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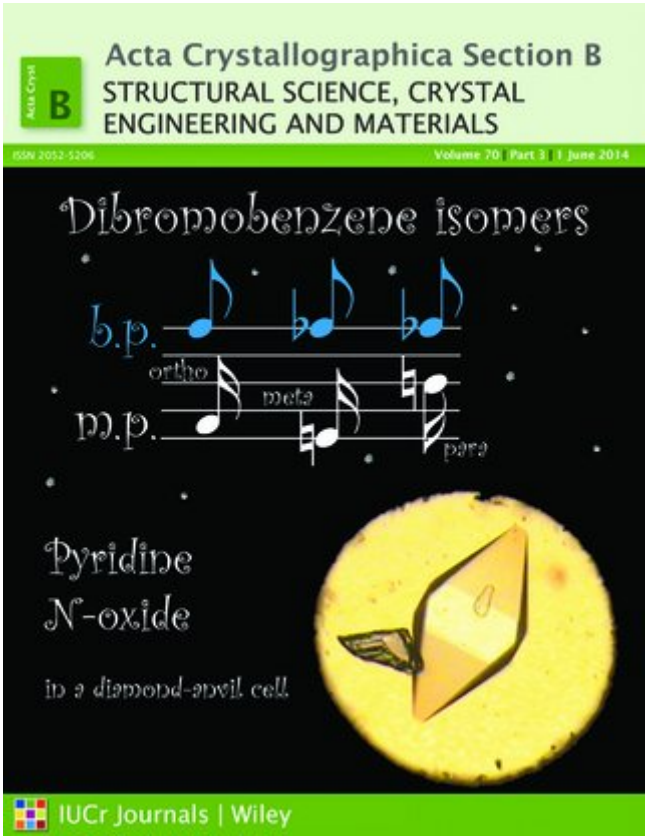
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IUCR JOURNALS NEWS

Non-ambient crystallography – is extreme becoming common?

Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials
Volume 70, Part 3 (June 2014)
(http://journals.iucr.org/b/issues/2014/03/00/issconts.html)

Special issue on Non-ambient Crystallography



One century of modern crystallography, celebrated in this year, 2014, has brought about many developments, some of which have involved the use of 'non-ambient conditions', which in their most severe form can be described as 'extreme-conditions' crystallography. In addition to recognizing this increasingly vibrant research field, this special edition also represents a refocusing of *Acta Crystallographica Section B* to become the journal of choice when it comes to publishing high-quality results from non-ambient crystallographic studies.

The first low- and high-temperature structural determinations were performed soon after the inception of X-ray diffraction structural analysis. One of the first low-temperature determinations was the structure of benzene in 1932, about the same time the first reports on high-pressure powder diffraction experiments

were published. These high-pressure experiments yielded results of low precision due to the thick walls of the pressure vessels.

It wasn't until 1959, when scientists invented the main device for high-pressure crystallography – the diamond-anvil cell (DAC) – that work at elevated pressure became more routine. This simple but ingenious apparatus still continues today to break all records of pressure, exceeding that at the centre of the Earth (364 GPa).

High-pressure techniques are constantly being developed and presently laboratory X-ray diffraction studies can be complemented by spectroscopy, also on the same sample in the DAC, as well as by experiments in specialized large-facility stations at synchrotrons, and at neutron spallation and nuclear reactor sources. Internally and externally heated DACs are available, as well as laser heating, allowing temperatures well over 1000°C. Other types of high-pressure devices have also been developed for various specific purposes, including physical, chemical, biological and most of all materials studies.

Endeavours in non-ambient crystallography have not been limited to structural characterizations at temperatures and pressures other than ambient. There are also studies of materials exposed to different gaseous environments or where the sample is subjected to various electrical or magnetic fields. Capillary-based sample cells have been particularly popular with these kinds of studies and a number of designs for the investigation of gas–solid interactions have been presented in the literature.

Clearly, non-ambient crystallography is a far broader field than can be done justice in a single Special Issue. The contents of this issue merely represent a small sampling of what is possible. Indeed, the number of non-ambient structure determinations, phase transformation and other non-ambient studies reported in the literature steadily increases annually. It indicates that researchers reach out for non-ambient conditions not only in their search for new materials but also to improve their understanding of the properties of matter under normal conditions, but also under various conditions, even at extreme depths inside the Earth or other planets and conceivably even stars.

It is our hope that the publication of this Special Issue on Non-ambient Crystallography will not only stimulate new research in all areas of non-ambient crystallography, but also that it would encourage publication of these results within *Section B*. We thank all the authors who have contributed directly to this issue and we encourage all researchers active in the field of non-ambient crystallography to consider *Section B* for the publication of their next research paper.

Dave G. Billing and Andrzej Katrusiak, Guest Editors

IUCR JOURNALS NEWS

IUCr Journals welcomes additional Main Editors

Acta Cryst D	**Randy Read** (Cambridge, UK) joins Ted Baker, Zbigniew Dauter and Soichi Wakatsuki as a Main Editor of *Acta Cryst. D*: *Biological Crystallography*.	
Acta Cryst E	**Luc Van Meervelt** (Leuven, Belgium) joins Bill Harrison, Helen Stoeckli-Evans, Edward Tiekink and Matthias Weil as a Main Editor of *Acta Cryst. E*: *Structure Reports Online*.	
Acta Cryst F	**Bill Hunter** (Dundee, UK) joins Howard Einspahr and Manfred Weiss as a Main Editor of *Acta Cryst. F: Structural Biology Communications*.	
Appl Cryst JAC	**Andrew Allen** (Gaithersburg, Maryland, USA; left) and **Janos Hajdu** (Uppsala, Sweden; right) join Anke Kaysser-Pyzalla as Main Editors of *J. Appl. Cryst.*	

IUCR JOURNALS NEWS

Acta Crystallographica Section E transforms from Structure Reports Online to Crystallographic Communications

At the start of the millennium, the IUCr launched its first fully electronic journal, *Acta Crystallographica Section E*: *Structure Reports Online*, with its founding Main Editors William Clegg (Newcastle, UK) and David Watson (Cambridge, UK). The first issue appeared on January 1, 2001, reporting crystal structure results across a wide range of inorganic, organic and metal-organic materials with access to the complete diffraction data, the submitted CIF and the full checking output.



To keep up to date with current trends and demand in the community, from January 2015 *Acta Crystallographica E*: *Structure Reports Online* will change its subtitle to *Crystallographic Communications*. The journal remains fully open access.

Acta Crystallographica Section E: *Crystallographic Communications* will publish two article types: longer format *Research Communications* and short *Data Reports*, similar in format to the current articles in *Acta E* you are already familiar with. Both of these will report crystal structure results across a wide range of materials, with a clear obligation on authors to highlight the science behind the structures.

A key step in realising the vision for *Acta Crystallographica Section E*: *Crystallographic Communications* has been the development of the *Research Communication* article format, with new text sections designed to help authors bring out the science behind the structures and their determinations. These

include *Chemical context*, *Structural commentary*, *Supramolecular features*, *Database survey*, *Synthesis and crystallization* and *Refinement*. Authors and readers will be pleased to find figures included in the published *Research Communications* rather than being confined to the supporting information. For the first time in the journal, individual reports are not limited to single structure determinations. In fact, authors are encouraged to describe the structures of two or more related compounds in a *Research Communication*. These changes will make *Acta E*: *Crystallographic Communications* the natural home for structure determinations with interesting science to report.

We look forward to receiving submissions in the new formats from authors old and new from July 1, 2014. Exemplar papers in the new formats will be online soon so keep an eye on the journal web pages.

In time, we envisage *Research Communications* and *Data Reports* to be covered by the Science Citation Index and the Data Citation Index, respectively.

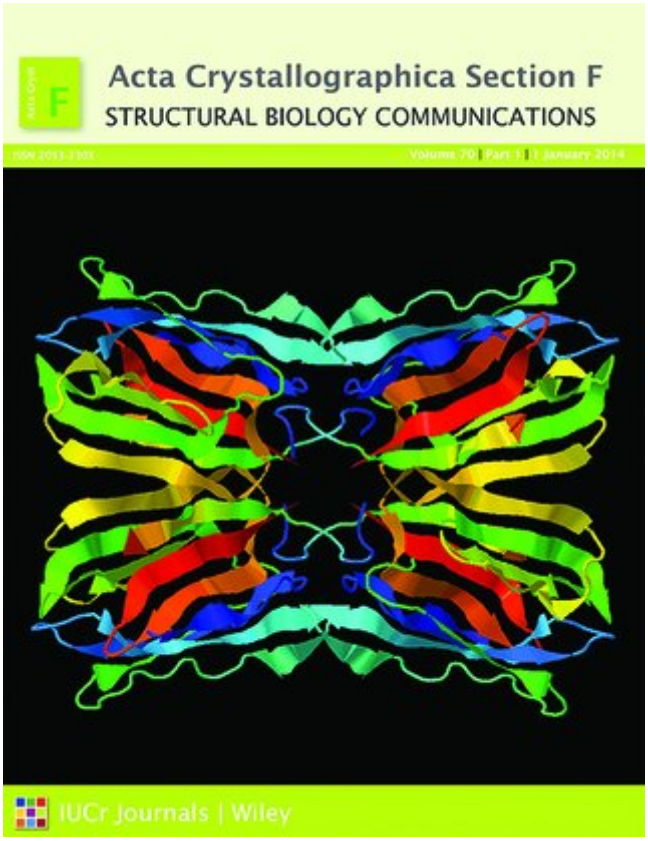
Read the full Editorial at http://journals.iucr.org/e/issues/2014/07/00/me0544/index.html.

Samar Hasnain, Editor-in-Chief, IUCr Journals

IUCR JOURNALS NEWS

publBio, an online tool for preparing biological data for publication

What better time than the International Year of Crystallography 2014 to review some of the useful tools available to help you submit your next paper to an IUCr journal?



The editors of *Acta Cryst. F* and staff at the IUCr Editorial Office in Chester have been working diligently at improving and updating *publBio* for authors. *publBio* (http://publbio.iucr.org) is designed to make the process of preparing and submitting your article to *Acta Cryst. F* as simple and as efficient as possible.

publBio consists of two parts: *publBio publisher* and *publBio annotator*. *publisher* is a tool for writing and submitting articles, whilst *annotator* is a tool for editing mmCIFs. The IUCr Word template now also has some of the functionality of *publBio* and, just like *publBio*, offers the option of utilizing data from an existing PDB deposition or an mmCIF file when creating the tables in an article.



Jonathan Agbenyega

The recently revised *publBio publisher* makes writing and submitting your *Acta Cryst. F* article much easier than before. It guides you through the article section by section, giving help and advice on what to include to produce a quality article that will interest readers.

publBio tables highlight all the items editors ask for, and data can be fetched automatically from your mmCIF or PDB file. Figures and supporting information can also be uploaded to complete your article. When you are ready to submit, one click takes you to *Acta Cryst. F* submission pages pre-filled for your article.

The editors of *Acta Cryst. F* welcome your feedback as you use these tools. If you would like to learn more or enquire about how you can sign up to a meeting or workshop where we'll demo the tools, please contact me at ja@iucr.org.

Jonathan Agbenyega, IUCr Business Development Manager

IYCR 2014

IYCr2014 South Asia Summit Meeting on Vistas in Structural Chemistry



Participants at the IUCr-UNESCO Summit Meeting in Karachi, Pakistan.

The IUCr-UNESCO Summit Meetings bring together scientists from countries in widely separated parts of the world, using a common crystallographic theme. There is a real necessity for scientists to think beyond political borders and other distinctions. Therefore the Summit Meetings, attended by scientists from academia and industry, and by science administrators, are planned between countries that have hitherto been divided on the basis of geography, ethnicity, religion and politics. These meetings focus on high-level science but also highlight the difficulties and problems of conducting competitive scientific research in different parts of the developing world.

April saw the first in the series of IUCr-UNESCO Summit Meetings, held in Karachi, Pakistan, April 28–30, 2014. The International Centre for Chemical and Biological Sciences (ICCBS) became the home to scientists and dignitaries from 19 countries (including India, China, Pakistan, Bangladesh, Iran, Jordan, Malaysia, Nepal, Saudi Arabia, Sri Lanka and Yemen). The President of the IUCr, Gautam R. Desiraju, the Editor-in-Chief of IUCr Journals, Samar S. Hasnain, and the Executive Secretary, Michael H. Dacombe, represented the IUCr, and Ahmed Fahmi represented UNESCO.

Entitled *Vistas in Structural Chemistry*, the South Asia Summit Meeting brought everyone together under the umbrella of chemical crystallography and pharmaceutical sciences. There were scientific sessions on Metal–Organic Framework Compounds, Crystal Engineering and Generic Pharmaceuticals, the Chemistry–Biology Interface and Drug Discovery and Design, Crystallography and Complementary Methods, and the Union and its Journals. The Plenary Lecture was given by Atta-ur-Rahman: *Promotion of Higher Education, Science and Technology and International Cooperation in Pakistan*. Panel discussions played a useful and informative part of the various sessions. The closing session focused on the way forward for regional cooperation, training centres, funding and how the IUCr and UNESCO could help with these goals.

An important outcome was The Summit Declaration, which was an Appeal to the IUCr to initiate actions to promote regional scientific collaboration; this was signed by over 50 of the participants.

The ICCBS formed an excellent venue for the event and the hosts made everyone very welcome – the organization was excellent. Dinner at Port Grand and the Gala Dinner were highlights of the evening activities. Particular thanks go to Professor Atta-ur-Rahman, Professor Iqbal Choudhary and Dr Sammer Yousuf.

The Summit meeting was followed by an OpenLab at the same location so that participants were able to meet renowned structural chemists and crystallographers.

Michael H. Dacombe, IUCr Executive Secretary

IYCR 2014

IUCr-UNESCO OpenLab in Karachi, Pakistan

Karachi, Pakistan, April/May 2014

The first of the IUCr-UNESCO OpenLabs was held at the International Centre for Chemical and Biological Sciences (ICCBS), U. of Karachi, Pakistan, from April 30 to May 8, 2014, in conjunction with the IYCr2014 South Asia Summit Meeting on Vistas in Structural Chemistry. The OpenLab Pakistan was organized in partnership with Bruker.

A keen interest was shown in the OpenLab from throughout the South Asian region and beyond, as was evident from the number of applications, which was close to 250. However, after careful consideration, 50 applicants were selected. The applicants were PhD students, early-career researchers and faculty members working in chemistry, physics and material sciences. Most of the participants were from Pakistan; however, there were also participants from Nepal, Sri Lanka, Saudi Arabia, Egypt, Bangladesh and as far afield as Cameroon. Most of the participants were provided with travel grants. The participants were also given luxurious accommodation in the ICCBS guest houses, meals and in-campus transportation. In addition, all participants were able to take part free of charge in the above-mentioned IUCr-UNESCO South Asia Summit Meeting, which was held April 28–30 at the same venue. This proved highly beneficial in creating awareness about the wider significance of the subject about which they were going to learn during the OpenLab. It also gave the participants a chance to interact with foreign delegates and renowned crystallographers.

The OpenLab Pakistan was organized into morning and afternoon sessions on each day. The morning sessions comprised theory lectures and use of various crystallographic software, and the afternoon sessions were dedicated to hands-on training on a Bruker SMART CCD area-detector diffractometer. The lectures were conducted in a state-of-the-art classroom where each participant was provided with a computer with high-speed internet access. Individual hands-on training ranging from crystal mounting, alignment and data collection to safety measures in the lab was provided.

The OpenLab topics were carefully selected and were aimed at enabling each participant to independently solve and interpret the structure and to prepare the CIF file for publication. The panel of resource persons was supported by Bruker's technical expert Mr Muhammad Hussain to assist in instrument handling and demonstration.



Gautam Desiraju lectures to the OpenLab Pakistan participants.

The day of inauguration of the OpenLab started with a very insightful and interactive lecture by Gautam R. Desiraju on 'Use of the Cambridge Structural Database in Analysis of Small-Molecule Crystal Structure'. A freely available teaching subset offered by the Cambridge Crystallographic Data Centre (CCDC) was used to teach preferred packing of molecules in the crystals. In addition, the participants

were connected to the online version of Prof. Desiraju's textbook *Crystal Engineering*. Using both online resources, Prof. Desiraju explained the role of various interactions in crystal packing and how it is ultimately responsible for the bulk properties of the material. Srinivasan Natarajan delivered an illustrative lecture on the basic theory of X-ray diffraction from crystals, polymorphism and metal–organic framework (MOF) compounds. Sammer Yousuf was responsible for demonstrations and providing hands-on training on crystal selection, mounting and alignment to all the participants. She also provided hands-on training on the use of *SHELXTL* to solve the crystal structure using X-ray data. Muhammad Nawaz Tahir demonstrated various advanced aspects of crystal structure solution specially dealing with difficult structures, disorder and twinning. Maqsood Ahmed delivered theory lectures on data reduction, space-group symmetry, structure solution and refinement, spherical and multipolar model approximations and X-ray charge-density analysis. He provided hands-on training on the use of *WinGX*, *Mercury*, *publCIF*, *MoPro* and the CCDC's Cambridge Structural Database. There was a lecture on reading and understanding *International Tables of Crystallography Volume A*. A full session was dedicated to powder X-ray diffraction and peak indexing in a powder diffractogram.

A short quiz was organized at the end to assess the level of understanding of the participants. The success rate was highly encouraging. Various prizes including cash prizes were given to those who performed well.

The closing ceremony of the OpenLab Pakistan was held on May 8. Certificates were awarded to the participants by the Director ICCBS, Karachi, Muhammad Iqbal Choudhary. The participants were very enthusiastic about introducing crystallography into their university curricula and about promoting it in their respective countries.

Maqsood Ahmed

Reports from other IUCr-UNESCO OpenLabs, such as those taking place in Morocco, Ghana, Cambodia, Uruguay, Turkey and Algeria, will appear in future issues of the *IUCr Newsletter*.

IYCR 2014

IUCr-UNESCO OpenLab in La Plata/Buenos Aires, Argentina

La Plata/Buenos Aires, Argentina, May 2014



Buenos Aires group



La Plata group

In line with the objectives of IYCr2014, professors and researchers from the Science and Engineering Schools of U. Nacional de La Plata (UNLP) and the School of Exact and Natural Sciences of U. de Buenos Aires (UBA), Argentina, had been organizing intensive courses, crystallization competitions and workshops since 2013 to better spread the knowledge of crystallographic techniques and methods within Argentina and across Latin America. With this background, the teams were ready to carry out the IUCr-UNESCO OpenLab initiative for IYCr2014 when Agilent Technologies and OlexSys Ltd offered to partner an OpenLab to be run in UNLP and UBA. The scheduled dates of the intensive course were from May 3 to 10, 2014. The OpenLab attracted about 80 applicants who were students, researchers and even some faculty from all over the world. The 37 selected delegates included post-docs, recent MSc, PhD graduate

students, MSc graduate students, one professor and three undergraduate students finishing their research work to get their undergraduate degree. They came from universities and research centers in Argentina (20), Bolivia (2), Brazil (4), Colombia (3), Costa Rica (1), México (2), Perú (2), Uruguay (2) and USA (1). The international team of lecturers and instructors was composed of O. Piro (OP), UNLP; L. Suescun (LS), U. de la República, Uruguay; L. Daniels (LD), Agilent Technologies; Horst Puschmann (HP), OlexSys Ltd; G. Echeverría (GE), UNLP; G. Punte (GP), UNLP; R. Baggio (RB), Comisión Nacional de Energía Atómica (CNEA) of Argentina; and F. Di Salvo (FDS), UBA. Massimo Nespolo (U. Lorraine, France) opened the OpenLab on behalf of the IUCr.

In the first three days, crucial theoretical and practical characteristics of small-molecule single-crystal X-ray crystallography were covered, interlacing traditional teaching with tutorial sessions. To solve practical exercises, students worked in small groups and discussed between themselves and with lecturers and tutors in a friendly environment. In this way, the physics of X-ray diffraction (OP), space-group determination (LS), structure solution methods (OP), data-collection strategies and data-reduction techniques (LD) and structure refinement (GP) were covered. For some of the topics, handouts with lecture notes were distributed to the participants, and discussions and questions were encouraged.

The attendees were introduced, online, to *OLEX2* by HP and worked with LD on solving a rather difficult structure applying the charge-flipping method. Before splitting into two groups, La Plata and Buenos Aires, the participants learned about the different crystallographic databases and their uses (LS). All the material is available at http://isfc2014.fisica.unlp.edu.ar/. For the rest of the OpenLab, the attendees were introduced to crystal-growth techniques and asked to form small groups for practical sessions on crystal-quality recognition, crystal selection, mounting on a goniometer head and getting a data set. These data were used to follow a step-by-step route to reconstructing the electronic distribution of an organic compound including a heavy atom from its single-crystal X-ray diffraction intensities. The procedure included the determination of the space group from the examination of the list of reflections and of the heavy-atom position from the Patterson map analysis, followed by the Fourier maps to obtain and refine the molecular model and, after reaching a good *R* factor, a Fourier synthesis to ensure the reliability of the solution achieved. At this stage the use of any graphical interface that might induce black box solutions was avoided. Finally, there was a discussion about the data interpretation, molecular geometry analysis and data presentation, along with the application of appropriate programs. These activities were led and coached by LD, GE and GP in La Plata and by LD, RB and GDS in Buenos Aires. They were performed in a warm-hearted and pleasant atmosphere that encouraged participation and helped form the basis for future collaborations between attendees and between attendees and lecturers. Those participants desiring credit points had to take an online examination within a month.

The successful development of the OpenLab was possible thanks to the full commitment of the lecturers, instructors and attendees and the financial support provided by the IUCr, ICTP, ICDD and CLAF for non-Argentine students, young scientists and lecturers, and Sistema Nacional de Rayos X (SNRX), Argentina, for local participants. ICSD and CCDC databases released their information to participants during the OpenLab. Organizational expenses were covered by Y-TEC (Argentina), UNLP, IFLP, CETMIC, LANADI, INQUIMAE and CONICET (Argentina).

Graciela Punte

IYCR 2014

Laue Memorial Plate dedicated in Poznań to celebrate IYCr2014



The Laue Memorial Plate (author: R. Sobociński). (photo G. Dutkiewicz)

In the years 1887-1891, Max von Laue (1879-1960) attended Friedrich-Wilhelms-Gymnasium, now St. John's Senior High School No. III (III LO im. św. Jana Kantego) in Poznań. About 20 years later, working at Ludwig-Maximilians-U. München, Max von Laue conceived of an X-ray diffraction experiment with a crystal as a three-dimensional diffraction grating. Such an experiment was successfully conducted under Laue's instructions by Walter Friedrich and Paul Knipping in 1912. Laue's discovery provided evidence about the wave nature of X-rays; proved the periodic lattice structure of crystals; and provided an estimate of the interatomic distances in molecules, which had to be of the same order as the X-ray wavelength, and won him the 1914 Nobel Prize in Physics). The discovery, in the hands of W. H. and W. L. Bragg (Nobel Prize in Physics, 1915) was soon converted into a powerful tool for the determination of the structure of chemical molecules. Today, the precise 3D structure of nearly one million chemical compounds is known, including molecular giants such as the ribosome.



The Laue Plate veiled with the IYCr2014 banner. (photo G. Dutkiewicz)



The unveiling act performed by (right-to-left) J, Gawroński (Polish Chemical Society), G. Desiraju (IUCr), A. Roodt (ECA), N. Jędrzejczak (student), J.-P. Ngome-Abiaga (UNESCO). (photo G. Dutkiewicz)



Poster prizes, sponsored by the Polish Synchrotron Radiation Society, announced by the chair of the poster jury, A. Wlodawer. The winners, right-to-left: W. Palczewska and A. Cieślak (1st Prize), A. Jarczyńska and O. Degórska (2nd Prize), D. Król and N. Pietruch (3rd Prize). (photo M. Ruszkowski)

As part of the celebration of IYCr2014, a Committee was established in Poznań, Poland, to commemorate Laue's time in Poznań with a Memorial Plate. The Committee included M. Jaskolski (Chair), W. Depmeier (IUCr Executive Committee), E. Framska, M. Gdaniec, K. Kordus, H. Koroniak, A. Legocki, A. Sakson and W. Kwiatek. The Plate, funded by the Polish Chemical Society and executed by sculptor Robert Sobociński, was unveiled on the School building on April 11, 2014. The dedication ceremony was attended by J.-P. Ngome-Abiaga (UNESCO), Bleicker (Chargé d'Affaires of the German Embassy), G. Desiraju (President, IUCr) and A. Roodt (ECA). It was followed by a Symposium, which showed Laue as a scientist and a champion of freedom, and his legacy as a source of inspiration for others. The lectures were presented by A. Więckowski, W. Schmahl, J. Lipkowski, W. Rypniewski, A. Wlodawer, J. Pełka, U. Heinemann, A. Kiliszek and D. Hoffmann. The School students presented a poster session dedicated to Max von Laue and various aspects of his discovery. The best poster, by A. Cieślak and W. Palczewska, was awarded with a prize sponsored by the Polish Synchrotron Radiation Society. Other sponsors of this function included the Ministry of Science and Higher Education, IUCr and ECA.

The importance of this Laue Day, when scientists, students, dignitaries and ordinary people from a number of countries came together in a secondary school, was eloquently summarized by Prof. Desiraju: 'Science is truly a way of bringing nations together and I join the community of crystallographers of Poland and Germany to celebrate the subject of crystallography and to honour the memory of one of our greatest sons.'

A concert of choral music was performed by the School Choir 'Proscenium' and the Poznań Chamber Choir, a Museum with a collection of original documents connected with Max von Laue was opened at the School, and a closing dinner was held.

Mariusz Jaskolski

FEATURE ARTICLE

The development of superspace crystallography and its application to the analysis of aperiodic crystals





Aloysio Janner



Ted Janssen

Professors Aloysio Janner and Ted Janssen (U. Nijmegen, the Netherlands) have made a remarkable contribution of exceptional distinction to the science of crystallography and are well deserving of the 10th Ewald Prize. What better time than during the International Year of Crystallography 2014 to recognize the tremendous achievement of these two eminent and highly regarded scientists?

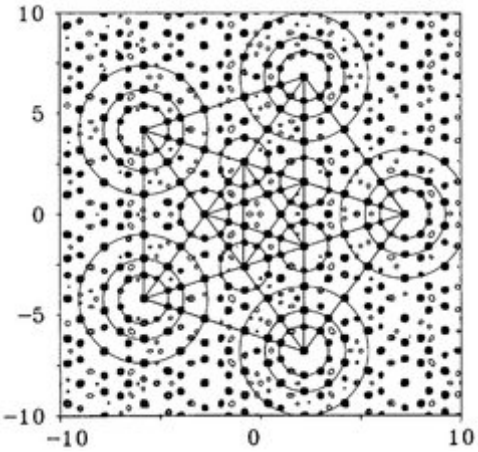
Aperiodic crystals are an interesting class of solids possessing long-range positional order yet lacking any defined periodicity. They are found in an ever-growing list of different systems: organic and inorganic compounds, minerals, metallic alloys, single elements under high pressure and recently also in soft matter consisting of large macromolecules, dendrimers, block copolymers, self-assembled nanoparticles in solution and even some proteins.

Aperiodic crystals are typically classified into incommensurately modulated crystals, where an underlying periodic crystal is modulated with a wavelength that is incommensurate with the lattice constant.

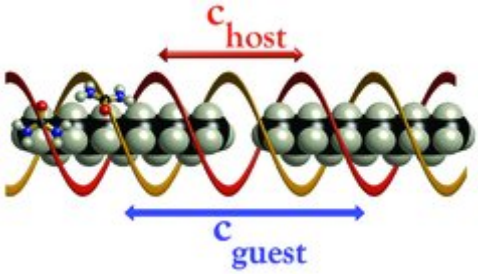
The lack of periodicity in these crystals precludes the use of standard crystallographic approaches for the study of their structure and physical properties; standard periodic space-group theory no longer applies. Phase retrieval methods and standard structural refinement tools do not work. With remarkable ingenuity, great creativity and mathematical rigour, the two Ewald Prize winners, along with the late P. M. de Wolff, were able to surmount all of these obstacles in a most beautiful way.

Together with de Wolff, Janner and Janssen – who were at the time working on the relationship between symmetry and physical properties in condensed matter – conceived and developed an approach to understand these incommensurately modulated structures, which de Wolff described as being superimpositions of basic periodic structures, with a symmetry that can be described by a three-dimensional space group.

Their work over the past 30 years has allowed for a rigorous analysis of the symmetry of aperiodic crystals and provides a unique route to understanding and solving their atomic structures. For this accomplishment de Wolff, Janner and Janssen shared the 1998 Gregori Aminoff Prize awarded by the Royal Swedish Academy of Sciences.



Fourier map of a decagonal plane of $Al_{78}Mn_{22}$ [A. Janner (1992). *Acta Cryst.* A**48**, 884–901; figure courtesy of W. Steurer].



Urea–alkane, an aperiodic crystal. Figure courtesy of Bertrand Toudic, U. Rennes, France.

Thanks to de Wolff, Janner and Janssen, the field of superspace crystallography evolved very quickly. The use of the superspace approach rapidly became the tool of choice for solving the atomic structure of incommensurately modulated and composite structures. In 1984, when Shechtman's discovery of quasicrystals was announced, Janner and Janssen were able to extend their superspace approach to deal with these new and puzzling structures.

Over their many years of research, it is perhaps difficult for these two scientists to select one crystal each that has particular significance; however, the IUCr can reveal their choices exclusively here and on the cover of this issue.

Janner wishes to share his affinity with the decagonal quasicrystal $Al_{78}Mn_{22}$. He describes how, by looking at the Fourier map of this quasicrystal, he recognized a pentagram from the Fourier spots, which he was not expecting. The pentagram had already been seen as far back as the Sumerian civilization (3rd millennium BC), was later adopted by the Pythagoreans as a secret sign of recognition, and is also considered to have magical properties. The history, as you can see, is rich. What amazed Janner was how this pentagram was not drawn by people but by nature on atomic positions of an aperiodic crystal.

Janssen highlights urea–alkane as his aperiodic crystal of particular interest. It consists of two mutually interpenetrating systems. One is a helix of urea molecules, which has broad channels in which the alkane molecules form another system; the systems do not fit each other. The combined system is a so-called incommensurate composite, and these materials are halfway between two other classes of aperiodic crystals: incommensurate modulated crystals and quasicrystals.

The award of the 10th Ewald Prize to Professors Janner and Janssen represents the tremendous achievement in the field of these two scientists and will change how crystallography is practised for many years to come.

Jonathan Agbenyega

FEATURE ARTICLE

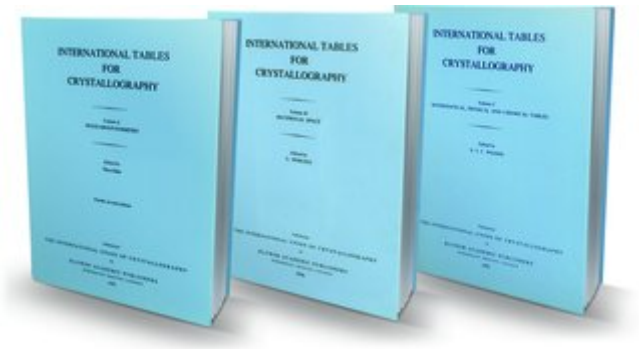
International Tables for Crystallography

International Tables for Crystallography is the oldest publication of the IUCr, with the first two volumes being published in 1935, *i.e.* twelve years before the establishment of the Union. Since then revisions and new volumes have appeared regularly. The current series, which is published in collaboration with Wiley, includes eight volumes as well as the *Brief Teaching Edition* of the space-group tables. A ninth volume, on powder diffraction, should appear in early 2015, and a tenth, on XAFS, is planned. The series as a whole attests to the very great scope and depth of the field of crystallography. The *International Tables* are much more than just a set of space-group tables.

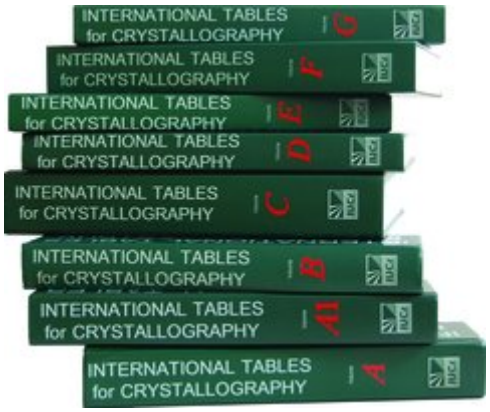
Early history



The first of the two original volumes of the 1935 edition and a volume of the 'red' series that began in 1952.



The 'blue' series of the 1990s.



The current series.



The next volume of *International Tables for Crystallography*; it is expected to appear early in 2015.



An example of electronic access to *International Tables for Crystallography*.
The series was conceived during a 1929 meeting in London when it was realized that standardization of notation and nomenclature was essential. From D. W. J. Cruickshank's history of the IUCr (www.iucr.org/iucr/history/aspects):
'... in 1929 there was a Faraday Society meeting in London on Crystal Structure and Chemical Constitution. Afterwards, Sir William Bragg convened a meeting to discuss the issues that required closer cooperation between crystallographers at an international level. Three committees were set up to investigate a coordinated abstracting scheme, the preparation of standardized space-group tables and the standardization of crystallographic nomenclature.'

Without the conventions that were developed in the early 1930s it would be impossible to assume, for example, that in monoclinic crystals it is the *b* axis that is unique and that in trigonal and hexagonal crystals it is the *c* axis that is unique. Without a standard reduced cell it is very difficult to know whether two triclinic cells with similar volumes are the same or not. Imagine the confusion there would be without these conventions.

The difference between the publication date (1935) for the first two volumes and the date given at the end of their preface (1932) is a reminder of how slow the publication process used to be.

A lively history of the tables is included in H. Kamminga's article [*Acta Cryst.* (1989). A**45**, 581–601] about the early days of the IUCr; this article can also be found at www.iucr.org/iucr/history/early-history.

Purpose

Each volume of the series covers a specific area of crystallography. In the early days most of the material was intended for working crystallographers. If the printed volumes were not so physically large each could be described as a *vade mecum*. With the advent of web access and small electronic devices, however, the size of the printed volumes is no longer so important; the series can now indeed function as a portable pocket reference.

The volumes contain useful material that is difficult, or perhaps even impossible, to find collected elsewhere. In many cases (*e.g.* space groups, scattering factors) it is important that there be a standard, authoritative reference. Furthermore, having the material collected is not only convenient but also allows a more unified approach than would otherwise be possible. In the online editions the many links within and between volumes simplify navigation and suggest connections between topics.

An educational role for the series was first mentioned in the General Preface to the second series (or 'red' series because of the color of its covers), which was launched in 1952:
'The aim of the present compilation is to facilitate the work of three categories of scientists: those who are actually engaged in the determination of crystal structures, those who are using X-ray methods in the study of crystals in general, and students of crystallography.' The educational role has expanded with time. While students using early volumes might have needed considerable help (I remember my own days as a graduate student), newer volumes have been written with the needs of the less experienced in mind. The publication in 1985 of *Brief Teaching Edition* of the space-group tables was an important step in bringing the tables to a wider audience.

Current Volumes

Volumes in the current series can be grouped under three headings:

1. Symmetry information

Vol. A *Space-group symmetry* (1st edition 1983; 5th edition 2002; online edition in 2006; editor Mois Aroyo, who succeeded Theo Hahn); Vol. A1 *Symmetry relations between space groups* (1st edition 2004; 2nd edition 2010; online editions in 2006, 2011; editors Hans Wondratschek and Ulrich Müller); Vol. E *Subperiodic groups* (1st edition 2002; 2nd edition 2010; online editions in 2006, 2010; editors Vojtech Kopský and Danny Litvin)
and the *Symmetry Database* (2011 onwards; also the responsibility of Mois Aroyo).

These volumes are the authoritative tabulations of symmetry groups. Vol. A includes the two-dimensional plane and three-dimensional space groups and is used regularly by most crystallographers; it is the successor of the first volume of 1935 but includes later revisions such as the 1995 introduction of the symbol *e* for a glide plane with translations in two directions (*e.g. Cmce*, formerly *Cmca*). The two-dimensional plane groups in Vol. A (and in the *Brief Teaching Edition*) are often used for teaching, perhaps in combination with Caroline MacGillavry's book of M. C. Escher's periodic drawings. The revised version of Vol. A that is expected to appear in 2014 will include new graphic representations of the cubic groups, and the online edition will include Seitz symbols [see Glazer, Aroyo & Authier, *Acta Cryst.* (2014). A**70**, 300–302].

Extended information about symmetry relationships is available in Vol. A1, which includes symmetry trees showing the relationships of the space groups. These trees are useful for tracing symmetry lowering, such as may occur during a series of phase transitions or as a result of chemical substitution.

The frieze, rod and layer groups are collected in Vol. E (see table on below). They are termed *subperiodic* because they are not periodic in all dimensions. The layer groups are needed for describing interfaces and also the structural layers that can be identified in many crystals. Rod groups are essential for

characterizing fibers (note that the cross sections of the 'rods' need not be circular) and are also useful for describing columnar packing units such as hydrogen-bonded chains.

Name	Dimensionality of the group	Dimensionality of the periodicity	Number of groups	Location
Space groups	3	3	230	Vol. A
Layer groups	3	2	80	Vol. E
Rod groups	3	1	75	Vol. E
Plane groups	2	2	17	Vol. A
Frieze groups	2	1	7	Vol. E
Line groups	1	1	2	

The *Symmetry Database* is an electronic resource that allows real-time manipulation of symmetry information, including all that found in the printed volumes of *International Tables*. The *Symmetry Database* facilitates studies of group–subgroup relations, domain structures and twinning, and relationships between members of crystal-structure families.

Information about superspace symmetry (*i.e.* for describing modulated, and especially incommensurately modulated, structures) is currently located in Vol. C.

A volume including a compilation of the magnetic space groups (or time-reversal groups or black-white space groups) is being discussed. In the meantime an e-book by Danny Litvin on magnetic space groups has been published by the IUCr (www.iucr.org/publ/978-0-9553602-2-0) and can be downloaded freely.

The 1983 edition of Vol. A was the first to be based on computer-generated space-group information. Computerization has increased steadily since then, culminating with the *Symmetry Database* and with computer generation and checking of the magnetic space groups.

Vol. D *Physical properties of crystals* (1st edition 2003; 2nd edition 2014; online editions in 2006, 2013; Editor André Authier). This volume is concerned with the influence of symmetry on the physical and tensor properties of crystals and on their structural phase transitions; it therefore describes applications of the symmetries described in other volumes (especially A and A1).
Part 1 introduces the mathematical properties of tensors and group representations and tabulates the independent components for each of the three-dimensional crystallographic groups. Several examples of tensor properties are described: elastic properties, thermal expansion, magnetic properties, linear and nonlinear optical properties, transport properties, atomic displacement parameters, and local electric susceptibility.
Part 2 is devoted to the symmetry aspects of excitations in reciprocal space: phonons, electrons, Raman scattering and Brillouin scattering.
Part 3 deals with the symmetry aspects of structural phase transitions and twinning. An important feature is the joint description of twinning and domain structures, which are usually presented in completely separate ways in handbooks of physics and of mineralogy.

2. Important information on other topics

Vol. B *Reciprocal space* (1st edition 1993; 3rd edition 2008; online editions in 2006, 2010; editor Gervais Chapuis, who very recently succeeded Uri Shmueli); Vol. C *Mathematical, Physical and Chemical Tables* (1st edition 1992; 3rd edition 2004; online in 2006; editor Richard Welberry, who succeeded Ted Prince and then Hartmut Fuess).

These two volumes can be traced back to Vol. II of the original series and Vols. II–IV of the 'red' series. Over the years, Vols. B and C have grown by accretion (especially C) to the point of being difficult to describe. Furthermore, many of the tables (*e.g.* X-ray scattering factors) need no longer be printed,

although having them available in an authoritative electronic form is important. The current editors of these volumes are working closely together on very major revisions. The original plan was for B to focus on topics more related to its current title (*Reciprocal space*) and for C to cover topics more connected to direct space, but it has become clear that such a simple division of topics is impossible.

3. Handbooks (in the sense of *Handbuch der Physik*)

Vol. F *Crystallography of Biological Macromolecules* (1st edition 2001; 2nd edition 2012; online editions in 2006, 2012; editors Eddy Arnold, Daniel Himmel and Michael Rossmann); Vol. G *Definition and Exchange of Crystallographic Data* (1st edition 2005; online in 2006; editors Syd Hall and Brian McMahon);
Vol. H (Powder Diffraction) (to appear in early 2015; editors Chris Gilmore, Henk Schenk and Jim Kaduk);
Vol. I (XAFS methods) (in development; editor Chris Chantler; joint main editors Federico Boscherini and Bruce Bunker).

These current and future volumes are in-depth handbooks designed for scientists interested in specific areas of crystallography. The volumes are intended to be indispensable for groups working and training students in these areas.

Vol. F takes the reader through all stages of structure determination and analysis for biological macromolecules, from those as small as short polypeptides and nucleic acid oligomers to those as large as a ribosome. Vol. F includes a historical perspective (along with many classic references), theoretical crystallographic background, descriptions of methods and information about experimental techniques. The articles are written by experts but should be accessible to anyone with a scientific background. Vol. F is the most authoritative single-volume collection available of articles on structural biology.

Vol. G provides an overview of the requirements for precise descriptions of crystallographic concepts and quantities in the design and execution of scientific software. While the volume concentrates on the specific interchange format (CIF) developed by the IUCr and provides a complete reference for CIF programmers and users, it is also of wider use in developing a formal language of crystallography to be used by computer programs and processes. The CIF data dictionaries, which are most easily searched electronically, account for half the pages. A historical introduction provides a perspective on why the CIF language has the form it does and how it is related to XML.

Vol. H is intended to be a one-volume summary of best practices and state-of-the-art applications of powder diffraction; its target audience includes both beginners and advanced practitioners. It will have sections on instrumentation and sample preparation, methodology, structure determination (including structure validation), defects, texture and microstructure, and software, as well as many chapters on applications in specific fields such as macromolecules, ceramics, cement, polymers, energy storage, petrochemicals and cultural heritage. The electronic version of Vol. H will include extra digital materials. Many authors have included raw diffraction data discussed in their chapters so that the reader may reproduce the data processing that is discussed.

Vol. I (XAFS methods) is still in the planning stage. A Vol. J is being discussed with the Commission on Magnetic Structures.

Access

The printed volumes can be purchased individually. Some of the newer volumes originally included a CD with accompanying software; more recently that software has been made available online.

Online access is for purchase by institutions and includes access to all volumes. Purchase of the package includes all the extra electronic resources associated with the volumes as well as access to the *Symmetry Database*.

The 'Guided Tour', available at http://it.iucr.org/services/guidedtour/, is highly recommended because it shows what is available electronically. Access to the Tables of Contents for all the volumes is free, as are sample pages (including author lists and prefaces); see the homepages for the individual volumes (*e.g.* http://it.iucr.org/F/). Links to published reviews for the individual volumes are given at the bottoms of their respective homepages.

Summary

The volumes of the *International Tables for Crystallography* are a marvelous resource for anyone working in, or interested in, crystallography. While the volumes have been developed individually over decades they are now richly interconnected *via* the many links in the electronic editions. Investigation of a question about the organizing principles behind a layered structure might well start with the space-group tables of Vol. A but then go on to the space-group relationships detailed in Vol. A1 and to the layer groups listed in Vol. E, and then perhaps to the tensor information in Vol. D. New students in macromolecular labs and powder-diffraction labs should find Vols. F and H very useful. Many of us think immediately of the space-group tables of Vol. A when the series *International Tables* is mentioned, but those tables represent only a small part of the information included.

In closing, it is essential to remember that these volumes would not exist but for the countless hours donated by the many editors and authors who have been involved with the series. It is difficult to thank them enough for their contributions.

Carol Brock

OBITUARY

Philip W. Hemily (1923-2014)

Philip W. Hemily (age 91), of Washington, DC, died January 7, 2014, in Sarasota, FL, of natural causes on the birthday of his partner of 37 years, Kathryn Arnow, a retired health policy analyst, who died in 2012. Born 1922 in Newaygo, Michigan, he loved France. He held a DSc cristallographie from the U. de Paris (1953) and was Chargé de Recherche at the French National Center for Scientific Research (CNRS) from 1953-1956. Following service in the US Army in WWII, he received a BS in Mechanical Engineering from the U. of Michigan in 1947. He held senior staff positions at NSF from 1957-1965, during which time he was instrumental in creating the international office of the Foundation and participated in establishing programs to strengthen science and mathematics education.

Hemily retired from the Senior Foreign Service of the Dept. of State (1983) after serving as Deputy Assistant Secretary General for Scientific Affairs of NATO (1976-1982) and Science Counselor to the US Mission to the Organization for Economic Cooperation and Development (OECD) from 1965-1974. Key accomplishments included providing leadership in the establishment of the NATO 'Science for Stability' program and the strengthening of National Science and Technology Policy structures in OECD nations.

From 1984-1995 as a Trustee of Americans for UNESCO, and Director of the Committee on International Organizations and Programs, Office of International Affairs, National Research Council of the National Acad. of Sciences, National Acad. of Engineering and the Inst. of Medicine, he gave priority attention to US scientific and engineering relations with UNESCO, the International Council of Scientific Unions, the establishment of international engineering organizations, and the follow up to the 1992 UN Conference on Environment and Development.

Philip is survived by children Philip, Valerie and Laurenne, and six grandchildren.

Brendon Hemily

MEETING REPORT

Workshop on Dynamic Structural Photocrystallography in Chemistry & Materials Science

Buffalo, NY, USA, June, 2013



Participants of the Workshop on Dynamic Structural Photocrystallography in Chemistry & Materials Science.

Photocrystallography combines X-ray diffraction with external light excitation of the sample. It is utilized for studying out-of-equilibrium phenomena in crystals, *i.e.* relaxation processes, long-lived metastable states, short-lived excited states and solid-state photochemical reactions. The rapid development of techniques and the availability of pulsed synchrotron X-ray sources have brought photocrystallography to the frontier of modern crystallography. It is now possible to conduct time-resolved studies of species with microsecond or even shorter lifetimes. Recent advances in the field show not only its potential and importance but also the need to train students and young researchers in the subject.

This workshop was initiated and organized by Philip Coppens (USA), and supported by members of his research group. The International Advisory Committee included E. Collet (France) and M. Takata (Japan). Fifty-five scientists, graduate and undergraduate students, young researchers, and invited speakers from American, European and Asian universities and research centers participated in the workshop.



Left corner: the in-house pump-probe photocrystallography instrument.

Light-induced processes such as photochemical reactions, linkage photo-isomers and photo-induced molecular excited states in crystalline solids – on timescales of hours to femtoseconds – were studied during the workshop. Development of experimental laser pump/X-ray probe techniques, used either for in-house experiments at high-intensity X-ray sources or for experiments performed at synchrotron beam lines or at free-electron laser sources, was a major focus. New computational techniques for time-resolved data processing and interpretation of results were also considered.



Software exercise class.

The workshop program was divided into two parts: an opening lecture by Philip Coppens and plenary lectures given by P. Naumov (NYU Abu Dhabi & U. of Kyoto), J. Benedict (U. at Buffalo, SUNY), E. Collet (U. of Rennes, France), A. Makal (U. of Warsaw, Poland), M. Messerschmitt (SLAC National Accelerator Laboratory), J. Spence (Arizona State U.) and F. Schotte (NIH, NIDDK). Software exercises followed.

The second part had three tracks: (1) Monitoring Chemical Reactions; (2) Pump–Probe Experiments of Excited State Structure (E. Trzop, A. Makal and B. Fournier), and (3) Treatment of Liquid-Jet Injection LCLS Data With Examples by N. Zatsepin (ASU). Manufacturer presentations were given by C. Ceccarelli (Agilent), L. Daniels (Rigaku) and C. Campana (Bruker AXS) on potential applications of commercially available X-ray diffraction systems for studying light-induced phenomena.

Thanks to support from the IUCr, travel grants were awarded to six young scientists.

Elzbieta Trzop and Katarzyna Jarzembska
Taken from ACA RefleXions, Fall 2013

AWARDS AND PRIZES

Huber receives Honorary Doctorate from Jagiellonian University



DHC Robert Huber (right) with his promoter Prof. K. Strzalka (left). (photo credit K. Strzalka)

On May 10, 2014, Robert Huber became Doctor Honoris Causa (DHC) of the Jagiellonian U. in Kraków, Poland. Prof. Huber is an iconic figure in protein crystallography. Now retired, he spent most of his career at the Max Planck Inst. in Martinsried, Germany, including 33 years as its director. At the end of the 1950s, Robert Huber helped to introduce protein crystallography to the European continent; although the X-ray diffraction experiment was first done in Munich, the method was actually developed in the British Isles (by the Braggs and for proteins by Perutz), to be reimported to Munich by Huber's mentor, Walter Hoppe.

Robert Huber is widely known for his titanic structural work on proteolytic systems and their inhibitory regulation, an area that also includes his pioneering work on the structure of the proteasome. Another milestone discovery, awarded with the Nobel Prize in Chemistry in 1988 (with Johann Deisenhofer and Hartmut Michel), was the determination of the crystal structure of the photosynthetic reaction center complex, which not only shed light on this light-to-chemical energy converter, but also demonstrated for the first time that integral membrane proteins can be successfully attacked by crystallography.

The name of Robert Huber is also associated with a number of other methodological advancements. All these numerous achievements were recited in Latin during the Honorary Degree award ceremony.

The ceremony was held at a special session of the Academic Senate of the Jagiellonian U., celebrating the 650th Jubilee of this majestic Alma Mater. The session was witnessed by ~1600 guests assembled in the Auditorium Maximum, including highest-ranking representatives of about 200 universities around the world, and the President of Poland.

The Jagiellonian U., one of the oldest in this part of Europe, was founded in 1364 by King Casimir III the Great. The inclusion of the DHC promotion in this remarkable celebration adds additional splendor to the Honorary Doctorate of Robert Huber.

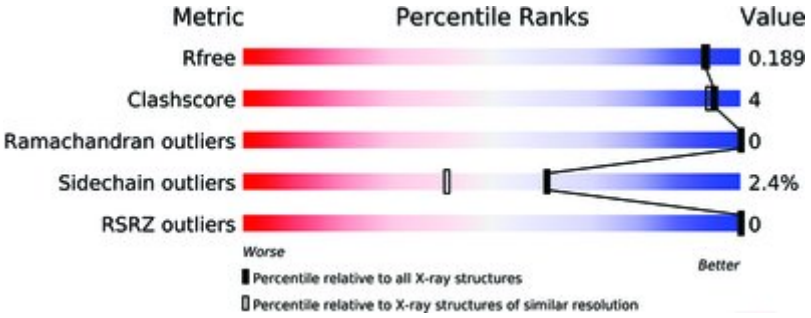
Congratulations and best wishes for continued success!

Mariusz Jaskolski

SPECIAL REPORT

Validation reports available for all X-ray structures in the PDB

The Worldwide Protein Data Bank (wwPDB) partners are pleased to announce that validation reports for all X-ray crystal structures in the PDB archive are now publicly available.



The validation reports provide at-a-glance summary information that compares the quality of a model with that of other models in the archive.



The reports contain residue-property plots. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ>2). 'The new validation reports are sure to become an indispensable resource for all X-ray crystallographers. Most importantly, we hope they will be really useful for all the end users of structural models, who increasingly need to critically assess and compare PDB entries,' said Anastassis Perrakis, Netherlands Cancer Inst., whose research focuses both on analysing macromolecular structures relevant for cancer, and also on developing the tools needed to decipher these structures.

The reports implement the recommendations of a large group of community experts on validation and include the results of geometric checks, structure-factor assessment and ligand validation. The reports include results from tried and tested software including *MolProbity*, *Xtriage*, *Mogul*, *EDS* and various CCP4 programs. They summarise the quality of the structure and highlight specific concerns by considering the coordinates of the model, the diffraction data and the fit between the two. Easily interpretable summary information that compares the quality of a structure with that of other structures in the archive is also provided.

Validating structures prior to publication and deposition

The new X-ray structure-validation reports have been provided to depositors as part of the structure-annotation process since August 2013. More recently, a stand-alone wwPDB X-ray structure validation server was launched (http://wwpdb-validation.wwpdb.org/). The server allows crystallographers to check

early, intermediate and near-final models on demand and helps identify any potential problems that need addressing prior to structure analysis, publication and deposition.

'The stand-alone validation server will run exactly the same validation tests that have recently been introduced for the annotation of new depositions,' says Randy Read of Cambridge U. Read chairs the wwPDB X-ray Validation Task Force (VTF) that has produced detailed recommendations to the wwPDB about how macromolecular crystal structures should be validated [1]. 'With the stand-alone server, crystallographers won't have any last-minute surprises when they deposit their structures just before submitting the paper,' Read adds.

Accessing validation reports for archived structures

Validation reports for X-ray structures archived in the PDB are accessible from the following FTP sites:

ftp://ftp.wwpdb.org/pub/pdb/validation_reports/ (wwPDB)

ftp://ftp.ebi.ac.uk/pub/databases/pdb/validation_reports/ (PDBe)

ftp://ftp.pdbj.org/pub/pdb/validation_reports/ (PDBj)

The reports have been developed in the context of a larger initiative, the new wwPDB Deposition and Annotation system (http://wwpdb.org/system_info.html), which was created to unify the annotation tools and practices used across all wwPDB deposition centres and for all common structure-determination methods.

Christine Zardecki

[1] Read R. J., Adams P. D., Arendall III W. D., Brünger A. T., Emsley P., Joosten R.P., Kleywegt G. J., Krissinel E. B., Lütteke T., Otwinowski Z., Perrakis A., Richardson J. S., Sheffler W. H., Smith J. L., Tickle I. J., Vriend G. and Zwart P. H. (2011). A new generation of crystallographic validation tools for the Protein Data Bank. *Structure*, **19**, 1395-1412. DOI: 10.1016/j.str.2011.08.006.

MEETING REPORT

Malaysian Crystallographic Association

On June 3, 2014, the Steering Committee of the Malaysian Crystallographic Association announced Government approval for the establishment of the Pertubuhan Kristalografi Malaysia.

The act signifies Malaysia's intention to participate formally in the IUCr, an on-going project led by the Malaysian Crystallographic Association under the guidance of Nadiah Halim of the U. of Malaysia.

The U. of Malaya held its first Chemical Symposium in Kuala Lumpur recently, which was the first formal commemoration of the International Year of Crystallography in Malaysia.

The event was sponsored by the Dept. of Chemistry, with thanks due to the Head of Dept., Sharifuddin Md Zain. The visit of Gautam Desiraju, President of the IUCr, to the event was largely supported by the U. of Malaya's High Impact Research scheme, administered by the University through the Ministry of Education.

To register your interest in joining the Association, send an email to Low Yun Yee (yylow@um.edu.my), interim Secretary. Plans for an Annual General Meeting later in the year are being made, where elections will be held for Office bearers and Committee members.

NOTICE

IUCr 2014: Montréal awaits…

After years of planning, your IUCr 2014 organizers are thrilled to be so close to welcoming you to Montréal, Canada. Thanks to the 2000 abstracts received, we are confident that you will find the scientific program robust, the community engaged and the atmosphere charged with intellectual curiosity.



In addition to the scientific program, there are numerous workshops, business meetings and industrial events scheduled, not to mention the special IYCr and social activities planned. As usual, rooms, times and dates are listed on the website and in the printed program you will receive when you arrive, but this year we are proud to introduce a mobile app to the mix. ***myIUCr2014*** is easy to use, can be accessed through our current website and will be updated throughout the entire congress.

This online congress tool and app is available through the iTunes App store or the Google Play Store, as well as through your built-in browser. Quick links will be provided on the congress website. Download it from your lab or office – it is free – and find out how you can get the most out of IUCr 2014. While students and early-career researchers typically need no introduction to apps, many others can still be hesitant to adopt this technology for fear it will involve more effort than benefit. Rest assured, however, that it will take no time at all before you will truly *app*reciate its convenience! It's simple:

Step 1: Activate and set up your myIUCr2014 profile

Import your photo, add a biography from LinkedIn or add your own

Customize your interests ('tags')

Share your LinkedIn, Facebook & Twitter links

Step 2: Start networking

Browse the myIUCr2014 app to find sponsors, exhibitors, and poster or oral presenters

Sort and filter companies and attendees by areas of interest, tracks, country and other combinations

Send messages to sponsors, exhibitors and other attendees, while keeping your email address private until you are ready to share it

Step 3: Keep up to date with the latest scientific presentations and events

Search by day, session track, keyword or type of event, to find exactly what interests you at IUCr 2014

View speaker profiles, abstracts and presentation schedules

Keep up to date with real-time changes throughout the entire congress

Step 4: Customize your IUCr 2014 experience

Plan your own personalized schedule for the time you spend at IUCr 2014

Add sponsors, exhibitors, sessions and events to your myIUCr2014 schedule to maximize your time

Access your event plan whenever, wherever, from your smartphone, desktop or mobile device

All registered attendees will receive an invitation to join this online community of crystallographers. Questions or requests for invitations can be sent to IUCr14abstracts@legendconferences.com.

And for those of you without a mobile device or simply wanting to see the program before the app is live, please visit the Program at a Glance online. Microsymposia, poster sessions and more are available now at http://iucr2014.org/side_program/scientific_program/program_at_a_glance_e.shtml (navigate: Program/Program at a Glance).



Several IYCr activities will be running in parallel to the IUCr Congress. A public display of Jean-Louise Hodeau's panels (www.iycr2014.org/resource-materials/voyage) will run during the Congress, on Level 1 of the convention centre. Near the conference registration will be another display, of IYCr posters from conference delegates and from national committees world-wide. Three public lectures are also scheduled to take place at McGill U. on Wednesday, Aug. 6, Thursday, Aug. 7, and Monday, Aug. 11.

For anyone interested in other IYCr activities, an international events calendar is available (www.iycr2014.org/events) and if you have any events planned, Louise Dawe (ldawe@wlu.ca) would like to hear from you. Finally, the American Crystallographic Association has an IYCr page that will be going live this week (http://iycr2014.org/aca/home), and a North American IYCr video contest for K-12 students has just been launched through Facebook (search for 'IYCr2014 Video Contest – USA/Canada'.)



With the program well in hand, you can now shift your thinking to the softer side of your trip to Montréal. Most hotels in our block are already sold out, and we understand that many of the properties within easy

walking distance of the Palais expect other large groups this summer. We only guarantee the remaining posted rates until July 14th, or until the blocks are sold out, so please book your rooms soon to avoid disappointment. To access the rates we've negotiated for you, you must make your reservation through our website: http://iucr2014.org/side_accommodations/accommodations_e.shtml.

And finally, we do hope that you will find the time to really take full advantage of your time here by combining business with pleasure. A good variety of independent suggestions and organized tours are outlined on our website at http://iucr2014.org/side_registration /touroption_e.shtml (navigate: Program/ Social activities). Activities to suit the tastes of delegates and their travelling companions alike are waiting to be discovered on this page.