

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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IUCr Journals get a fresh change of clothes



The online version of the IUCr's research journals was launched at the 1999 Congress in Glasgow under the masthead of **Crystallography Journals Online**. It was an innovative platform, providing full-text HTML with high-quality mathematical typesetting, easy access to CIFs and other supporting information associated with any article, and links out to cited literature and structural database entries.

Now, 16 years later, to accommodate new hardware devices and to meet the desire for more information about significant new publications, the IUCr Journals website has been given a fresh new livery and enhanced functionality. The new design is clean, bright and adaptable to different screen sizes. Exactly the same information is served up to mobile phone, tablet and desktop devices, but the format will change to suit the limitations or advantages of each class of device.

New article format



Citation record and cumulative download statistics for an article published in *Acta Crystallographica* Section A.

The straightforward, linear presentation of individual articles has not altered - readers still find this the most natural and efficient way to read articles. However, a new default sans-serif typeface and changes to the design of tables and figures improve the clarity of the HTML text. There is also clearer marking of the article's category, citation and digital object identifier (DOI), together with its copyright and licensing

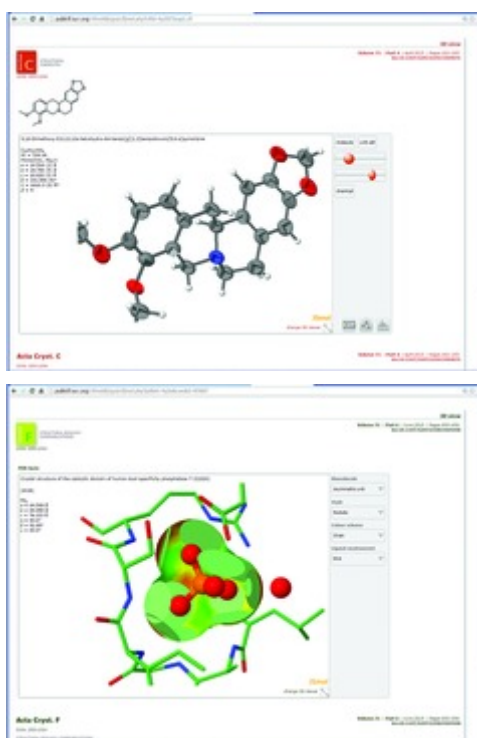
information and a clear indication if it is open access or free-to-read. Prominent at the top of each page is an obvious link to the article's status and publication history as certified by the CrossMark system.

As before, technical terms in crystallography and chemistry are hyperlinked to, respectively, definitions in the *Online Dictionary of Crystallography* and the *IUPAC Compendium of Chemical Terminology* (the 'Gold Book'). Also, the reference list links out to cited articles and database entries indirectly through CrossRef, the Web of Science, Chemical Abstracts Service and the CCDC, or directly in the case of IUCr Journals.

A toolbox of useful features takes the form of a set of buttons. Whenever appropriate, the same buttons appear on the summary (abstract) page or table of contents associated with the article. This allows the reader to obtain relevant information about the article (e.g. citation format, usage statistics, supporting information) from the most convenient entry point. So you do not have to be actually reading an article, for example, to obtain a three-dimensional visualisation of the structures it describes - particularly useful for non-subscribers who wish to learn more about a non-open-access article.

An especially useful new feature is the detailed usage information available for every article, showing numbers of citations as recorded by a number of monitoring services, as well as a detailed interactive graph of all article downloads in both PDF and HTML formats from the IUCr Journals server.

New supporting information format



3D visualisation of small molecules (top) (on the IUCr Journals server) and biological structures (bottom) (from the PDB).

IUCr Journals have always excelled in providing free and easy access to supporting information, especially the structural data files (CIFs, structure factors or Rietveld profiles). Now, experimental, coordinate and geometry data from the CIF can be viewed inline at the end of any article reporting a small-unit-cell structure.

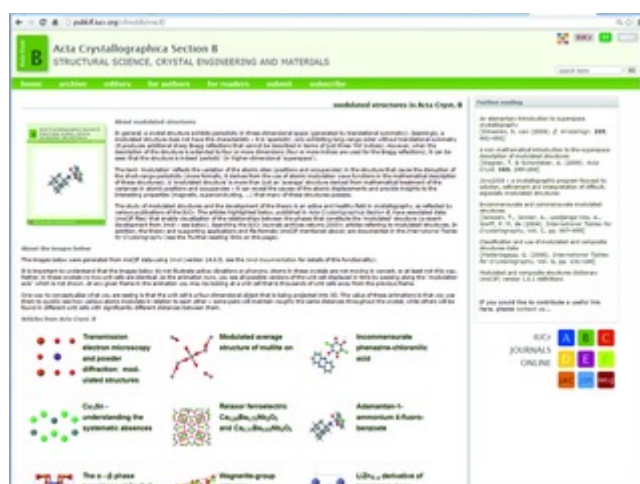
The '3dview' visualisation interface has been improved and provides a common interface for three-dimensional interactive images of all classes of structure: biological macromolecules, inorganics, small molecules, metal-organic complexes. For small structures, there are also tools to view or predict powder profiles, and to perform similarity searches among other structures published in IUCr Journals.

New journals information format



Each journal home page highlights significant new content.

The colourful bold design of the new site emphasises that each journal is part of the same high-quality publishing stable, but at the same time brings out the distinctive qualities of each title. Each journal home page highlights a number of recent articles of particular interest or significance. In many cases, these highlighted articles have accompanying commentaries establishing their importance, either in featured articles on the general IUCr home page or as commissioned companion pieces in the journals themselves.



The gallery of incommensurate structures.

Sidebar allow for a variety of content related to the specific focus of each journal. For example, *Acta Crystallographica* Section B has a sidebar link to a gallery of amazing visualisations of incommensurate modulated structures published in the journal. These use *JSmol* to produce animations in time that correspond to lattice distortions in space. *Journal of Synchrotron Radiation* focuses on beamline papers in a sidebar, while other journals provide links to special or virtual issues, or provide access to article listings according to keywords categorising the journal's scope.

The journal home pages also feature constantly updated lists of latest, most-read and most-cited articles. For each journal, a new 'about' page provides a detailed synopsis of that journal's main features, and includes an interactive map showing the distribution of authors worldwide.

Preserving the virtues

Table. The IUCr journals in 2015

	IUCrJ Editors: Edward N. Baker, Gautam R. Desiraju, C. Richard A. Catlow, Sine Larsen and John C. H. Spence
	Acta Crystallographica Section A: Foundations and Advances Editors: Simon J. L. Billinge and Jianwei Miao
	Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials Editors: Alexander J. Blake and Marc de Boissieu
	Acta Crystallographica Section C: Structural Chemistry Editors: Anthony Linden and Paul Raithby
	Acta Crystallographica Section D: Biological Crystallography Editors: Zbigniew Dauter, Jenny L. Martin, Randy J. Read and Soichi Wakatsuki
	Acta Crystallographica Section E: Crystallographic Communications Editors: William T. A. Harrison, Helen Stoeckli-Evans, Edward R. T. Tiekink, Luc Van Meervelt and Matthias Weil
	Acta Crystallographica Section F: Structural Biology Communications Editors: William N. Hunter and Manfred Weiss
	Journal of Applied Crystallography Editors: Andrew Allen, Janos Hajdu and Anke Kaysser-Pyzalla
	Journal of Synchrotron Radiation Editors: Gene Ice, Ilme Schlichting and J. Friso van der Veen

The refreshing new look also reflects the changing dynamic of the journals' aims and scope. In the last couple of years, IUCrJ has been launched as an open-access journal publishing high-profile articles with wide appeal across all the fields of science where crystallography plays an important role. Many of the journals have gained new Editors, bringing expertise from new areas, and many of the sections of *Acta Crystallographica* have revised their subtitles to reflect more accurately their subject areas (see Table).

While the presentation of scholarly research in IUCr Journals has been enhanced enormously by this makeover, the journals themselves maintain their commitment to high-quality peer review, expert editorial guidance, and careful copy-editing, proof-reading and typesetting that has always been their hallmark.

As is clear from the incredibly diverse range of inputs into the International Year of Crystallography (chronicled on <http://iycr2014.org>), crystallography is a science that penetrates deeply into many other disciplines: structural chemistry, materials science, mineralogy, solid-state physics, structural biology, mathematical group theory ...

More than ever, IUCr Journals seek to be a natural home for articles describing any relevant area of molecular, structural and materials properties research. They remain true to the vision of *Acta Crystallographica*'s Founding Editor, Paul Ewald, who wrote in the very first editorial of 1948: '*Acta is intended to offer a central place for publication and discussion of all research in this vast and ever-expanding field. It borders, naturally, on pure physics, chemistry, biology, mineralogy, technology and also on mathematics, but is distinguished by being concerned with the methods and results of investigating the arrangement of atoms in matter, particularly when that arrangement has regular features.*'

While the scholarly publication landscape is changing in the 21st century, IUCr Journals' commitment to quality, to capturing, reviewing, critiquing and disseminating the most important advances in the structural sciences, and to promoting interdisciplinary research is unwavering. And we hope, with this refreshed online platform, this will become more apparent than ever to the widest range of discerning readers.

IYCr 2014

The IYCr2014 crystal-growing competition for schoolchildren



Design: S. Allaey.

Crystal-growing competitions have been run successfully for many years in a number of countries. As one of the objectives of the International Year of Crystallography was to introduce students to the exciting, challenging and sometimes frustrating world of growing crystals, the organizers of a number of national and regional competitions wanted to share their experience with future organizers around the world. The IYCr in 2014 provided perfect timing to start many new regional and national competitions.



Some of the proud winners from schools in Argentina, Australia, Belgium, India, Lithuania, Portugal, Spain, UAE and UK.

A brochure was produced to provide newcomers with the necessary information to join this exciting venture of growing single crystals. Not only a scenario to set up a competition and some basic tips on how to get started with crystal-growing experiments were provided, but also support was offered by a small working group of coordinators of existing national competitions. In addition a new animated video 'How to grow a single crystal - with Johanna' was created to show the basic steps of growing large single crystals at the level of schoolchildren. These materials are available at the IYCr2014 website: www.iycr2014.org/participate/crystal-growing-competition-2015. At the end of 2014 we were able to locate at least 34 regional and national crystal-growing competitions.

To establish a vibrant worldwide network of schools participating in crystal-growing experiments, a worldwide competition open to all schoolchildren up to 18 years old was set up. It is of course not realistic to grow during the same period of time single crystals of the same compound in every country. Instead the participants were asked to convey their experiences through videos or essays. A panel of judges has evaluated all the entries - 134 entries in total from 25 countries - using the following criteria: creativity, aesthetic value, description of working plan and experimental work, clarity of explanations and scientific background. A difficult job, as the quality of the submissions was amazingly good!

Five gold, silver and bronze medals, together with 12 honorary mentions and four creativity prizes, were awarded for the videos category, whereas for the essays category, three gold, silver and bronze medals and seven honorary mentions were awarded. The official announcement of the laureates took place during the IYCr2014 Legacy launch conference in Rabat (April 22-24, 2015). Medals, certificates and prizes were sent by mail to the laureates by the end of May. All winning entries are available at the website of the competition. Have a look - some of the videos are really professional and can be used in motivating others to start their own crystal-growing experiments!

Following the great success of the IYCr2014 competition, the IUCr has announced the 2015 edition of the worldwide crystal-growing competition for schoolchildren. This time only videos can be submitted; the closing date for submissions is November 22, 2015.

The IUCr has also organized, together with UNESCO, a special crystal-growing competition for selected schools belonging to the UNESCO Associated Schools Network, which ran for a period of four weeks in October-November. A total of 51 crystals were submitted to UNESCO headquarters from participants in Singapore, Benin, Argentina, Cote d'Ivoire, France, Zambia, Cape Verde and Switzerland. The laureates of this competition were participants from Yishun Town Secondary School in Singapore, Benin Université in Benin and Colegio Juan Demonte No. 2701 in Argentina.

Luc Van Meervelt, Coordinator of the IUCr Crystal-growing competition for schoolchildren

The IYCr team asked the winners of the 2014 crystal-growing competition for schoolchildren how they had heard about the competition and how they would like to learn more about crystallography-based topics at school. Here are some of their replies:

I heard about the competition on the website and as I had been growing crystals for over 5 years I thought that it would be good to enter. I have been inspired to grow bigger Alum crystals but in saying that I want to learn how the study of crystallography can be used to make more effective medicine, better tasting food and more. I love growing crystals.

Sam Gorrie, St Andrew's School, Walkerville, SA, Australia

We heard about the competition through known contacts at the Indian Institute of Science (IISc) in Bangalore. We hope to learn more about crystallography-based topics through your website and hands-on working in IISc. It was a great learning experience and a very interesting and challenging project for both of us.

Aditya Bhargava and Arundhati S., Sharada Vidyanikethana Public School, Mangalore, India

We heard about the IYCr2014 worldwide crystal-growing competition through the Assistant Principal of Holy Family Primary School. She was made aware of the local state competition by the organiser, Dr Ashraf Ghanem (University of Canberra - Royal Australian Chemical Institute). Dr Ghanem organises the local competition and invited the winners to submit their reports to the IYCr2014 website. It would be nice to have lectures given by experts in the field, even short internet-based presentations where schools can log in from all around the world. These could be provided in real time or afterwards as a YouTube video. We thought maybe a series of weekly or monthly lectures introducing the topic of crystallography with basic details and some experiments that would, over a period of time, delve further into the wonderful world of crystallography. These videos would have to be carefully tailored for the appropriate age group.

Benjamin and Aidan Rothenfluh, Holy Family Primary School, Gowrie, ACT, Australia

I am very much interested in participating in the competition this time around also, as it was great fun and an excellent learning experience for me. I have informed many of my friends who are interested. I heard about the crystal-growing competition when I was browsing the Internet for some interesting science project ideas. I saw the competition introductory video and found it very interesting. Then, as I learnt more about crystals I found it quite fascinating and decided to participate in the competition. I learnt a lot during the research on crystals and uses of crystallography during last year's competition. I learnt how crystallography underpins all sciences from biology and genetics to structural, IT and automobile engineering. At school, I would love to experiment to see how the structure of matter and arrangement of atoms changes the core properties of the materials. I would like to learn how crystallography is helping develop new drugs. As I am in middle school exploring various avenues for my future career, learning about crystallography has opened new horizons of opportunities and unlimited possibilities.

Prerana Pai, Delhi Private School, Sharjah, United Arab Emirates

IYCR 2014

IUCr awarded ICSU grant for 'Building Science Capacity in Africa via Crystallography' project

We are proud to announce that the IUCr has been awarded a grant for the project 'Building Science Capacity in Africa via Crystallography' under the ICSU Grants Programme 2015. The proposal was prepared as a follow-up to the IYCr Pan African Summit meeting (Bloemfontein, October 2014) and submitted by the IUCr (as an ICSU member) on behalf of Andreas Roodt, President of ECA and chair of the Summit meeting, and Michele Zema, IYCr Project Manager and IUCr representative for the proposal.

The IUCr project is supported by:

- ECA
- UNESCO
- ICSU Regional Office for Africa
- INDABA Series of meetings
- SAASTA (South African Agency for Science and Technology Advancement) Public Engagement with Nanotechnology

The project aims at further cementing the African Crystallographic Association (AfCA), whose Steering Committee was established at the Summit meeting in Bloemfontein in October 2014. The programme will be conducted as part of the IUCr Crystallography in Africa initiative.

The main actions will be:

- (i) to set up a follow-up meeting to the Summit, preferentially in Northern Africa, to further work towards the formal formation of AfCA;
- (ii) to arrange the First Pan African Conference on Crystallography (PCCr1), which will be held at the University of Dschang in Cameroon (Central Africa), October 6-11, 2016. This conference aims to bring together African crystallographers, mineralogists and solid-state and structural scientists to increase the awareness of crystallography and improve the educational opportunities for African researchers and students of all levels;
- (iii) to bring African scientists to the INDABA series of conferences in South Africa (in the latter part of 2015) to expose them to high-level international interdisciplinary science.

Moreover, the project includes many additional actions, which will be undertaken pending the availability of funds, infrastructure and human resources.

For more information, please visit www.iycr2014.org/capacity-building/icsu2015.

IYCR 2014

International Year of Crystallography 2014 Resolution

Issued on the occasion of the IYCr Legacy Conference, Rabat, Morocco, 22-24 April 2015

Crystallography for the next generation

In January 2014, the United Nations Educational, Scientific and Cultural Organization (UNESCO) and the International Union of Crystallography (IUCr) launched a number of activities to support the United Nations Resolution A/RES/66/284 of 3 July 2012 proclaiming the International Year of Crystallography.

The significance of the International Year was summarised in a booklet entitled '*Crystallography matters!*', distributed worldwide in 16 different languages. Over the course of the year, hundreds of activities, initiatives and publications brought the importance of crystallography to new audiences, actively trained new crystallographers, and raised the profile of a science that is central to so much of our understanding and interaction with the world around us.

The conference '*Crystallography for the next generation*', held in Rabat, Morocco in April 2015, under the High Patronage of His Majesty King Mohamed VI, reviewed with pride the accomplishments achieved during the International Year, with a forward-looking focus on how to sustain momentum and build on success. At a time when scientific endeavour is critical for societal benefit and the importance of crystallography is greater than ever, crystallography remains a science that still has lower visibility than it should.

We, the undersigned, therefore **commit**:

1. to enhance the stature of crystallography

- by maintaining close liaison and representation between our individual organisations
- by collaborating on relevant programmes of science policy at regional, international and global scales
- by forging closer links between the IUCr and other International Scientific Unions
- by encouraging the recognition of crystallography as an essential component of physics, materials science, chemistry and structural biology, and of its inclusion in curricula for secondary and tertiary-level education
- by continuing to protect the integrity of science through publication of peer-reviewed journals and reference works of the highest quality;

2. to build capacity in developing regions of the world

- by continuing implementation of the OpenLabs and related training initiatives
- by coordinating strategic projects based on available funds and resources, such as the IUCr 'Crystallography in Africa' and the IUCr-ICSU 'Building Science Capacity in Africa via Crystallography' programmes, and supporting similar initiatives in Latin America and South-East Asia
- by encouraging talented students to take advantage of opportunities such as the TWAS Fellowships for Research and Advanced Training
- by continuing to transfer expertise through Visiting Professorship programmes and regional schools or workshops
- by working to reduce barriers to the free movement of scientists;

3. to extend further the public understanding of science in general and crystallography in particular

- by maintaining and expanding educational and public awareness materials and making them freely available in many languages
- by direct engagement of practising crystallographers with active school outreach programmes such as UNESCO Associated Schools Network
- by ongoing development of local crystal-growing activities for schoolchildren and the permanent establishment of a global coordination;
- and we call upon our associates, scientific practitioners and educators worldwide to join our organisations in these efforts to sustain and build on the momentum of the International Year of Crystallography in the spirit that now 'Crystallography matters ... more!'



To endorse the actions and goals set out in the IYCr2014 Legacy Resolution go to <http://iycr2014.org/declarations/legacy-endorsement>



IYCR 2014

Bruker OpenLab Algeria, May 9-14, 2015



The IUCr-UNESCO OpenLab Algeria, which was held at the Université frères Mentouri in Constantine from May 9-14, 2015, and organized in partnership with Bruker, was a great success. A total of 80 students (40 from Constantine and 40 from other Algerian as well as Tunisian and Moroccan universities) attended the OpenLab, which also included several hands-on tutorials and the exhibition 'Voyage dans le Cristal'.

The programme book and photo gallery can be seen at www.iycr2014.org/events/openlabs/bruker-openlab-algeria.

This school was organized in the format of an OpenLab, within the scope of the International Year of Crystallography celebrations. It was sponsored by the IUCr and actively supported by the Bruker AXS company and the Cambridge Crystallographic Data Centre (CCDC).



The school was open to all researchers from the Maghreb and the rest of Africa, and most particularly to PhD students who are regular users of crystallography in their research work, and to young crystallography professors.

Due to space limitations, the workshops were restricted to 80 registered PhD students. The geographic student distribution was the following: 12 foreigners from Africa (including citizens of the Maghreb), 28 Algerians not from Constantine and 40 from the Université de Constantine.

Lectures and seminars were open to the general public, in particular to MSc students of all areas of chemistry (60 students). Raising awareness about crystallography among the students in their final year in the Master programme, and refreshing the crystallography knowledge of all the staff involved in using crystallographic methods as their main analytical tool, were some of the main objectives of the school. Many people who had already some knowledge in crystallography participated, and we spared no effort to spread knowledge of this science around, beyond our fellow crystallographers.

Teaching and training were carried out by local specialists and invited distinguished crystallographers. Overall, 10 foreign invited guests, 10 invited Algerians (all of whom are crystallography professors and members of the Algerian Association of Crystallography) and 20 crystallographers from CHEMS, our research unit, combined their efforts to provide the required teaching and training.

The first day started with the opening ceremony and presentations for the dissemination of the science of crystallography to the general public, including a description of the history of crystallography, its evolution and its importance in research and in industry. One of the highlights of the first day was the award ceremony for the winners of the crystal-growing competition for middle-school and high-school students.

The programme of the other days consisted of seminars, lectures and workshops. Eminent scientists presented the cutting edge developments in crystallography.

Shows, on display in a hall of the building reserved for the OpenLab, were accessible at all times during the week. The following topics were presented:

- a voyage back in time to show the equipment and ancillary devices used by crystallographers throughout the history of this science;
- a voyage in the crystal in order to make the onlooker discover the multiple facets of crystals, not just literally, but also their beauty, their many marvels, in science for their contribution to the understanding of the structure of matter and of life itself, and an incredible material for its numerous application in modern life;
- a display of works, related to the structure of crystals, made by high-school and middle-school students in the scope of a design competition (various objects: ornaments, drawings, models, designs, ...).

The activities undertaken by our research unit CHEMS in order to promote the science of crystallography were not limited to the one-week school described above. Three other events were organized, solely in 2014: (1) With the support of the Université de Constantine, we celebrated the International Year of Crystallography by organizing open houses. Inauguration took place in March 2014, when the Minister of Higher Education and Scientific Research came to do the unveiling. (2) Open houses also took place in April 2014, (3) followed in combination by the Student Day on May 19, 2014. On this occasion, we were honoured by the presence of the General Secretary of the Minister of Higher Education and Scientific Research, together with the General Director of Scientific Research and Technological Development.

Hocine Merazig

Currently, crystallography has become almost a 'press-button' science because of the rapid progress of computer technology. Nowadays, crystallographers, and especially young crystallographers, are increasingly trapped by the technology which hides behind the science of crystallography. Yet this delicate science requires particular attention to detail in order to obtain good research results. For this reason, it is essential to attend schools like this, to strengthen basic knowledge before setting to work on computer processing, and to go further in research.

Andriamanantena Laza, participant

IYCR 2014

Bruker OpenLab Tunisia, May 14-23, 2015



The IUCr-UNESCO OpenLab Tunisia was organized in partnership with Bruker France and held in the form of a travelling lab, making use of the portable Bruker D2 powder diffractometer. Logistical organization and lecturing were provided by members of the Tunisian Crystallographic Association (ATC) with the support of local universities and laboratories. Two stops were made: Monastir, May 14-17, 2015, and Nabeul, May 20-23, 2015.

First stop: Monastir



Participants at the Bruker OpenLab in Monastir.

The first stop was held at Hotel El Habib in Monastir. Due to space limitations, the workshops were limited to 33 participants, including 27 PhD, 3 Master students and 3 technicians, coming from different Tunisian universities (Sfax: 13; Monastir: 7; Tunis: 5; Bizerte: 2; Borj-Cédria: 1; Gabès: 2; Gafsa: 1; Mahdia: 1; Sidi-Thabit: 1) plus one from Algeria. The main objective of this event was to improve both the crystallographic theoretical knowledge and the experimental skills of the participants. The training sessions were carried out by local experts of the ATC (Mohsen Graia, Mohamed Oumezzine, Habib Nasri and Nasr Sdiri), supported by five crystallographers from the physical-chemistry of materials research units of Monastir (Hassen Bachoua, Marwene Oumezzine, Amel Hassine) and Sfax (Issam Omri, Fadhila Edhokkar), who ensured a smooth functioning of the workshops. The opening ceremony was hosted by the ATC President, Mohamed Oumezzine; the organizer of the OpenLab, Mohsen Graia; and the Bruker France delegate, Loïc Le Dréau. The lecturers successfully developed the theoretical part: theory of diffraction of X-rays, X-ray diffraction from powder, pattern matching, structure refinement by the Rietveld method, preparation of the CIF file and use of the *pubCIF* and *checkCIF* tools, the CCDC *ConQuest* software, and resolution and refinements of large molecules with disorder. Workshop 1 was dedicated to demonstrating the diffraction equipment and hardware, *i.e.* X-ray tubes, filters, monochromators and detectors (fluorescent screens, photographic films, Geiger-Muller and scintillation counters). Workshop 2 was devoted to preliminary operations, such as choosing crystals at the microscopes and mounting. Workshops 3 and 4 were held by Loïc Le Dréau, who introduced the D2 Phaser diffractometer and demonstrated its use. In workshop 5, Mohsen Graia held a tutorial about structure resolution and refinement from single-crystal XRD data. First, two simple structures were processed. Subsequently, five other compounds, characterized by occupational disorder, were presented.

Second stop: Nabeul



Participants at the Bruker OpenLab in Nabeul.

The second stop was held at the Institut Préparatoire aux Etudes d'Ingénieur de Nabeul (IPEIN) of the University of Carthage in Nabeul. In addition to support from the IUCr, UNESCO and Bruker France, the IPEIN contributed partially to financial, human and material resources for running the OpenLab. Nineteen participants from Algeria, Tunisia and Côte d'Ivoire were present (47% female). The opening ceremony was hosted by Abdessattar Barhoumi, head of the IPEIN, Loïc Le Dréau from Bruker France and Habib Boughzala from the Laboratory of Materials and Crystallochemistry (LMC), first Vice-President of the ATC and organizer of this OpenLab. Three sessions on single-crystal diffraction were tutored by Loïc Le Dréau, with the support of Tarek Rhaïem from the LMC. Habib Boughzala gave six lectures on powder diffraction, symmetry and the CIF tools, helped by Khalil Bouzazi from the LMC. At the end of the tutorial sessions, participants could take advantage of the Bruker D2 diffractometer to collect XRD data from their own samples. The last day of the OpenLab was dedicated to analysis and treatment of these data.

The OpenLab Nabeul was very much appreciated by the participants, who sent very positive feedback. 'It was one of my best professional experiences and I have received a large amount of knowledge in X-ray diffraction,' said Sofien Saidani from Bizerte (Tunisia); Eric Ziki from Côte d'Ivoire expressed his gratitude for a very fruitful and enjoyable experience: 'it is like having a second family, the atmosphere was pleasant, everyone was so kind and the lecturers made difficult topics accessible to anyone thanks to their skills and humour'.

Mohsen Graia and Habib Boughzala, Local Organizers in Monastir and Nabeul, respectively

IYCR 2014

Building a legacy for IYCr2014 in Africa



The Cambridge Crystallographic Data Centre (CCDC) has a mission to make the wealth of structural chemistry data contained in the Cambridge Structural Database (CSD), the world's repository for organic and organometallic small molecular crystal structures, accessible to all researchers, including those operating in more challenging environments. In 2007, at the instigation of Professor Luc Van Meervelt of K. U. Leuven, Belgium, the CSD was provided for use in the structural chemistry research group of Professor Zéphirin G. Yav at the University of Kinshasa, Democratic Republic of Congo, as part of a year-long British Council-financed Science Training Laboratory project.



Group photo from a CSD workshop at UNIKIN.

The relationship between the CCDC and the University of Kinshasa (UNIKIN) has developed further from 2012 onwards, with CCDC staff spending time with our colleagues in Kinshasa in June 2012, 2013 and 2014. The CCDC provided training through seminars and practical workshops to a number of UNIKIN academic and research staff as well as MSc/PhD students covering the following topics:

- using the CSD for research and teaching purposes in crystallography and structural chemistry;
- probing molecular geometries and interaction energies using the CSD's Mercury interface to the semi-empirical quantum chemistry program *MOPAC*;
- applying molecular modelling and structural chemistry in drug design;
- identifying an active molecule through protein binding site analysis, and docking, with the CCDC's *SuperStar* and *GOLD* programs.

These annual visits led to the establishment of joint research goals and ultimately to the launch of the CCDC Student Scholarship Programme in Kinshasa, beginning in the academic year 2013-2014. This programme provides a framework of financial support and academic co-supervision to two postgraduate structural chemistry students based in Kinshasa: an MSc student during his final-year research project,

and a PhD student for the duration of his three-year degree (to include some periods of research undertaken at the CCDC in Cambridge, UK). These two research projects are concerned with using the CSD and quantum mechanical calculations to investigate sigma-hole and hydrogen-bond intermolecular interaction geometries and energies in selenium-containing compounds.

This on-going collaboration shows that structural chemistry research can be successful in places where the lack of equipment, of reliable internet access and of access to resources for teaching and research make for a challenging environment. The CCDC is also helping to build crystallography expertise more widely in the Democratic Republic of Congo by training more scientists at UNIKIN, and is attempting to source a second-hand single-crystal diffractometer to be donated to the University of Kinshasa to enable the research groups to run their own diffraction experiments rather than having to send their samples to other countries to be analysed.

The CCDC is contributing to the development of crystallography and structural chemistry in other parts of Africa and thereby strengthening the legacy of the International Year of Crystallography 2014 by working with Lewis Whitehead of the Novartis Institutes for Biomedical Research in Massachusetts, with further input from lecturers at the University of Nairobi and Kenyatta University, to put together a one-week series of lectures and workshops which will provide an introduction to computational chemistry and *in silico* visualisation for Sub-Saharan African scientists. Additional funding has already been secured from the IUPAC, the ACS and the IUCr, and this training event is now scheduled to be held in Nairobi, Kenya, in early September 2015. The overall aim of this OpenLab event is to train the teachers to use software suites and build structural chemistry knowledge so they can then train others, and knowledge transfer becomes self-perpetuating.

Juliette Pradon, Research and Application Scientist at the CCDC, Cambridge, UK

IYCR 2014

USNC/Cr Young Observers Program Participant



Anastasiya Vinokur from the U. of Wisconsin wrote extensively about her experiences as a Young Observer at the IUCr meeting in Montreal:

Young Observers opened a window for me to a wider community. I sat one afternoon at the USNCCr booth and listened to an impromptu history of crystallography from people who witnessed it unfolding. I attended talks by crystallographers about whom I had only read in textbooks. I watched the Union delegates waltz through the challenges of politics and science. This is a vibrant ever-changing community and I felt excited to become part of it. I am just at the beginning of my scientific career, but I see the path that I want to take: there is a place for me among the world's crystallographers. Attending the IUCr 2014 this summer widened my horizons, taught me new concepts, introduced me to a new people and made me, I hope, a better scientist. I look forward to attending the ACA meeting in Philadelphia next summer so as to learn more and to grow more.

(ACA RefleXions, Winter, 2014)

MEETING REPORT

BCA-BSG Winter Meeting Research Infrastructures in Structural Biology

BCA-BSG Winter Meeting Research Infrastructures in Structural Biology

Grenoble, France, December 2014



The European Photon and Neutron (EPN) facility in Grenoble hosted the 2014 BCA Biological Structures Group winter meeting, December 15-17. The first session, Research Infrastructures, chaired by V. Fulop (Warwick), began with a presentation by H. Reichert, the ESRF Director of Research for Physical Sciences. There are 21 member countries and 8 associate members. Approximately 30% of the proposals are biological. An upgrade to improve the facilities for structural biology and soft matter, analysis of extreme conditions, time-resolved studies, nanotechnology and X-ray imaging is underway. Phase 2 will involve building a new storage ring to provide a two-orders of magnitude increase in intensity. Studies including low-dose *in vivo* tomography for high-resolution imaging of cells involved in the neurobiology of ageing and high-resolution neutron diffraction studies of pyrophosphatase, fatty-acid binding protein and HIV protease were described.



Participants at the BCA Biological Structures Group winter meeting December 15-17, 2014.

The next session began with a presentation on recent developments in single-particle electron cryo-microscopy by C. B. Schaffitzel (EMBL). P. Williams (Astex Pharmaceutical, Cambridge, UK) gave an intriguing account of how protein crystallography has been utilized for high-throughput fragment screening in parallel with biophysical, spectroscopic and other techniques. With the advent of XFEL and developments in in situ data collection and compound handling, the future looks particularly bright for crystallography as a drug-screening technique. Studies of bacterial DNA ligase, a good target for new antibiotics due to a difference in its cofactor requirement from the human host enzyme, were described. D. Scott, (Nottingham) described the use of neutrons to study intrinsically disordered proteins and their interactions with DNA. G. Leonard (ESRF) explained how fully automated data collection from 'sludges' of micro-crystals mounted in loops and processed by techniques that are currently being developed for XFEL serial crystallography are likely to make major breakthroughs in structural biology. Fast-readout detectors may allow us to go back to room-temperature data collection as a routine technique. T. Forsyth (ILL) described the LADI-III instrument using a quasi-Laue beam and perpetuated samples to allow work on crystals as small as 0.1 mm^3 . Time-of-flight spectroscopy, back-scattering and spin-echo studies have all allowed the dynamics of proteins to be studied and complement X-ray, NMR and EM techniques.

In a session on Structural Biology on the EPN campus, S. Cusack (EMBL, Grenoble) explained that influenza is a segmented negative-strand orthomyxovirus, which uses ribonucleoproteins to package its eight mini-chromosomes. The swapping of these chromosomes between different strains of the virus causes new and serious epidemics or even global pandemics to occur. The successful crystallization of the enzyme from a strain of virus affecting bats allowed the structure to be solved. The structure shows how 16-18 bp of RNA interacts with the cap-binding domains and how the 3' end of the RNA sits in the active site.

In a session on Emerging Techniques in Structural Biology, A. Florent (IBS) described a study of urate oxidase that gave fabulous insights into how the substrate binds as a peroxo-intermediate, although increasing the X-ray dose was shown to cause the bond to the oxygen to break. L. Duke (Diamond) described soft X-ray microscopy, which is being developed as a tool for ultra-structural studies. Individual cells can be imaged in fabulous detail by freezing in liquid ethane without any of the staining, drying and sectioning procedures which are common-place in the EM community. Gold particles are used as fiducials for the image analysis. A study of autophagy demonstrated the outstanding potential of this technique.

The meeting was closed by the BSG chairman, V. Fulop, who presented the poster prize to A. Yee (ILL/Keele) and thanked the local organizers (G. Leonard, T. Forsyth and E. Mitchell).

taken from an article by Jon Cooper, BCA Crystallography News, 132, March 2015

MEETING REPORT

15th BCA/CCG Intensive Teaching School in X-ray Structure Analysis

Durham, UK, March 2015



The 15th BCA/CCG Intensive Teaching School in X-ray Structure Analysis was held in Durham from March 21-29, 2015. The course consists of a mixture of lectures interspersed with tutorials in which the students get a chance to apply concepts they have just learned to sets of problems. The lectures and tutorials were held at Trevelyan College. Each tutor group consisted of eight students and had a tutor who stayed with them throughout the week to act as their first port of call for help throughout the course.



Participants at the 15th BCA/CCG Intensive Teaching School in X-ray Structure Analysis held in Durham from March 21-29, 2015.

This course was attended by 80 students studying in the UK, Canada, Finland, Denmark, Slovenia, India, Poland, USA, Germany, Ireland, United Arab Emirates, Brazil, Australia, Japan and Italy. The participants had a range of crystallographic experience. The majority of the participants are PhD students, with a small number of PDRAs and academic/industrial researchers.

New tutors K. Fucke, L. Hatcher, M. Senn and H. Shepherd had previously attended the course as students. The main lecture topics tackled during the seven-day course were in the following order: Introduction (Prof. W. Clegg), Maths (D. Sivia), Symmetry (W. Clegg), Data Collection from Instrumentation through to Data Collection Strategies (R. Copley), Fourier/Patterson Methods (W. Clegg and S. Moggach), Charge Flipping and Direct methods (L. Palatinus), Uncertainty and Inference (D. Sivia), Refinement (R. Cooper), Derivation of Results and Twinning (S. Parsons), Validation (R. Copley) and a Disorder Workshop (A. Thompson). In addition to the main lectures and tutorials there were two optional lectures, one on Incommensurate Structures (L. Palatinus) and one on Synchrotrons and Neutrons (M. Warren and K. Fucke), both of which were essentially fully attended and appreciated by the students.

Evening activities designed to enable the students to mix with each other included an introductory mathematics lecture (D. Sivia), a bar quiz (R. Cooper), a talk on databases (P. Wood) and student group presentations (M. Probert and K. Fucke). For their group presentations, each tutor group was assigned a different crystallographic topic, which they had to present in as entertaining a way as possible while still being educational. An elite panel of the lecturers judged the presentations and, as with previous years, the standard of the presentations was very high and amusing. On the final evening we had the course dinner, which was a chance to thank all of the contributors to the school, the local staff, organizers, lecturers, tutors and students, all of whom led to another very successful school.

For the first time, on Sunday, March 29, we held an optional hands-on *Olex2* workshop that was run by H. Puschmann and O. Dolomanov (*OlexSys*). This workshop was attended by ~40 students, some of whom had previously used *Olex2* while for others it was new software. For all of the participants it was a chance to apply concepts they had learnt to structure solution and refinement in *Olex2*. Previous participants of the school had requested this kind of hands-on session.

The school was heavily oversubscribed due to the growing use of crystallography by a wider range of users as a result of the development of easy-to-use software for data collection, structure solution and refinement, much of which does not require a large amount of crystallographic expertise to obtain a result. Consequently, schools such as this are essential to provide users of crystallography with a solid understanding of the underlying theory so that they can identify and treat any problems they may run into, as well as checking the validity of their results prior to publication.

We would particularly like to thank all of the organizations that provided financial support for the course and without whom we would not have been able to run the school so successfully. These are Diamond, IUCr, ECA, CCG, ICG, Oxford Cryosystems, Agilent Technologies, CCDC, Rigaku, ISIS, Bruker and Incoatec.

The funds kindly provided by the IUCr (7000 USD, ~£4680) were used to help the following students with contributions towards their subsistence (see IUCr Financial Report for full details): A. Nayak (Indian Inst. of Technology, Bhubaneswar, India), K. Czerwinska (Warsaw U. of Technology, Poland), V. Carta (U. of British Columbia, Canada), M. Ursic (U. of Ljubljana, Slovenia), R. R. Ternavisk (U. Estadual de Goias, Brazil) and P. Vinicius de Sousa L. Fook (U. of Trento, Italy).

Judith A. K. Howard and Hazel A. Sparkes (Local Organizers)

MEETING REPORT

International School of Biological Crystallization (ISBC2015)

Granada, Spain, May 24-29, 2015

<http://www.isbcgranada.org>



Jose Antonio Gavira welcoming the participants of the School.



A group of students attending one of the 19 practical demonstrations.



Participants at the entrance of the Alhambra.

Since 2006, during the last week of May Granada has been home to a series of Crystallization Schools: the International School of Crystallization (ISC) and the International School of Biological Crystallization (ISBC), which are organized by the Laboratory of Crystallographic Studies (LEC) of the Spanish National Research Council (CSIC) in alternating years. These schools are aimed at postgraduate and postdoctoral students, as well as research scientists from industry and academia: all those who deal routinely with

crystallization issues but need fundamental knowledge of crystallization phenomena and the behaviour of crystallizing solutions.

This year it was the turn of the International School of Biological Crystallization (ISBC2015), which took place May 24-27, under the auspices of the IUCr through the Commission on Crystal Growth and Characterization of Materials and the Commission of Macromolecular Crystallography. Of the total 82 registered participants, 52 were students, 20 academics, six industry representatives and four exhibitors from as many as 23 different countries. They came to Granada to learn from 27 top quality international speakers, to hear case-study presentations, to watch practical hands-on demonstrations, and to discuss their own research results in lively sessions where 44 posters were presented. All of the 32 grant applications were accepted for funding.

ISBC2015 covered five days of lectures and demonstrations related to the crystallization of biological macromolecules and also to biomineralization. Lectures on the first day focused on the fundamentals of macromolecular crystallization, including solubility, nucleation theories, and crystal growth kinetics and mechanisms, as well as the basis of screening and high-throughput technology. On the second day, lectures and discussions revolved around current and new technologies, from seeding to *in vivo* crystallization and preparation of micro- and nanocrystals for free-electron lasers and synchrotron radiation or large crystals for neutron diffraction. The morning of the third day we learned about the use of fluorescent labelling and microfluidic chips, as well as the handling of protein crystals, SAXS, gel growth and electron microscopy. In the afternoon, after an introduction to the subject of biomineralization, we explored the pathway to non-classical nucleation and the importance of protein/peptide interactions in biomineralization. Thursday was entirely dedicated to our Demonstrations Fair, where 19 specialists offered practical sessions periodically at scheduled times. As in previous years, our Demonstrations Fair proved to be an excellent teaching tool as it provided students with plenty of opportunities to interact on a personal basis with instructors and to watch closely how to perform crystallization experiments.

On Friday, we returned to biomineralization with different hot topics in the field. As a novelty to be maintained in the future, the closing talk of the programme was devoted to acknowledging the contribution of one of the pioneers of the field. This year we invited Richard Giege, who performed a fascinating personal overview of the history of biological crystallization. The last scientific activity of the school was the oral presentations of the six winners of poster prizes, which were sponsored by the IUCr, Elsevier and Bernhard Rupp.

In addition to the scientific programme, there was an enticing social programme starting with a welcome cocktail on Sunday, followed by a night tour around the outstanding beauty of the Moorish palaces of The Alhambra on Wednesday. Each evening, the participants enjoyed the lively atmosphere of the city, its tapas bars and historical buildings, except for Thursday when we organized our classical flamenco and dinner party in Carmen de la Victoria, a traditional property of the University of Granada located in the historic quarters of Granada from where we could admire magnificent views of the Alhambra hill.

José Antonio Gavira and Juan Manuel García-Ruiz

MEETING REPORT

International School of Crystallography 48th Course

Engineering Crystallography: from Molecule to Crystal to Functional Form

Erice, Italy, June, 2015, <http://crystalerice.org/Pastactivity/2015/2015.htm>



Prize winners (left to right): Kevin Roberts (Director), Isabel Olson, Stuart Kennedy, Ran Drori, Erin Davis, Fred Boyle, Elena Meirzadeh, Paola Spadon, Marlena Gryl, Annalisa Guerri (Organizer), Sameer Modi, Anneke Klapwijk and Filip Topić.



Participants at the 48th Crystallographic School in Erice, June 2015.

The 90 participants from 33 nations who attended the 48th Crystallographic School in Erice were selected from 170 applications. They came from universities (PhD students, postdoctoral and young researchers), and chemical and pharmaceutical companies. The course was supported by the IUCr, ECA and CCDC, as well as by private companies Dectris, Abbvie, Merck and PANalytical.

A typical day included a morning session with four lectures and an afternoon session with two lectures, tutorials, workshops or round-table discussions. The first day provided a complete overview plan for the course (Roberts). The opening talk (Docherty) presented the translation of molecule to crystal to product in the pharmaceutical sector. This was followed by lectures on supramolecular assembly and solid-form architecture (Aakeroy), and the link between the crystal structure and mechanical properties of organic materials (Malla-Reddy). In the afternoon the crystallization route map was introduced (Roberts) and the importance of supersaturation as the driving force for nucleation and growth was comprehensively covered (T. Hoorst). The influence of interfaces during the crystal growth process was elegantly captured (Ward).

In days 2 and 3 the concepts of morphology and chirality were introduced. The link between growth and habit was covered in detail (Roberts). The definition of molecular chirality and the importance of the resolution of chiral molecules were given in a series of lectures (Kuroda, Tamura, Coquerel). The theme of

stability was introduced, focusing on chemical reactivity and crystal defects (Jones) and the physical stability of polymorphs and solvates (Griesser).

Molecular and solid-state modelling techniques were then introduced. Molecular to crystal modelling techniques were described in detail (Hammond), and solid-state computational modelling including crystal structure prediction was reviewed (C. Cabeza). The information available in the Cambridge Structural Database (CSD) and the impact of solid-state informatics on solid-state structure design (Feeder) were reviewed. Additional talks concerned phase diagrams (Coquerel), chiral liquid crystals (Tamura) and solid-state architecture of energetic materials (Aakeroy). Leading exponents in the field introduced crystallization process modelling concepts (Mazzotti) and crystallization process control (Nagy). Different crystallization processes including evaporation and cooling (Myerson), as well as comparing and contrasting batch and continuous processing (Price), were presented.

On days 5 and 6, Discrete and Finite Element Modelling (DEM/FEM) was introduced to show the connection between the particles formed in primary manufacturing and their possible impact on secondary processing (flow, mixing) (Wu). Other topics included solution and solid-state characterization (Kwokai), as well as co-crystal formation through grinding (Jones), solid-state and surface characterization (Feeder, Heng), and crystallization screening and process scale-up (Griesser and Nagy). Software tutorials (*Mercury* by the CCDC and *Visual Habit* from Leeds U.), and the Crystal 16 crystallization workflow (Avantium), an always popular feature of the Erice Schools, rounded off these sessions.

The final day consisted of an overview of analytical technology applied to crystallization and powders (Kwokai), and to crystal optical characterization (Kuroda), and the application of ultrasound to induce nucleation (Price). The formal teaching was concluded with the deconstruction of a product back to component parts and the impact of science of scale tools on product design (Docherty). The final afternoon was dedicated to panel discussions on all aspects of the course with seven of the speakers. Throughout the week students submitted questions so that the panel could address broad themes.

Over the course of the School about 70 posters were presented in two sessions. Six 15-minute oral presentations by young participants (selected from the poster abstracts) were included in the programme: Thomas Gee (U. of Southampton, UK), F. George (U. Catholique de Louvaine, Belgium), G. Lloyd (Heriot-Watt U., UK), M. Gryl (Jagiellonian U., Poland), A. Tilborg (U. of Namur, Belgium) and M. Viertelhaus (BASF SE, Germany).

On the afternoon of the last day several awards were presented. Parallel awards were given for each of the two poster sessions. First place awards went to S. Kennedy (Durham U., UK) and R. Drori (New York U., US); second place to F. Topić (U. of Jyväskylä, Finland) and I. Olson (New York U., US); third place awards to S. Modi (NIPER, India) and A. Klapwijk (U. of Bath, UK). The Lodovico Prize, acknowledging the most active student inside and outside the lecture hall, was given to Elena Meirzadeh (Weizman Inst. of Science, Israel), with special mention going to Marlena Gryl (Jagiellonian U., Poland).

Participants completed a survey on the quality of the Course. Their responses indicate that a similar meeting should be held at least in 3-4 years' time, and that the course was successful in most of its objectives (score 85/100).

Annalisa Guerri

See [here](#) for information on the 49th Course, 'High-Pressure Crystallography: *status artis* and emerging opportunities'.

MEETING REPORT

MultiPoles meet (again) in Warsaw

Warsaw, Poland, May 2015, <http://multipole-meetings.org/>



The MultiPoles gathered in May 2015 at the monument to Nicolaus Copernicus in Warsaw. Crystallography has a prominent place in the academic landscape of Poland, and many Poles (MultiPoles) are quite active in the field throughout the world. They work at prestigious universities and research institutes and at advanced synchrotron centers, and contribute to methods development and large-scale initiatives. The reason for this may be that in Poland crystallography is still taught to undergraduate students, and exact sciences used to be (the Past Tense intentional) strong at the secondary-school level. Another idiosyncrasy is that crystallographers with Polish roots stick very much together and somehow have been able to overcome one of our national 'virtues', summarized as 'where there are two Poles, there are at least three opinions'.

Polish crystallographers from around the world, and a contingent of bioinformaticians, met together, for the second time, in Warsaw on May 10-13, 2015 (multipole-meetings.org), in the beautiful Staszic Palace, with Copernicus' statue in front of it. A committee chaired by Janusz Lipkowski as a coda for the International Year of Crystallography IYCr2014 organized the conference, titled 'Multi-Pole Approach to Structural Science'. The Program Committee headed by Alex Wlodawer invited ~50 speakers. The acceptance ratio of nearly 100% generated a very exciting program. The meeting was held under the patronage of the Minister of Science and Higher Education and was supported by the Polish Academy of Sciences and its President, Jerzy Duszyski.

Alex Wlodawer gave a historical review of crystallography, and Zbyszek Dauter presented the MultiPoles in a subjective looking glass. The Keynote Lecture was delivered by Ada Yonath. She described her family's journey from Zduńska Wola (a small town in Poland) to Israel and her own scientific journey under the flag of the ribosome. The remaining talks were divided into sessions on Proteins and Nucleic Acids, Structural Enzymology, Signaling and Immunology, Large and Challenging Structures, Macromolecular Modeling, and Methods and Validation. Although the program was dominated by structural biology, it also included talks on small-molecule and supramolecular structures, nanocrystallography, and crystallography beyond the independent-atom model. In addition, over 100 posters were presented by the younger participants. Two poster prizes, sponsored by the FEBS Journal and HKL Research, went to Maria Górna (CeMM Vienna, Austria) and Nadia Opara (Paul Scherrer Institute,

Switzerland), respectively. The total number of over 200 registered participants vastly exceeded the original plans.

An important session organized in the middle of the conference by Andrzej Legocki was focused on Poland's accession to EMBL. The session started with a lecture by Iain Mattaj, Director General of EMBL, and was continued as a panel discussion, with the participation of Maciej Żylicz from the Foundation for Polish Science (FNP), and Włodzisław Duch, representing the Ministry of Science and Higher Education. At present, Poland has the status of Prospect Member State, and is committed to becoming a Full Member within three years.

The conference banquet was held in a beautiful chateau in Jabonna, 20 km north of Warsaw. The participants left Warsaw with lots of new ideas, new and rekindled contacts and friendships, nice photographic albums, a biography of Maria Skłodowska-Curie, another predecessor of the MultiPoles, and with a firm pledge to meet in a few years again, most likely in Poznań.

Mariusz Jaskolski

MISCELLANY

IUCr Newsletter survey



There is still time to take part in our *IUCr Newsletter* survey with a chance to win an Amazon voucher.

Results to date from the survey are beginning to show some interesting trends.

Current format and content

The preferred format is overwhelmingly the digital page-turn edition with more than 60% preferring this particular format over the print (30%) and HTML (25%) versions. Of those surveyed, 75% access the electronic version of the *Newsletter* on desktop computers, 30% on smartphones and 29% on tablets.

Of the sections read, readers enjoyed IYCr2014 content the most (54%), followed by the meetings calendar (44%), future meetings (39%), IUCr Journals (38%), IUCr News (38%), Letter from the President (36%), cover story (35%), awards, news and notices (21%) and crystallographic meeting reports (21%).

Community

The *Newsletter* plays a very important role in making readers feel connected to both the IUCr (88% of readers surveyed) and the crystallographic community at large (91%).

Suggestions for improvement

There does not seem to be an overwhelming need from our readers to increase the frequency of the newsletter from four to six or even twelve issues; however, readers did indicate a wish to see more commissioned opinion pieces from leading names in the field (78%).

Other content suggestions

Moving forward, readers surveyed would like to see generally more research news stories from approximately 400 words upwards. They would also like to see more book reviews, profiles of scientists and related news from other sources.

Other content ideas shared by respondents included more multimedia, such as videos, photos, and podcasts in the online version, as well as commissioned articles covering important milestones in crystallography, a wish to see more high-quality articles and articles from leading investigators, more learning content, a software corner, more opinion pieces, a section covering news from each Regional Associate, more interdisciplinary content, more outreach content, and generally more visibility through social network channels.

Title

We asked respondents to suggest a new name for the *Newsletter*. The majority felt the current title was sufficient; however, we did receive the following suggestions for new titles: *IUCr World News*, *Crystal Stories*, *CRYSTALNEWS*, *CrystalWorld*, *IUCrNews*, *Crystallography Matters!*, *Crystals Today*, *Crystallography Today in the World*, *Crystallography Worldwide*, *Crystallography World* and *IUCrN*.

Do you broadly agree with these interim findings? If you would like to have your say, then please follow this link and take part in our survey today!

www.surveymonkey.com/r/iucrnewsletter2015

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

AWARDS AND PRIZES

8th Max Perutz Prize Awarded to John Helliwell



The 8th Max Perutz Prize of the European Crystallographic Association has been awarded to John R. Helliwell, Emeritus Professor of Chemistry, U. of Manchester, UK, for his long, generous and fruitful dedication to developing all aspects of the use of synchrotron radiation for crystallography.

John Helliwell received his undergraduate degree in physics in York, taught by Michael Woolfson and Peter Main. He then embarked on a PhD in protein crystallography at Oxford U., supervised by Margaret Adams. He was mentored by Charlie Bugg and Guy Dodson in the laboratories of Dorothy Hodgkin and David Phillips. He has been Professor of Structural Chemistry at the U. of Manchester from 1989 till 2012 and he is now Emeritus Professor of Chemistry.

John has given significant support to the global development of synchrotron and neutron facilities through his research publications, his books and his extensive advisory committee work. He led the development of the world's first dedicated protein crystallography beamlines at SRS Daresbury and in the 1980s he developed the instrumentation and methods that allowed the collection of the first broad-band Laue diffraction patterns for protein and virus crystals using synchrotron radiation. Using this method he carried out a pioneering time-resolved study of enzyme action on hydroxymethylbilane synthase. Later John developed an innovative combination of biochemistry, spectroscopy, microscopy, protein crystallography and small-angle scattering to study the crustacyanins, chromophoric proteins that are responsible for the coloration of lobster shells. John also pioneered some of the first developments of synchrotron radiation for phasing based on optimised anomalous scattering. He began the investigations of the effects of radiation damage and its potential use for phasing and he has recently demonstrated the use of MAD phasing for *ab initio* structure determination from powder diffraction data.

John Helliwell has also made major contributions serving the global crystallographic community through numerous Advisory Committee responsibilities to ensure a speedy and effective growth at as many synchrotrons and neutron facilities as possible; he was also the first Chair of the IUCr's Commission on Synchrotron Radiation. He was president of the European Crystallographic Association (2006-2009) and served as Editor-in-Chief of the IUCr journals (1996-2005).

He is the author of a classic book on protein crystallography, *Macromolecular Crystallography with Synchrotron Radiation* (Cambridge Univ. Press, 1992) and is a founding editor of the *Journal of Synchrotron Radiation*.

In addition to his pioneering achievements and to the key role he played in the development of experimental beamlines for structural biology worldwide, John has trained a generation of

crystallographers through the many students that he supervised, including some of the finest of the world's beamline scientists, and is constantly engaged in outreach of the science to crystallographic communities worldwide.

John Helliwell received the award at the 29th European Crystallographic Meeting in Rovinj, Croatia, August 23-28, 2015.

Alessia Bacchi, Vice President of ECA, Chair of the 8th Perutz Prize Committee

MISCELLANY

Did you know?

More than 11 million printed items and 70,000 e-journals in the Oxford Bodleian Library include one of the first books to appear in print: Pliny the Elder's *Historia Naturale* (1476), Euclid's *Stoicheia*, the oldest manuscript of a classical Greek author to bear a date (888), and an exquisite map of the insulin molecule attributed to Dorothy Hodgkin and dated 1968.

A paper with 5,154 authors was published in *Physical Review Letters* in May 2015. (from *Nature*, **521**, May 21, 2015)

At an auction in the spring of 2015 an anonymous bidder paid \$395,000 for Heinrich O. Wieland's 1927 Nobel Prize medal. Wieland was credited along with Adolf O. R. Windaus with determining the chemical structure of cholesterol. The structure was wrong. J. D. Bernal showed that the Wieland and Windaus structure could not be correct on the basis of the cell dimensions of cholesterol crystals. Hodgkin went on to determine the correct molecular structure.

Alisher Usmanov, a Russian entrepreneur, paid \$4.8 million for James Watson's 1962 Nobel Prize in Physiology or Medicine medal, and returned the medal to Watson. Watson is said to have given the money to research.

Australia's government has cut AUS\$263 million (US\$211 million) from university grants over the next three years to keep key national Research facilities running.

In a recent film, 'Just Eat It: a Food Waste Story', Grant Baldwin and Jen Rustemeyer revealed that between 20 and 70% of bananas, celery and nectarines are thrown away immediately after harvest and that a third of the food produced globally is wasted, including 15 to 25% of the food we purchase in our regular trips to the supermarket. (from *Science*, **348**, p. 629, 2015)

The number of people in the United States who spend more than US\$100,000 a year on medicines tripled to 139,000 in 2014 compared with 2013. (from *Nature*, **521**, May 21, 2015)

NOTICE

High-pressure crystallography: status artis and emerging opportunities

Erice, Italy, 27 May to 5 June, 2016

www.crystalerice.org

The 48th Course of the International School of Crystallography will take place in Erice from 27 May to 5 June, 2016. The course will give a general overview of the ever-expanding use of high pressure: from the very modest pressure required to induce the denaturation of proteins and modify intermolecular interactions, through the higher pressures required to synthesise new materials for technological application, to the ultra-high pressures required to radically alter the chemical and physical properties of simple elements and materials or recreate the conditions found in Earth's and other planets' interiors. All these aspects make it a versatile and central tool in condensed matter science. The objective of this course is to educate young researchers in the interdisciplinary aspects of high-pressure crystallography research and to inspire the next generation of high-pressure scientists to leave their own stamp on the field. Fundamental topics covered in the course include experimental techniques for pressure generation, X-ray and neutron diffraction on single-crystal and powder materials, comparative structural studies, and combined high-temperature and low-temperature experiments. Lectures will be complemented by demonstration and workshop sessions. The course will provide a platform for young and senior scientists to interact, and to identify and discuss new challenges in this rapidly evolving and vibrant research area. Please visit the still in-progress and renewed website (www.crystalerice.org).

Directors: Francesca F. Fabbiani, Malcolm Guthrie and John Parise

NOTICE

2016 Annual Meeting



Denver, Colorado, 22-26 July, 2016

www.americalassn.org

The 66th Annual Meeting of the American Crystallographic Association (ACA) will be held in Denver, Colorado, 22-26 July, 2016. The transactions symposium will highlight Structural Dynamics across the disciplines represented by the ACA. The rest of the meeting will continue to reflect the wide reach of crystallographic research, with sessions on sources, methods and results. These include opportunities from new and improved instrumentation, single-/multiple-crystal, powder and solution methods, and hot structural results. There will be sessions highlighting those results requiring complementary techniques, including cryo-electromicroscopy. Invited speakers include 2016's honorees, Jason Benedict (SUNY Buffalo), Axel Brunger (Stanford U.), Elspeth Garman (U. of Oxford) and Benno Schoenborn (Los Alamos National Lab.).

The meeting will include a strong educational component for early career scientists, with specific talks designed to introduce research areas in addition to presenting results. Related evening sessions include a mixer, career fair, career development, and diversity in the laboratory. The conference will end with a closing banquet and the award of poster prizes for the best presentations. We hope to see you in 2016.

Chairs: Amy Sarjeant and Edward Snell