presentation was determined based upon the audience wildly rattling plastic hand clappers (provided by STOE as measured on an applause meter. At the end of this session, the 8th Erwin Felix Lewy Bertaut Prize (ECA/ENSA) was awarded to Linda Reinhard (Hamburg, Germany) for her extraordinary "pioneering contributions to the crystallographic analysis of enzymes and the optimization of protein preparations for diffraction studies".

ECM30 included eight satellite meetings held at universities or research centers:

- PSI Powder Diffraction School PDS2016 – Modern Synchrotron Methods (Villigen, Switzerland)
- Robert F. Stewart School on Electron Density and Related Properties (Nancy, France)
- Young Crystallographers ECM-30 Satellite Meeting (Basel)
- Crystallography in the Pharmaceutical Industry Workshop (Basel)
- The CSD Python API: A Foundation for Innovation (Biocenter, U. of Basel)
- High Data Rate MX Satellite Meeting (Biocenter, U. of Basel)
- A Workshop on Methods in Crystallographic Computing (Lossburg-Wittendorf, Germany)
- SMARTER 5 Meeting – Structure Elucidation by Combining Magnetic Resonance, Computational Modelling and Diffraction (U. of Bayreuth, Germany)

A special microsymposium, "Teaching and Education," chaired by H. Flack (Geneva, Switzerland) and H. Stoeckli-Evans (Neuchâtel, Switzerland) and the creation of a general interest group on the topic reflects the intention of the ECA to support teaching young scientists.

At the closing session prizes were awarded to 21 young scientists. A list of the winners and the sponsors will be published on the ECA website (www.ecanews.org). After the conference, 70 participants used the opportunity to join a tour to visit the Swiss free electron laser SwissFEL at the Paul Scherrer Inst., inaugurated on December 5, 2016. ♦

Photo credits: ECM30 and W.L. Duax.

Joel Bernstein, Jack Dunitz and Carol Brock.

Officers of the ECA and the delegates from member countries.

Science Slam Contestants: (l-r) Barbara Wicher, Stanislava Todorova, Falk Meutzner, Gregor Hofer, Stefano Checchia and Alankriti Bajpai with Katharina M. Fromm. Inset: The hand clappers used by the audience to applaud the contestants.

SGK/SSCr General Assembly.

Young crystallographers before the conference dinner at the zoo.

Full house.

Coffee break.

MS37 “Molecular compounds and MOFs at ambient conditions and under high pressure”. (l-r) Wendy Lee Queen (chair), Piero Macchi, Ewa Patyk, Boris A. Zakharov, Stephen Moggach, Francesca Fabbianni (chair) and Xiaodong Zou.

MS34 “Molecular recognition, supramolecular chemistry and crystal engineering”. (l-r) back: Carl Henrik Görbitz (chair), Scott J. Dalgarno, Chiara Massera (chair), Luigi Renzo Nassimbeni; front: Marijana Dakovic, Consiglia Tedesco and Carol Brock.

MS13 “Hot structures in biology”. (l-r) Udo Heinemann (chair), Valtentin Chabert, Jan Dohnalek and Chwan-Deng Hsiao, missing N. Soler and C. Davey.

MS4 “New developments in phasing and refinement”. (l-r) front: Massimo D. Sammito, Eleanor Dodson, Jon Agirre; back: H. Jenkins, Randy J. Read and Pavel Afonine.

MS47 “Teaching and education”. (l-r) John R. Helliwell, Adam Michalchuk, Howard Flack (chair), Jean-Louis Hodeau, Michele Zema, Suzanna Ward, Helen Stoeckli-Evans (chair).

Pohang, South Korea, September 2016

http://2016iucrhpworkshop.yonsei.ac.kr/

by Yongjae Lee, Chair of the Organizing Committee and Andrzej Katrusiak, Chair of the IUCr CHP and Program Committee

The 14th IUCr Commission on High Pressure (CHP) Workshop was held at the Pohang Advanced Laboratory (PAL) in South Korea, in Sept 2016. The Organizing Committee was chaired by Yongjae Lee (Yonsei U., Seoul). The Workshop focused on recent advances in high pressure techniques. Lectures and posters covered structural phase transitions and their kinetics, new materials synthesis, Earth and planetary science, soft and biological matter, physical and chemical properties, theory and computation, and techniques for high-pressure studies at synchrotron, neutron and laboratory-based facilities. The workshop was attended by 120 participants from 19 countries.

The workshop started with a welcoming speech by Kibong Lee (Director of PAL). Plenary Talks were given by Ho-Kwang Mao (Director of HPSTAR, China) on Pressure and X-Radiation, Chi-Chang Kao (Director of SLAC, National Accelerator Laboratory, USA) on The Potential of X-ray Free Electron Laser for High Pressure Research and by Takehiko Yagi (U. of Tokyo, Japan) on Synchrotron Facilities and High Pressure Science in Japan.

Special sessions were focused on PAL and High Pressure Research in Korea. Before the excursion to the PLS-II and PAL-XFEL facilities, J.-Y. Kim (PAL) described the current status of PLS-II beamlines, and an introduction to PAL-XFEL was given by its Director, I.S. Ko. High Pressure Research in Korea was reviewed by Y.-H. Kim (Gyeongsang National U.), and current high pressure research and activity were reviewed by researchers from Korea; Y.-H. Ko (Agency for Defense Development, Korea), Research on materials under high pressure or temperature; S.K. Lee (Seoul National U.), Glasses and melts under compression and extreme confinement; K.H. Kim (Seoul National U.), Critical behavior in quasi-1D organic conductors as investigated by a cubic anvil cell up to 8.5 GPa; J. Kim (Hanyang U.), HYU-HPSTAR-CIS High Pressure Research Center; G.W. Lee (KRISS), Study of High pressure and High temperature in KRISS; Y. Lee (Yonsei U.), Construction of Max-X (Matter in eXtreme conditions X-ray) beamline at Pohang Accelerator Laboratory.

Six young scientists received IUCr awards, and presented short talks: T. Pakornchote (Chulalongkorn U. Thailand), Role of peculiar *d*-spacing variations of scandium trihydride under high pressure using *ab initio* method; J. Kim (U. Texas, Austin), High Pressure Effects of few- and monolayer $MoWS_2$ van der Waals alloy; C. Childs (UNLV, USA), Laser annealing after a kinetically hindered phase transition in the pyrochlore $La_2Sn_2O_7$: A method for true structure determination; S.K. Singh (Aryabhatta Group of Institutes, India), High Pressure Phase Transition Properties of Lutetium Monopnictide: A DFT Study; K. Kotmool (Mahidol Wittayanusorn School, Thailand), Superhard Semiconducting Phase of Osmium Tetraboride Stabilizing at 11 GPa; I Danilov (Institute for High Pressure Physics, RAS, Russia), Striking dependence of the properties of glassy propylene carbonate on the P-T way of synthesis.

Young scientist poster awards went to H. Hwang (Yonsei U.), Water Insertion in Kaolinite under Moderate Pressure and Temperature; E.J. Kim (Seoul National U.), Effect of pressure on the structural changes of silicate network of fluid-bearing silicate melts: Insights from multi-anvil press and multi-nuclear solid-state NMR; J. Im (Yonsei U.), High Pressure Chemistry of MIL-47(V) and ZIF-8 in Different Pressure Transmitting Media; X. Liu (U. of Edinburgh), High-pressure crystallisation of biodiesel.

Meetings of the CHP, chaired by A. Katrusiak, featured discussions of Diffraction-data deposition (K. Dziubek), future workshops, historical reviews, and rules regarding the participation of CHP members in the workshops and elections.

The Workshop was sponsored by a number of institutions including YONSEI-SLAC-USC Global Research Laboratory and HYU-HPSTAR-CIS High Pressure Center, funded by the Korean Ministry of Science, ICT, and Planning (MSIP) and the BK21Plus Institute at Yonsei U., funded by the Korean Ministry of Education. Especially the support from the IUCr, HPSTAR, and PAL is gratefully acknowledged. ♦

The Workshop excursion to the PAL site.

Douglas (Doug) Dorset 1942–2016

BY LISA BAUGH, MARK DISKO, BILL DUAX, JOHN FRYER, SVEN HOVMÖLLER, WILLIAM LAMBERTI, LAURIE MARKS, STAVROS NICOLOPOULOS, KARL STROHMAIER AND XIAODONG ZOU

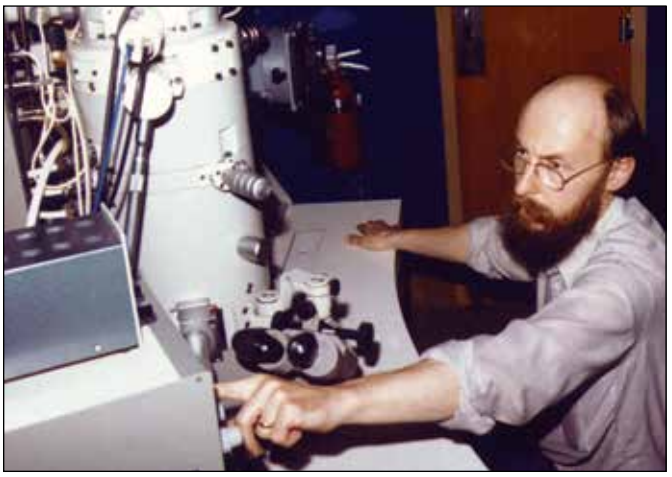
Douglas Dorset passed away on December 8, 2016. He was born in southeastern Pennsylvania on August 29, 1942. He attended Juniata College, majoring in Chemistry and received his Ph.D. degree in Biophysics from the U. of Maryland in 1971 with Albert Hybl. He joined Donald Parson's electron crystallography laboratory at Roswell Park Cancer Institute that year and in 1973 moved to the Medical Foundation of Buffalo – now the Hauptman Woodward Medical Research Institute – where he headed the Electron Diffraction Department and did the fundamental work for which he is best known. Douglas worked on challenging, electron beam-sensitive materials that required strong experimental skills to record representative patterns, and specialized sample preparation methods.

Douglas moved to ExxonMobil Research and Engineering Company in 2000, investigating the structure of wax crystals and how these change in the presence of modifiers. His research encompassed new methods (e.g. use of maximum entropy techniques with Chris Gilmore) and an array of crystallographic studies on zeolites, polyolefins and other materials. While at ExxonMobil, Douglas quickly assumed a leadership role in helping to establish a new materials discovery capability. This included many new catalytic materials that showed promise in separations and catalysis applications, and led to many patents in the area.

In the face of those who said that electron diffraction data could not yield quantitative results, he argued that the problem of dynamical scattering could be overcome and that electron diffraction data could yield *ab initio* structure determinations. He was responsible for bringing the work on electron crystallography of Vainshtein and Zvyagin in Moscow to the attention of a larger western audience. He developed techniques to overcome the problems of the missing cone of data, dynamical scattering, radiation damage and sample problems. His breadth of applications included polymers, waxes, zeolites, fibers, cholesterol derivatives, fullerenes, phthalocyanines, solid solutions of paraffins and proteins at low resolution. He was the first to carry out an *ab initio* solution of a membrane protein structure using electron diffraction data at 6 Å resolution.

In 1995 he published "Structural Electron Crystallography," the first definitive text on the subject and still an invaluable source. This book, together with his pioneering work in electron crystallography, laid the foundation for an explosion of the field in the twenty-first century. Many of his methods are the basis for powerful methods of solving the structure of crystals which are not readily amenable to study using X-ray diffraction methods, employing techniques such as Precession Electron Diffraction, Automated Diffraction Tomography and methods for solving surface structures.

Douglas received the A.L. Patterson Award in 2002 from the American Crystallographic Association. He was within the top 1% of most-cited authors in the chemical literature, world-wide, 1981-1997. He was a member of the IUCr Commission on Electron Diffraction (now Electron Crystallography) 1993–2002 (Chair 1999–2003), and a Co-Editor of *Acta Crystallographica A* 1999–2011. He was on the Editorial Board of the *Journal of*



Electron Microscopy Technique, 1988–2010, and Associate Editor, *Microscopy Society of America Bulletin*, 1992–1994.

Douglas was involved in organizing several of the IUCr International Schools of Crystallography in Erice, Sicily as well as other Schools on Crystallography around the world. He was a good teacher and co-supervised research students in several countries, an enthusiastic supporter of many young researchers – who are now active electron crystallographers. He encouraged many of us in our work during the early years of electron crystallography, when its power was not fully embraced by the global crystallography community. His impressive knowledge of all aspects of crystallography will be remembered by all who met him.

Apart from his interest in science, he was also very interested in politics, environmental causes, culture, history and languages. Discussions with Douglas would start out on a scientific note, then end up encompassing music, languages, typefaces, geography and a multitude of other subjects. Music was important in his life, not the least because his son Erik is a professional violinist. He was also an avid collector of old books. He taught himself Dutch to better understand the medieval printing techniques, and despite his illness over several years had nearly completed a book on the Dutch printing methods.

His wife Bonnie was at his side always. Bonnie was a generous host for those who had come from various parts of the world to work with Douglas. We will forever remember his scientific integrity, knowledge and humor. Douglas is survived by his beloved wife of 49 years, his son, and two grandchildren. ♦

INDEX TO ADVERTISERS

ADVERTISEMENT FEATURE

Silver X-ray source

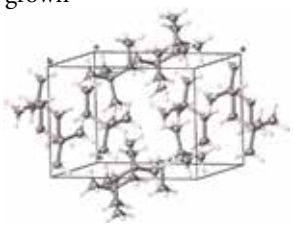
Have you ever faced the conundrum of which wavelength to choose? Most single crystal diffraction labs now have access to more than one X-ray wavelength for small molecule crystallography thanks to the introduction of Rigaku Oxford Diffraction's dual wavelength Gemini in 2005.

In many cases, the decision is clear cut. If it's a light atom containing sample which are often weakly diffracting, containing chiral centres, copper radiation offers both high diffraction intensity and the ability to accurately measure the anomalous signals. Gallium and molybdenum wavelengths struggle to achieve the required measured differences in the phases and amplitudes of Friedel pairs of reflections, a key factor in determining the correct absolute configuration. Traditionally samples that suffer from absorption can be looked at with a molybdenum source, which also enables charge density experiments, as well as high pressure studies.

The new Rigaku Oxford Diffraction microfocus silver source, **Silva,** extends the ability to study a wider range of samples than using traditional copper or molybdenum wavelengths. This shorter wavelength allows the possibility to measure very highly-absorbing samples or to obtain better completion on high pressure setups. Here we describe a variety of experiments with the Silva source and its enhancements over other wavelengths, with the results showing that, in many cases, silver radiation outperforms in terms of data quality and data collection time over other available wavelengths.

High Pressure with Silver

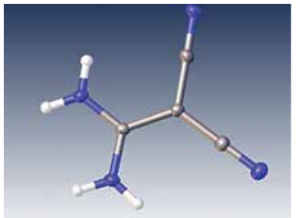
The shorter wavelength of Ag compared to Mo and Cu allows more reflections to become accessible in the limiting window of diamond anvil cells (DACs). This is a huge advantage when it comes to solving the structure with incomplete data. A single crystal of 2,2-dimethylbutane or DMB were grown from liquid in a DAC at Warsaw University, Poland. The sample, having the space group Pnma, was then measured using the **Silva** source at 2.7 GPa. A completeness of nearly 60% was achieved out to 0.8 Å, with a final R1 of 5.0%. The same sample, when run using Mo, did not prove successful.



The final refined structure of DMB and a Diamond Anvil Cell.

Single Theta Charge Density with Silver

A silver source allows for measurement of charge density on samples to a resolution of 0.28 Å, but an additional benefit is the ability to perform a single-theta charge density experiment out to 0.41 Å with the active area of an Atlas S2 CCD detector. Having a single theta position means fewer images and fewer runs, which improves the scaling statistics and reduces overall experiment time.



Crystal picture and refined structure of organic sample from charge density experiment.

An experiment was performed with a crystal of diaminomaleonitrile using the **Silva** and the Atlas S2 CCD detector. The predicted experiment time was 54 hours when using correlated 200 second exposure times. However, due to the intelligent measurement system of all S2 CCDs, any frames with overloaded reflections were automatically re-measured at ¼ of the exposure time, and the binning mode was switched from 4x4 high gain mode to 1x1 standard gain mode. This method utilises the highest detectivity mode of the detector for the weakest reflections at high angle, whilst making sure no information is lost by switching to the highest dynamic range mode for the brightest reflections. This way it is possible to collect strong and weak reflections in the same image, and maintain high data quality.

Experiment details	
Experiment time (hrs)	59
Correlated Exposure time (s)	200
R_{int} (inf – 0.4 Å)	0.055
R_{int} (inf – 0.8 Å)	0.020
I/σ(inf – 0.4 Å)	8.7
I/σ(inf – 0.8 Å)	29.6
R_1 (%)	5.49

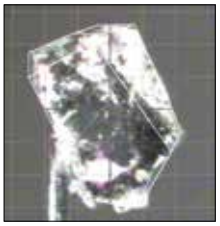
Table 1: Statistics for charge density experiment measured on diaminomaleonitrile, which was kindly provided by Chris Frampton, Brunel U., UK.

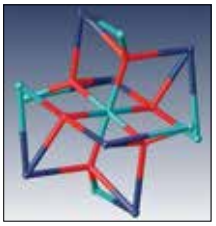
Absorbing samples with Silver

When using silver X-rays, the absorption coefficient (μ) of most samples can be approximately halved. Table 2 below shows the statistics for a crystal kindly provided by Wrocław University, Poland that was run on Mo and Ag microfocus sources with a 1 hour time limit. Although the redundancy was lower for the Ag data due to the longer exposure time per image needed to achieve good statistics, the reduction in absorption actually increases overall I/σ, and improves the final R1 value.

	Mo (μ = 20 mm-1)	Ag (μ = 11 mm-1)
Exposure time per frame (s)	20	40
Redundancy	170	130
I/σ	25	34
R1 (%)	2.29	1.28

Table 2: Details of experiment run on inorganic $Y_3Al_5O_{12}$ crystal with Ia-3d symmetry. Microfocus Mo and Ag sources were used for both experiments and full face-indexed absorption correction applied via CrysAlis^{Pro}.





Crystal image with wireframe model used for the numerical absorption correction, and final structure model

In summary, silver radiation can offer a variety of solutions to the home chemical crystal laboratory. In fact, combining Cu and Ag into a dual wavelength system such as the SuperNova offers allows for protein, absolute configuration, charge density, (very) highly absorbing samples, and weakly diffracting samples to be measured with the highest quality. It offers the widest range of capabilities from a single machine. ♦

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www.Rigaku-OD.com

Advertisement Feature

From your project to our product


Jeanette Hobbs

At Molecular Dimensions, we develop many products in collaboration with academics. Our collaborations with the research community are important as they result in innovative solutions to current issues in structural biology. Claire Naylor spoke to our Product Development Manager, Jeanette Hobbs, about how it works.

How many products did Molecular Dimensions launch last year?

Last year we launched 10 new products, a mixture of screens and other consumables, of which at least 6 came from academic collaborations.

How do you get new ideas for products?

You have to be open to asking customers what they would like to see on your product line and you get some good ideas that way. Communication is the key and I have scientists that I regularly speak to about new ideas and products. I used to seek out collaborations for new products but now we have a lot more customers approach us to help commercialize their idea.

How do you decide if an idea is commercial?

We have a strategy meeting where we go through product ideas and score them for how easy they are to do and their impact on the company and the structural biology world. Everyone has to agree that your product idea is fantastic!

What proportion of the ideas eventually become products?

Probably only 20% of ideas that go into a planning meeting will continue to the product development pipeline.

What is the most useful thing that your collaborators can do to make their product successful?

Have published examples of successes with that product or an application note for it.

How long does it take for a product to go from idea to being on Molecular Dimensions website?

Depending on complexity, type of product and the amount of legal people involved – a few weeks to over a year.

Why should researchers develop their idea with you?

It's fun and we make the process fun for you, plus you get your name in lights and that goes around the world and you'll have kudos forever!

Finally, what is the best thing about your job?

The work I do changes so often I never get bored, and I'm in a unique position to interact with many different types of people from lots of different backgrounds. The daily life of a Product Manager is challenging to say the least, but I probably wouldn't be attracted to it if I was looking for something easy. ♦

Molecular Dimensions

www.moleculardimensions.com

Pioneering SESAME light source circulates first beam

A beam circulated for the first time in the pioneering SESAME synchrotron on January 11. The next step will be to store the beam. This is an important milestone on the way to research getting underway at the first light-source laboratory in the Middle East. SESAME was established under the auspices of UNESCO before becoming a fully independent intergovernmental organization in its own right in 2004. SESAME's Members are from Bahrain, Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, the Palestinian Authority and Turkey. Its mission is to provide a world-class research facility for the region, while fostering international scientific cooperation. The first call for proposals to carry out research at SESAME was recently issued.

"This is a very proud moment for the entire SESAME community," said Khaled Toukan, SESAME Director. "SESAME is now opening for business."

SESAME, which stands for Synchrotron-light for Experimental Science and Applications in the Middle East, experiments will enable research in fields ranging from medicine and biology, through materials science, physics and chemistry to healthcare, the environment, agriculture and archaeology.

The SESAME main ring.

"This is a great day for SESAME," said Sir Chris Llewellyn-Smith, President of the SESAME Council. "It's a tribute to the skill and devotion of the scientists and decision-makers from the region who have worked tirelessly to make scientific collaboration between countries in the Middle East and neighboring regions a reality."

The first circulating beam is an important step on the way to first light, but there is much to be done before experiments can get underway. This process is likely to take around six months, leading to first experiments in the summer of 2017.

Members of the SESAME beam commissioning team led by Technical Director Erhard Huttel (centre) after successfully circulating SESAME's first beam.

In the meantime, scientists wishing to carry out research at SESAME are encouraged to submit their proposals, following the procedure described at www.sesame.org.jo/sesame/component/content/article/85-uncategorised/440- cfp.html. ♦

American Crystallographic Association 2017 award winners

The following awards will be presented at the American Crystallographic Association (ACA) annual meeting in New Orleans, LA, USA, May 26–30, 2017.

Patterson Award to Zbigniew Dauter

Zbigniew Dauter

For over 30 years, Zbigniew Dauter has been one of the leading proponents of the use of synchrotron radiation for macromolecular crystal structure determination. Zbigniew has worked at the EMBL Outstation in Hamburg, the National Synchrotron Light Source at Brookhaven and the Advanced Photon Source at Argonne. He has been an innovative developer of methodology with highly influential studies on the use of anomalous diffraction in biomolecular structure analysis at true atomic resolution. He has strongly influenced the development of phasing methods based on native anomalous scatterers. He has analyzed many structures at exceptional resolution and detail that provided new insights in biological chemistry.

He applies his crystallographic expertise to correct errors in published macromolecular crystal structures. His extraordinary depth of understanding also comes to the fore in his longstanding work as a Section Editor of the biological crystallography section (D) of *Acta Crystallographica*. Zbigniew has delivered many plenary lectures at international conferences where he educates and entertains.

Zbigniew has published in all the sections of *Acta Crystallographica*. He embodies the positive spirit of scientific research at all levels, in depth and in breadth, and fulfills the vision of the ACA Patterson Award to recognize and encourage outstanding research in the structure of matter by diffraction methods, including the methodology of structure determination and/or innovative application of diffraction methods.

David Rognlie Award to Helen M. Berman

Helen M. Berman

Helen M. Berman received her PhD in Chemistry in 1967 from the U. of Pittsburgh. In 1969, she joined the Fox Chase Cancer Center, where her research program focused on nucleic acid crystallography. In 1989, she joined the faculty at Rutgers, the State U. of New Jersey, where she is now a Board of Governors Professor of Chemistry and Chemical Biology.

Helen played an influential role in the early development of the Protein Data Bank (PDB). For nearly five decades she maintained the PDB archive as a resource created by, and for, the community. As head of the Research Collaboratory for Structural Bioinformatics (RCSB), Helen became the Director of the PDB in 1998, and developed the RCSB PDB into a vital and key resource for biology and education. The primary reference for the RCSB PDB was included in *Nature*'s 2014 list of the 100 most cited papers.

In 2003, Helen formed the Worldwide PDB with groups in the UK and Japan to ensure that a single PDB archive would

continue to be freely and publicly available to the global community. She has fostered the development of other bioinformatics resources, ontologies, and community-driven validation standards. These include the Structural Biology Knowledgebase, an online resource that combines the results from the NIH-funded Protein Structure Initiative research with external data annotations to provide comprehensive information about proteins.

Berman serves on many advisory committees and editorial boards. Helen has numerous awards, including the DeLano Award for Computational Biosciences from ASBMB (2013); the Carl Brändén Award from the Protein Society (2012); a Fellow of the ACA (2011); the Martin J. Buerger Award from the ACA (2006); and a Distinguished Service Award from the Biophysical Society (2000).

Elizabeth Wood Science Writing Award to James O'Brien

James F. O'Brien

James F. O'Brien began his academic career as a physical chemist at Missouri State U. (MSU) in 1969. He won three teaching awards including the Governor of Missouri's Award for Teaching Excellence (2001). In 2002 he was granted the status of Distinguished Professor – the highest status awarded to faculty at MSU. Early in his career O'Brien began presenting general lectures as part of the American Chemical Society speaker series. He has given 293 invited talks at seminars, banquets, meetings, etc., including 135 Sherlock Holmes lectures and 136 "Famous Mad Hatter" talks about mercury poisoning. In 2010 he was elected to the MSU Wall of Fame. O'Brien's writing for the general public has focused on Sherlock Holmes. The book *The Scientific Sherlock Holmes* won an Edgar Award from the Mystery Writers of America as the best book of 2013 in the critical/biographical category.

Etter Early Career Award Christine Dunham

Christine Dunham is the recipient of the 2017 Margaret C. Etter Early Career Award, which recognizes "outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career."

Christine Dunham

Christine is using X-ray crystallography and cryo-EM to understand how proteins are synthesized in bacteria and how the process is regulated in conditions of stress. She is interested in the molecular basis of frameshift errors, which arise when the ribosome reads a shifted sequence of the messenger RNA, producing an alternative protein sequence, the role of the toxin-antitoxin system in persistency, a latent state that bacteria enter under stress, and the link between RNA modification and antibiotic resistance.

Christine obtained a bachelor's degree at Barnard, a PhD from the U. of California, Santa Cruz, and was a post doc at the MRC in Cambridge, UK, with Venki Ramakrishnan and is currently at Emory U. ♦

Further information on these awards can be found at www.amercrystalassn.org/2017-award-winners.

T.K. Sidey Medal: Getting a clearer image of biomolecules and tissue

www.royalsociety.org.nz/2016/11/23/tk-sidey-medal-getting-a-clearer-image-of-biomolecules-and-tissue/

Rick Millane from the U. of Canterbury has been awarded the T.K. Sidey Medal from the Royal Society of New Zealand for his contributions to methods for imaging biological molecules. His theoretical and computational methods for imaging biological molecules and tissue using X-rays and optical radiation allow their structures to be determined.

Millane was "delighted and honored" to receive the award, particularly since the first Sidey Medal was awarded to Ernest Rutherford in 1933. "I am grateful to the many students and colleagues around the world who have supported and contributed to my research."

Millane is well known internationally for his work on 'phase retrieval' methods,

Rick Millane receives the T.K. Sidey medal from Barry Scott. *Photo credit: Royal Society of New Zealand.*

an important component of X-ray diffraction imaging. His phase retrieval algorithms have been applied to the latest imaging technology: X-ray free electron lasers (XFELs), which use X-ray pulses short enough and intense enough to image biomolecules that have defied conventional imaging methods, and use nanoscale crystals with just a few unit cells in each direction. This technology has the potential to greatly advance understanding of disease processes and drug design.

The selection committee acknowledged him as a leader in advancing algorithms that are suitable for this new technology. Millane has also worked on fiber diffraction analysis for imaging and determining the structures of disordered or non-crystalline substances, including biopolymers such as DNA and sugars in connective tissue.♦

Eleventh Ewald Prize awarded to Sir Tom Blundell

The eleventh Ewald Prize has been awarded to Sir Tom Blundell (U. of Cambridge, UK) for his work as 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, he determined an exceptionally broad array of medically critical human protein structures; championing methods enabling drug design and discovery through structural optimization, crystallographic fragment screening, and computational modelling; and for being a leader in advanced crystallographic education internationally.

The presentation of the Ewald Prize will be made during the Hyderabad Congress Opening Ceremony on August 21, 2017.

A fuller tribute will be appearing in the next issue.♦

On the Cover

Aspects of IUCr2017: (clockwise from top left: IUCr2017 logo; Ewald Prize winner, Sir Tom Blundell (see article above); the world's largest crystal structure model will be on display at the Congress (http://worldrecord.r-krickl.com/, *photo credit: Robert Krickl*); The Charminar, a monument and mosque in Hyderabad; the Programme Committee; and two views of the Hyderabad International Convention Centre (HICC).

Special Issue of Polish Biochemical Society Quarterly dedicated to Alexander Wlodawer

www.postepybiochemii.pl/#Archiwum?./cont/3_2016.html

BY MARIUSZ JASKOLSKI

This year, Alexander Wlodawer, a renowned figure in structural biology, is celebrating his 70th Birthday. Alex graduated from the U. of Warsaw, and received his PhD from UCLA. Since 1987 he has directed a protein crystallography laboratory at the National Cancer Inst. in Frederick, MD. Alex maintains very close ties with Polish science, supporting scientists from and in Poland, engaging in collaborative research, and participating in scientific panels. In 2005 he was elected a foreign member of the Polish Academy of Sciences. Alex is famous for contributions to the structural biology of the HIV virus and of other biomedical targets. He is a dedicated mentor and promoter of science, and an exemplar of the highest standards in scientific conduct and research.

A Special Issue of the Polish Biochemical Society Quarterly, *Postępy Biochemii* (www.postepybiochemii.pl/#Archiwum?./cont/3_2016.html), dedicated to Alexander Wlodawer has contributions from his many coworkers, mentees, and friends.♦

24th Congress and General Assembly of the International Union of Crystallography

Hyderabad, India, August 21 – 28, 2017
www.iucr2017.org/

The 24th Congress and General Assembly of the IUCr will be held in Hyderabad, India, August 21–28, 2017, at the Hyderabad International Convention Centre (HICC). The opening ceremony will be held during the early evening of August 21 and will include the Ewald Prize lecture.

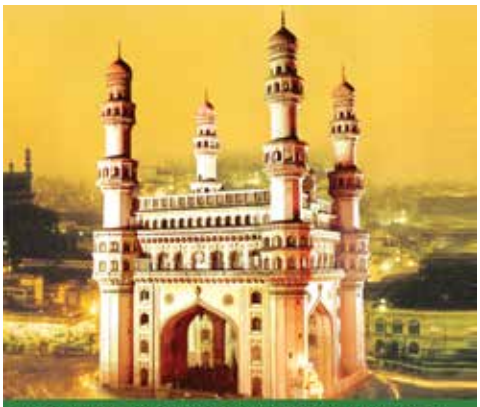
The program will be cutting edge with 3 plenaries, 40 keynotes, 119 microsymposia and also posters, commercial exhibits, satellite meetings, workshops and official meetings of the IUCr. The Congress will present the latest and most exciting crystallography research in fundamental areas, chemistry, physics, biology, pharmaceutical sciences and materials research.

This Congress will offer several new and unique features for registered participants. These include spot presentations by young investigators for *ad hoc* research grant awards, formal arrangements for face-to-face interactions between students and established crystallographers, and the setting up of collaborations between scientists from developing countries and others. Additional new features are e-posters and e-abstracts linked to IUCr journals and free access for all our journals from HICC during the days of the Congress. Pre-conference outreach activities all over the world, including India, are already underway to promote crystallography and science in general among young students, including school children, to take forward the legacy of the International Year of Crystallography and of the 24th Congress.

Several scientists and students from Africa, South America and smaller Asian countries are expected to attend the Congress and we will make all efforts to ensure their participation.

The Local Organizing Committee is pleased to inform you that the online registration and abstract submission forms are now available on the Congress website, www.iucr2017.org/, which is being updated regularly. ♦

Registration and abstract submission now open



The Charminar in Hyderabad, inspiration for the IUCr2017 logo.

Important dates

February 28, 2017	Abstract submission deadline (registration is required for abstract submission but payment is not mandatory at this stage)
March 15, 2017	Bursary application deadline (bursaries are given to partially support travel and subsistence, not registration)
April 15, 2017	Bursary and abstract acceptance announcement
May 7, 2017	Payment deadline for bursary recipients
May 31, 2017	Early bird registration closes (participants and students whose abstracts have been accepted must complete payment formalities before this date)
August 10, 2017	Regular registration closes

67th Annual Meeting of the American Crystallographic Association

New Orleans, LA, USA, May 26–30, 2017
www.amercrystalassn.org/2017-meeting-homepage

Sir James Fraser Stoddart

The meeting will launch with a full day of workshops on four different topics followed by an Opening Ceremony and Reception on Friday, May 26. We are honored to have Sir James Fraser Stoddart, 2016 Nobel Laureate in Chemistry, scheduled to give a plenary lecture at the Opening Ceremony, on Friday, May 26.

The theme of this year's Transactions Symposium is Cryo Electron Microscopy that will feature lectures by the world's leading researchers and experts. New this year will be a session on NMR crystallography. Both are dedicated to covering topics of importance to scientists with a wide range of professional backgrounds and designed to emphasize our need for collaboration and cooperation.

The meeting will provide multiple opportunities for networking: Opening Reception, Networking Mixer, Closing Awards Banquet, as well as vendor lunches and evening poster sessions.

Young researchers will benefit from special and free events such as Career Development, Networking Mixer, Diversity and Inclusion, Communicating Science to Public, Undergraduate Research Symposium and educational sessions and workshops. You are encouraged to apply for funding support through travel grants, by volunteering, or contact us if there are many students coming from the same lab.

Information on this year's awardees can be found on Pages 20–21. For detailed information about this conference, visit www.amercrystalassn.org/2017-meeting-homepage. ♦

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

May 2017

22-26 ♦ ACA 2017. New Orleans, LA, USA. www.amercrystalassn.org/. See Page 23

July 2017

2-7 ♦ 4th European Crystallography School (ECS4). Warsaw, Poland. http://ecs4.ecanews.org.

August 2017

14-15 ♦ International Satellite Meeting on Improving Data Quality in XAFS Spectroscopy. Oxfordshire, UK. www.diamond.ac.uk/Home/Events/2017/Q2XAFS2017.html.

15-20 ♦ Crystallographic Computing School. Bangalore, India. www.iucr.org/resources/commissions/crystallographic-computing/schools/bangalore2017.

18-20 ♦ PPXRD-15: Pharmaceutical Powder X-ray Diffraction Symposium. Hyderabad, India. www.icdd.com/ppxrd.

19-20 ♦ Electron Diffraction for Materials Science and Pharmaceutical Applications. Brussels, Belgium. http://www.iucr17edsat.com.

21-28 ♦ 24th IUCr Congress and General Assembly. Hyderabad, India. www.iucr2017.org. See Page 23.

29-30 ♦ Crystallography and Society. Pune, India. www.iucr2017.org/program/satellite-meetings.

29-30 ♦ SASCheM 2017: Structural Aspects in Studying Chemistry of Materials. Kolkata, India. www.iiserkol.ac.in.

30-4 ♦ Int'l School on Fundamental Crystallography and Workshop on Structural Phase Transitions. Odisha, India. http://nitrkl.ac.in/Academic/1Department/ph/CEP/Structural%20Phase%20Transitions.aspx.

October 2017

8-13 ♦ Int'l School on Fundamental Crystallography and Electron Crystallography. Sofia, Bulgaria. www.crystallography.fr/mathcryst/sofia2017.php.

November 2017

20-21 ♦ ICG – Italian Crystal Growth. Milan, Italy. http://sites.unimi.it/ICG2017/index.html.

13-23 ♦ Macromolecular Crystallography School 2017. Montevideo, Uruguay. http://pasteur.uy/mx2017.

Bruker OpenLab Albania, May 30 – June 3, 2016 *continued from Page 9*

tion for the Promotion of Crystallography in Albania) working group, which was then extended thanks to the participation of crystallographers from Kosovo, and finally converged into the AAC. The AAC is now a member of the ECA and has applied for membership of the IUCr.

The idea of organizing this activity was then to further disseminate and raise awareness about the importance of crystallography, and highlight the fact that Albania and Kosovo would definitely benefit from a proper crystallography education at the academic level. In conclusion, the OpenLab Albania encouraged close cooperation in the South-East Europe and Balkan region, provided advanced knowledge and technology, and made the public aware of the importance of studying and advancing crystallography, because it matters! ♦

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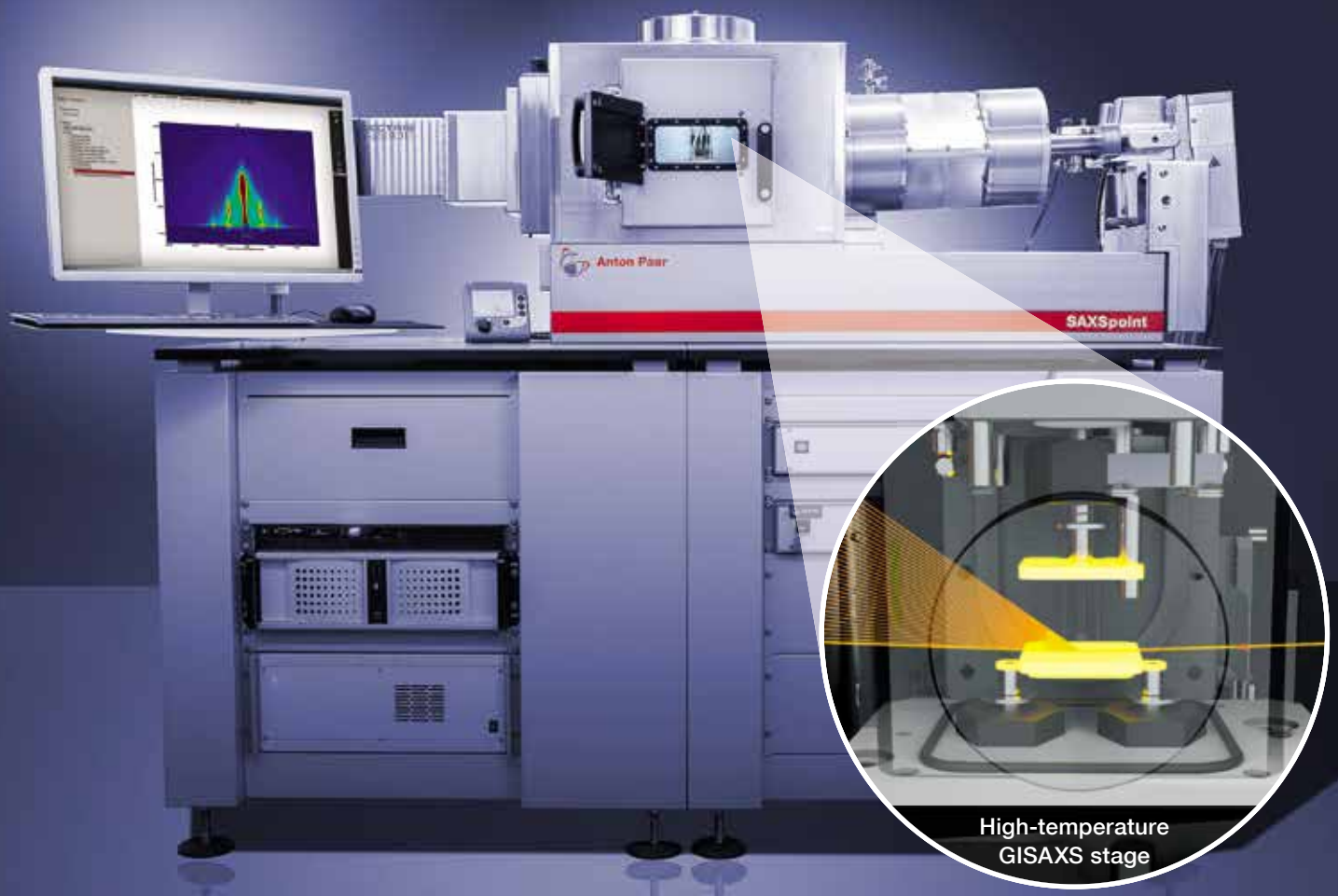

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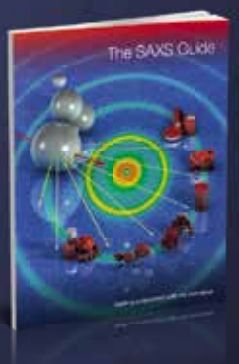

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