

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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LETTER FROM THE PRESIDENT

Facing challenges

Sven Lidin



Left: the spice market in Oaxaca in October. Right: a beautiful day in Novosibirsk in early February.

After a little more than a year as the President of this Union I'm still struck and amazed by the richness of this organization. During this year, I've had the privilege to attend many types of meetings in many parts of the world, from the large, global or regional meetings such as the IUCr Congress in Hyderabad, India, and the ECM in Oviedo, Spain, to smaller local meetings like the inaugural meeting for the crystallographic facility in Abidjan, Côte d'Ivoire, and the conference on crystallography, microscopy and synchrotron radiation in Oaxaca, Mexico. From meetings of well established scientists at the German Crystallographic Association meeting in Essen to young and aspiring students at the Russian Chemistry Olympiad in Novosibirsk. We are truly global, representing crystallographers worldwide. I'm proud to be part of this organization.



Nobel Prize winner Dan Shechtman together with young crystallographers in Abidjan.

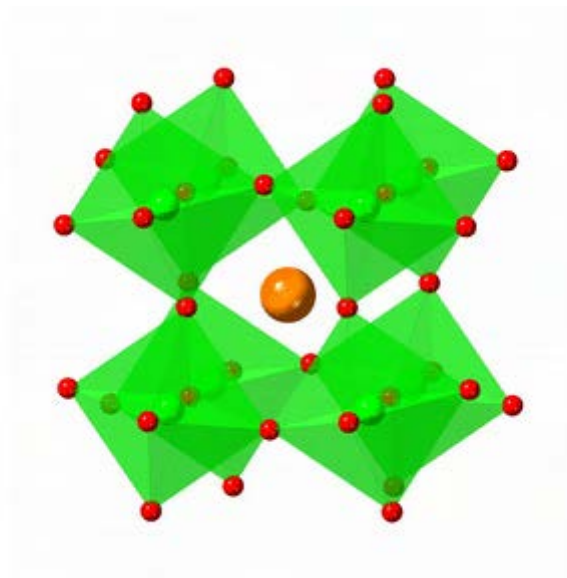
Still, we are facing many challenges. One is the different opportunities offered to scientists in different places. Access to high-quality X-ray, neutron and electron facilities is one of the prerequisites for high-quality science. Many things can be accomplished with in-house sources, and it was a very positive experience to see the new facility in Abidjan. It is an important feature of synchrotrons and neutron sources that they tend to be open to users from all over the world, often with travel support as an additional feature. This has the additional benefit of providing the sources with the best experiments. Large-scale facilities are, however, not available everywhere and not to everyone and in order to qualify for beam time, you must first be experienced enough to put together a good proposal. Our challenges are not only geographical. Science in general has a history of being a pursuit dominated by men. Crystallography is no exception, and even if the situation has improved, we still have a long way to go. A small, but significant step is the formation of the IUCr Gender Equity and Diversity Committee headed by Jenny Martin. The terms of reference for this group may be found [here](#).

Finally I would like to raise the issue of Plan S and what it may mean for IUCr publishing. Plan S is an initiative that is aimed at curtailing excessive publishing costs by forcing a wholesale conversion to open access rapidly. While I understand the need to curb exorbitant prices and sympathize with the general idea, I am worried that plan S is going ahead too quickly. Plan S rules out the use of hybrid models, where some articles are published open access and others require subscription for viewing. This is a model frequently used in learned society publishing, such as many of the IUCr journals. Using this model we are able to maintain relatively low subscription fees and manageable open-access fees and it is a way for us to manage a slow transition from one model to the other. Small publishing houses such as the IUCr are vulnerable to sudden changes and there is a significant risk that a rapid implementation of Plan S will be devastating for small-scale operations such as the IUCr. The effect will then be a reduced diversity of journals. This will be one of several important points to cover at our next Journals Management Board meeting.

EDITORIAL

Lasting legacies

Mike Glazer



It is with considerable sadness that I have to announce that, since the last issue of the *Newsletter*, the crystallography community has lost yet another of its most distinguished members, Joel Bernstein. He was an entertaining speaker and was the world's leading expert on the subject of polymorphism. I knew him well as a personal friend, and I mourn his passing. You can read his obituary in this issue of the *Newsletter*, together with those of Tom Steitz, Aaron Klug and Håkon Hope.

Following [my article on quartz in the last issue](#), I was pleased to receive several comments by email and so we decided to publish an article by Shigeru Ohba, showing how to use the so-called Airy's spiral to determine the hand of a quartz crystal. It seems that one can talk endlessly about quartz. We also publish comments by Wulf Depmeier on [the interesting ideas proposed by JuanMa García-Ruiz](#) on the effect of the observation of crystals, such as quartz, on the development of ancient hominid brains. Wulf suggests that these early humans were probably attracted initially by the high reflectivity of crystals.

We also have a couple of interesting articles on the history of crystallography. Some time ago, while I was looking through my old files, I discovered a printed copy of Max von Laue's address to the 1st Congress of the International Union of Crystallography in 1948. In it, Max described the early work in 1912 that led to the discovery of X-ray diffraction and includes an amusing account of how their electrical apparatus caused the lights in the university to buzz! This nearly got them into trouble. The second article is on the life and scientific works of Auguste Bravais in the mid-19th century. Although I knew about his work on the theory of lattices (we all know of the 14 Bravais lattice types, don't we?), I had not realized before just what a formidable polymath he was. Well worth reading!

The IUCr awards at each of its international congresses a prestigious prize, the Ewald Prize, to an established crystallographer of distinction. During the Hyderabad Congress, it was suggested that we should set up another prize, this time in honour of W. H. and W. L. Bragg, to be awarded to one or two *early-career* researchers. The first such award(s) will be made at the next [Congress in Prague in 2020](#). A special committee under the chair of Elena Boldyreva has been set up tasked with choosing one or two promising early-career scientists. You can help in getting this award established by nominating candidates to the [IUCr Executive Secretary](#).

Another important contribution in this issue is by Gervais Chapuis and Carol Brock on the IUCr Online Dictionary of Crystallography. As they explain, this is set up as a wiki to enable anyone to contribute definitions of crystallography-related terms. If you need to find a definition this is one of the first places to go.

Finally, in this issue we have an important opinion piece by Massimo Nespolo on the growing problem of so-called predatory journals. Massimo is well known for not pulling his punches! I am sure that most of us have received emails inviting us to publish papers, or to become a member of the editorial board/reviewing team and so on. I get roughly two of these per day. As explained by Massimo, you need to be aware of this and how to spot them. There are so many journals being advertised these days it is sometimes difficult to know which are reputable and which, to put it simply, are just money-making scams.

There is another type of scam that we need to watch out for, namely “predatory conferences”. Again, I must receive at least two email invitations to these every day. They often have grandiose titles including the words “World” or “International” or “Advanced” and seem to be sent by representatives of commercial companies, often adopting a (possibly fake) female name (I assume this is intended to attract my attention). Often the venue is simply the name of a city, but no mention of the actual location within the city. I recall one of them had a photograph of the University Museum in Oxford, referring it to as being in London! One that I received recently had on its website a list of “Major Associations around the Globe” which included the IUCr! This is obviously a cynical attempt at trying to lend an air of respectability to their conference. The email that I received said “the conference is going to get you inspired beyond your wits and head to a new destination to encounter your creative circuit”! Not sure what that means, and whether at my age I still have any creative circuits! Moreover, you have only to look at the names of the organizers on their websites to see that most of them refer to minor figures. Often the standard of English is very poor, and even more importantly displays a complete lack of knowledge of the science. Here, for your amusement, is an example from the website of one such recent conference announcement on crystallography:

Chemical Crystallography is a use of diffraction methods to the investigation of basic science. An incessant reason for existing is the recognizable proof of common items, or of the results of manufactured science tests; however point by point sub-atomic geometry, intermolecular collaborations and supreme designs can likewise be considered. Structures can be examined as an element of temperature, weight or the utilization of electromagnetic radiation, or attractive or electric field: such studies involves just little minority of the aggregate. The utilization of single precious stone X-beam diffraction to decide the structure of a concoction compound has been generally delegated 'Substance Crystallography'. The strategies, the exactness in analyses combined with the modern PC contraptions and advances in innovation makes this branch of science an unequivocal supplier of precise and exact estimations of sub-atomic measurements. Structure assurance by powder diffraction, precious stone designing, charge thickness examination and studies on atoms in energized states are the late additional items.

What? Unfortunately, and this is serious, I have heard of cases where people have been led into paying money to attend these types of “conference”. You can find many websites on the internet that discuss this problem: just search the web for “Predatory conferences”. You have been warned!

Finally, Massimo Nespolo and I have been on the warpath regarding publications in which the terms ‘lattice’ and ‘structure’ (and corresponding ‘superlattice’ and ‘superstructure’) appear to be incorrectly used interchangeably. You can read Massimo’s latest paper on this [here](#). This should be required reading by all crystallographers (anyone in fact discussing crystal structures).

IUCR JOURNALS NEWS

New opportunity for Commissioning Editors for IUCr Journals



The International Union of Crystallography publishes nine leading journals in crystallographic research, including crystallographic instrumentation and methods, and crystallography-based application sciences. As the Union enters its eighth decade, we are announcing an exciting opportunity for a category of editor new to IUCr journals: Commissioning Editors in the fields of **Chemistry and Materials**, **Biology**, and **Methods and Instrumentation**. The three Commissioning Editors will work with the Main Editors, Managing Editors and Editorial Boards of all IUCr journals, as well as with the Editor-in-Chief, to commission, send out for review, and edit high-quality articles from leading researchers that will highlight both the role of crystallography in cutting-edge research and new science where crystallography can advance the state of the art.

As well as handling commissioned articles, the role of the Commissioning Editors will include development of Special Issues involving one or more of the journals, and working with IUCr journal Main Editors to recruit new Co-editors to join the various IUCr journal Editorial Boards. In all aspects, please note that the IUCr is committed to improving gender and geographical balance while maintaining the highest scientific standards.

The nine [IUCr journals](#) are (fully open-access journals are denoted by an asterisk, others are hybrid):

IUCrJ* (cross-cutting and high profile)

Acta Crystallographica A: Advances and Foundations

Acta Crystallographica B: Structural Science, Crystal Engineering and Materials

Acta Crystallographica C: Structural Chemistry

Acta Crystallographica D: Structural Biology (especially biological macromolecules)

Acta Crystallographica E*: Crystallographic Communications

Acta Crystallographica F: Structural Biology Communications

Journal of Applied Crystallography (applied crystallography and interdisciplinary research)

Journal of Synchrotron Radiation (synchrotron radiation, free electron lasers)

In addition, there is the IUCr's open data publication: **IUCrData***.

Candidates for Commissioning Editors should meet similar appointment criteria to those for IUCr journal Main Editors given [here](#).

Please write in confidence **by 31 March 2019** to the [Editor-in-Chief](#) and [Executive Managing Editor](#), enclosing your CV, a list of up to 20 of your most important publications, your vision for the role of the Commissioning Editor appointment you are applying for (*Chemistry and Materials, Biology, or Methods and Instrumentation*) in 500 words and a full list of publications.

IUCR JOURNALS NEWS

Welcoming three new Editors for IUCr Journals



From left to right: Angela Altomare (*Acta A*), Janet Newman (*Acta F*) and Karena Chapman (*JAC*).

IUCr Journals are delighted to announce the appointment of three new Editors.

Having served for several years as a Co-editor for *Acta Crystallographica Section A, Foundations and Advances*, Angela Altomare will now be working alongside Simon Billinge in defining and developing the role of the journal as a whole.

Angela graduated *cum laude* in Physics at the University of Bari, in the beautiful Puglia region of Italy. She now oversees a highly active team of researchers at the Institute of Crystallography of the Italian National Research Council (CNR), where her work is focused on developing innovative crystallographic methodologies for structure solution from single-crystal and, mainly, powder diffraction data. The computer programs written by Angela and her team (notably *EXPO* and associated algorithms) are used worldwide to characterize the structures of a huge range of materials.

Angela is well known for her passion for sharing her knowledge and research with fellow scientists, frequently speaking or lecturing at national and international meetings and schools. She is an active member of the IUCr's Commission on Powder Diffraction and the Italian Crystallographic Association, and has served on several international programme committees, recently as Chair of the highly successful 15th European Powder Diffraction Conference.

Simon says he is delighted that Angela has agreed to take on this new role, as "her wealth of crystallographic experience and knowledge will help us take *Acta A* to the next level, as the community develops the theory for the much broader definition of crystallography that is needed in the 21st century - the crystallography of 'real' materials".

Janet Newman, Director of The Collaborative Crystallisation Centre (C3) at CSIRO, and a long-time Co-editor on our biological journals, has been appointed as a new Section Editor for *Acta Crystallographica Section F, Structural Biology Communications*.

Janet obtained a BSc (Hons) in inorganic chemistry from the University of Sydney, a PhD from the Swedish University of Agricultural Sciences, as well as post-doctoral fellowships at Columbia University and Los Alamos National Laboratory. After a stint in industry in California, Janet returned to Australia 13 years ago to set up and run the C3 macromolecular crystallization facility in Melbourne.

Janet's main interest is in developing tools to help make macromolecular crystallization more robust, including designing new crystallization screens, using machine learning to classify the outcomes of trials and developing software to help design optimization experiments. And she has a lifelong commitment to help everyone spell 'sulfate' correctly!

On hearing of her appointment, her fellow *Acta F* Section Editor, Mark van Raaij, welcomed Janet and said that 'it's great to have Janet's deep expertise, broad experience and her contagious enthusiasm on board at *Acta F*'.

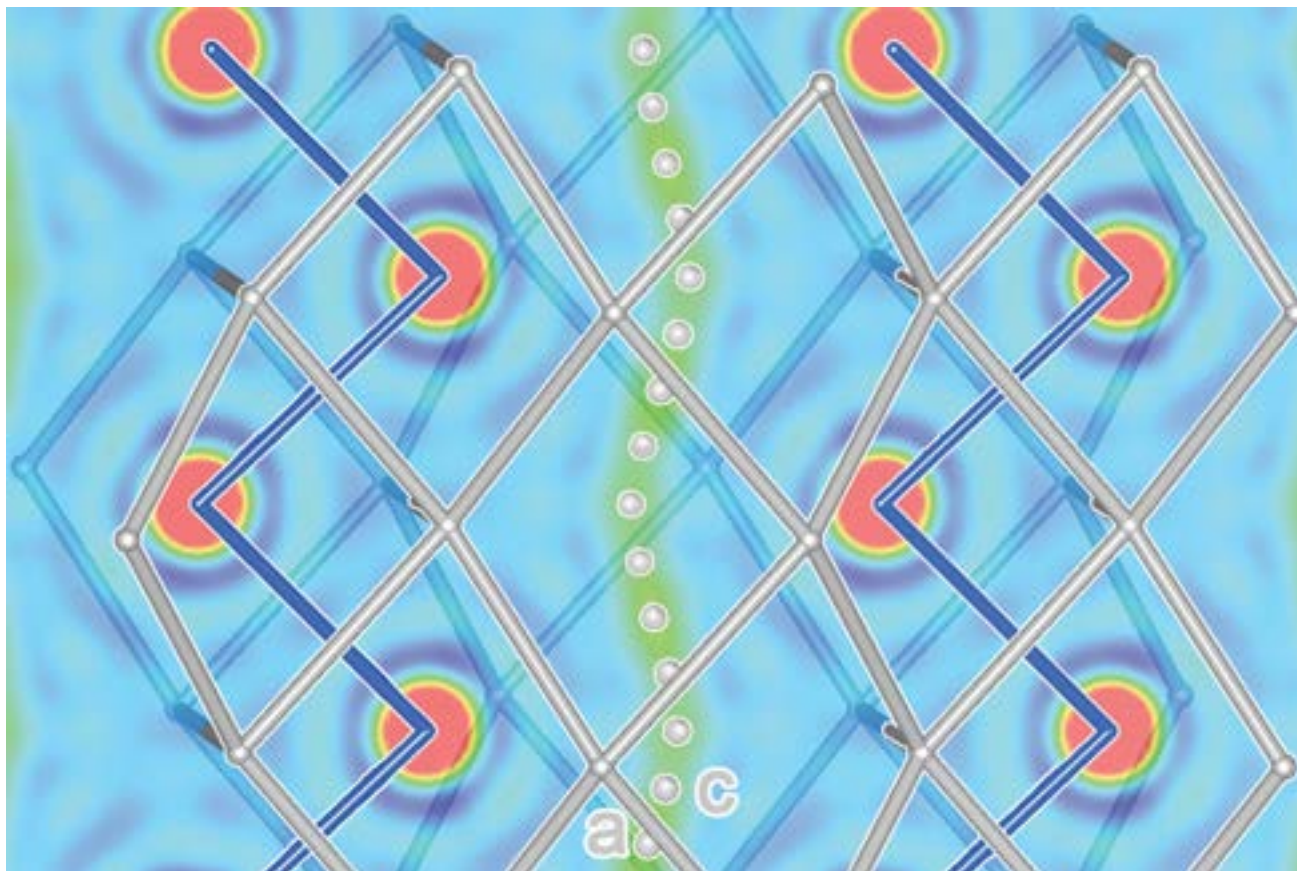
Karena Chapman has been appointed as a Main Editor of *Journal of Applied Crystallography*, joining existing Editors Janos Hajdu and Garry McIntyre. Karena has been a valued member of *JAC*'s Editorial Board since 2014.

Another chemistry graduate of the University of Sydney, Karena went on to join the X-ray Science Division at Argonne National Laboratory. There her research involved developing fundamental insights into the structure-function relationship in complex energy-relevant materials, as well as developing and supporting the world-leading Pair Distribution Function beamline, 11-ID-B, at the Advanced Photon Source. In her role as coordinator of the X-ray and Neutron Summer School she has also played a part in mentoring the next generation of crystallographers and scatterers. In September 2018 Karena took up the role of Professor in Materials Chemistry at Stony Brook University.

Garry commented 'We all look forward to working with Karena as a Main Editor of *JAC*, to continue the growth initiated by past editors and staff in the relevance, reach and impact of the journal. Janos added 'Karena's presence and critical input will help this exciting field of science and I hope it will also bring fresh air to the journal in general.'

IUCr Journals Editor-in-Chief Andrew Allen said 'While, sadly, this also marks my 'retirement' as a Main Editor of *JAC*, I really look forward to continuing to work with Karena, Janos and Garry. I know that *JAC* is in good hands, and will continue to prosper!'

Acta Cryst. A: Aperiodic 2018 special issue



This [virtual special issue of *Acta Crystallographica Section A*](#) features some highlights of the [9th Conference on Aperiodic Crystals](#) (Aperiodic 2018) held at Iowa State University (Ames, USA) in July 2018, and brings together articles originally published in the January and March 2019 issues of the journal. The Aperiodic meetings are held every three years and are the flagship meetings of the [IUCr's Commission on Aperiodic Crystals](#). Aperiodic 2021 will take place in Sapporo, Japan.

Aperiodic crystals, once regarded as anomalies or outliers in the field of crystallography, have taken centre stage since Dan Shechtman's discovery of icosahedral quasicrystals in an Al-Mn alloy in 1982. Controversy followed centred on the proper definition of crystalline materials. Ultimately, quasicrystals and, more generally, aperiodic crystals were 'validated' and assumed their place among the vast array of crystalline forms when the definition of a crystal was modified to include them: "A material is a crystal if it has **essentially** a sharp diffraction pattern" (see the IUCr Online Dictionary of Crystallography entry on '[Crystal](#)').

Among the exciting research presented at Aperiodic 2018, some of the best was presented by students and young investigators. Four formal awards were given in recognition of these excellent studies, two of which are described in this open-access issue. Ashwin Shahani (University of Michigan, Ann Arbor, USA) recounts beautiful X-ray tomography experiments, in which growth and dissolution of the decagonal quasicrystal Al-Co-Ni (from the liquid phase) were observed as a function of time, and Paul Klar (Universidad del Pais Vasco, Spain) tackles the complex, and long-mysterious, mineral known as mullite.

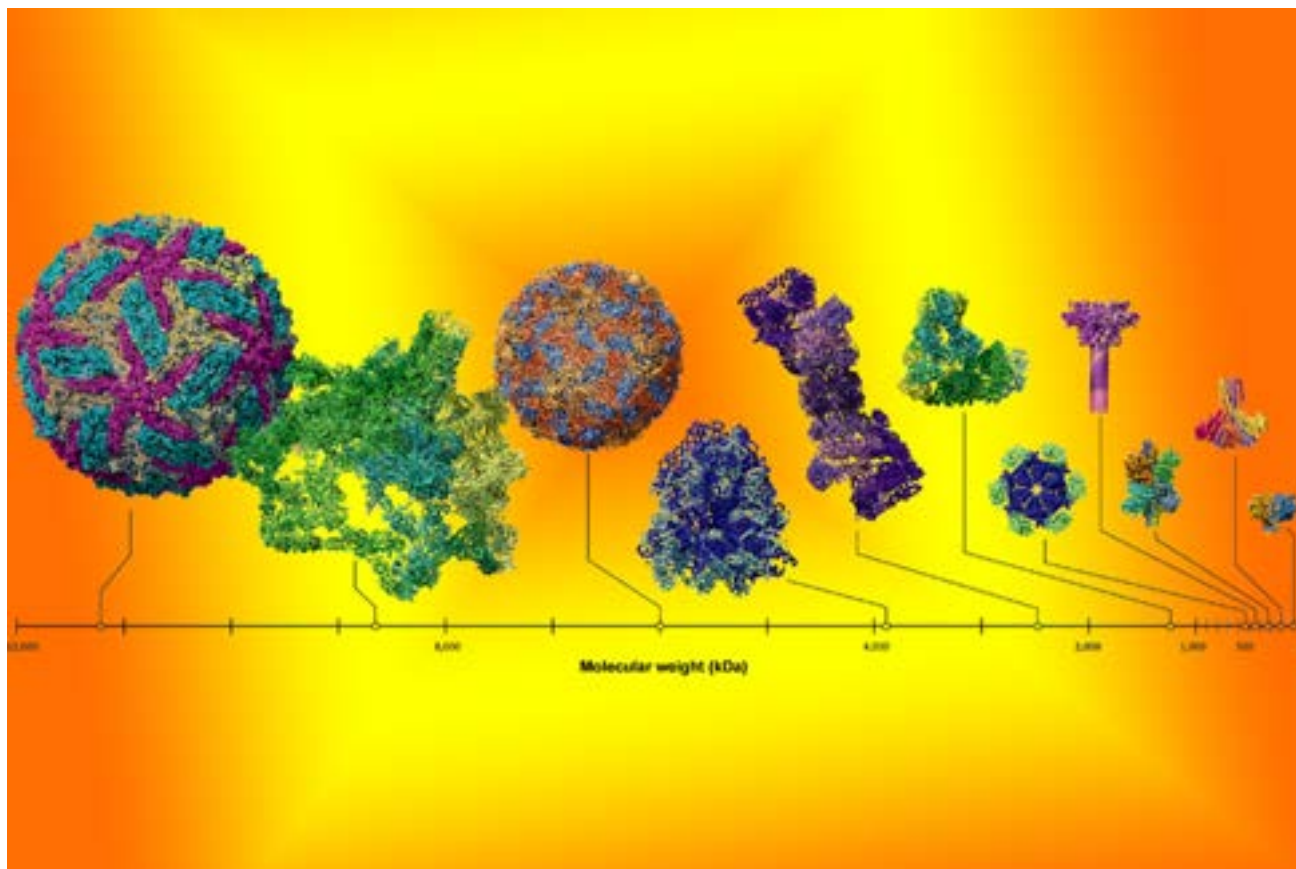
Other exciting directions in aperiodic research presented at the conference are featured in this issue, along with a tribute to one of the founding fathers of superspace crystallography, Ted Janssen, whose contributions to the field are reviewed by Marc de Boissieu.

This article contains material extracted from the Guest editorial by Gloria Borgstahl, Alan I. Goldman and Patricia A. Thiel, "Aperiodic order coming of age: from inorganic materials to dynamic protein superstructures".

EDITORIAL

The cryo-EM revolution: fueling the next phase

Sriram Subramaniam



In January 2016, exactly three years ago, *Nature Methods* featured cryo-electron microscopy (cryo-EM) as the 'Method of the Year' on its cover. The acknowledgment was not intended to imply that cryo-EM was a new method. Near-atomic resolution structures obtained using cryo-EM were already reported a decade ago. Microscopes capable of operation at cryogenic temperatures and generating images interpretable at atomic resolution were available two decades ago, and methods for analyzing low-dose cryo-EM images were being developed three decades ago. The most significant advance that made this revolution in structural biology possible was the development of direct electron detectors that ushered in the current era of electron counting and the recording of electron microscopic images as movies. By collecting a series of images instead of a single projection image, the motion of the proteins and specimen stage during the exposure could now be partially compensated. The integration of these detectors into electron microscopes suddenly made it possible to determine structures of proteins and protein complexes at unprecedented resolution.

If the access to these advanced tools and methods was restricted only to specialized practitioners of cryo-EM, this revolution in resolution would not have led to cryo-EM becoming the true revolution that it has, with the prospect of transforming all of structural biology, and perhaps cell biology too, in the years ahead. What is at the origin of this groundswell of unabated growth and adoption of cryo-EM that we have been witnessing in the last three years? There are at least three factors that are helping drive this next phase of the cryo-EM revolution.

First, the advances in streamlining many of the steps in the cryo-EM workflow have enabled non-specialists in adjacent, but closely related disciplines to take advantage of cryo-EM methods in their own research programs. The intricate steps involved in specimen preparation, data collection, data processing and interpretation have been broken down into sufficiently clear instructions that the barrier to entry is now lower than in previous years, especially at places where there is adequate availability of microscopes and the related accessories for specimen preparation and computing. The biggest beneficiaries at present have been X-ray crystallographers and NMR spectroscopists, but there is little doubt that this envelope will expand to include scientists in many other disciplines in modern biology.

Second, cryo-EM has transitioned from being a method that is only capable of handling a small subset of cryo-EM worthy specimens to a very large spectrum of proteins and protein complexes of broad general interest. This transition of cryo-EM from being a technology that was billed as a tool to analyze large and/or highly symmetric specimens, to one that can successfully tackle a range of proteins and protein complexes of broad general interest has been transformative. The structures of an impressive number of proteins, small and large, sometimes with extensive conformational spread, have been successfully analyzed by cryo-EM. Many of these protein complexes may never be coaxed to produce well ordered crystals for study by X-ray crystallography. It is important to recognize that in almost every instance, these selected successes in the application of cryo-EM rest on decades of advances in biochemistry, biophysics and protein science that laid the necessary groundwork. Nor can we overlook the fact that the landscape of macromolecular entities that are still intractable to analysis by cryo-EM remains immense. Yet, the future looks bright and there is every reason to hope that an ever-increasingly complex array of biological assemblies will be tackled by cryo-EM.

A third factor, perhaps a consequence of the first two, and with long-term impact, is the creation of national scale facilities that provide access to the latest cryo-EM technology. Modern electron microscopes are expensive, and the cost of their purchase and maintenance are often beyond the reach of many academic institutions. Besides, these are still finicky instruments; their mere purchase does not guarantee performance, and the expertise to get the best performance out of them is crucial, but not sufficiently widespread. Consequently, there is a very important role for federally funded facilities in ensuring adequate access (Stuart *et al.*, 2016). These facilities are necessary to supplement capacity at institutions that may have some infrastructure for cryo-EM, but even more so to those that do not have easy local access to data collection on advanced electron microscopes. The national center at Diamond Light Source (<http://www.diamond.ac.uk/Science/Integrated-facilities/eBIC.html>) has been exemplary in this regard, leading the way for democratizing access to cryo-EM technology. Many others such as the NeCEN center in the Netherlands (<http://www.necen.nl>), the Janelia Farm campus of the Howard Hughes Medical Institute (<https://www.janelia.org/support-team/cryo-electron-microscopy>) have also been instrumental in driving the adoption of cryo-EM by structural biologists. In the US, the first pilot national cryo-EM facility providing broad access was launched by the National Cancer Institute in 2017 (<http://www.cancer.gov/research/resources/cryoem>), and has already supported over 170 data collection sessions from 28 institutions across the US with just one Titan Krios microscope. The recent creation of three NIH-funded national centers (<https://www.nih.gov/news-events/news-releases/nih-funds-three-national-cryo-em-service-centers-training-new-microscopists>), each equipped with numerous modern electron microscopes, is certain to have a transformative impact by ensuring adequate access to cryo-EM instrumentation for US researchers.

The creation of synchrotrons catalyzed the dramatic growth of X-ray crystallography. National electron microscopy facilities will have a similar impact on the growth of cryo-EM. The emergence of cryo-EM as a powerful tool for structural biology led funders of biomedical research to ponder the question of the best model for enabling growth of this discipline, debating the relative merits of institutional, regional and national centers. The experience over the last three years teaches us that all three variants will be essential to sustain growth in the next phase of cryo-EM. Institutional investments are necessary to ensure adequate resources for training and providing access to screening instruments. Regional centers

will facilitate concentration of expensive instrumentation, while also offering opportunities for on-site training and easy access. National centers, funded at the right scale will be necessary not just to function as user facilities, but also as hubs for innovation that help advance the frontier of the field, and take on important, long-term challenges of broad interest to the biomedical research community. It is clear that we need growth at all three levels. Maintaining a healthy equilibrium between institutional, regional and national resources will be essential to fuel the next phase of the cryo-EM revolution.

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This article was originally published in [IUCrj \(2019\)](#). **6**, 1-2.

RESEARCH NEWS

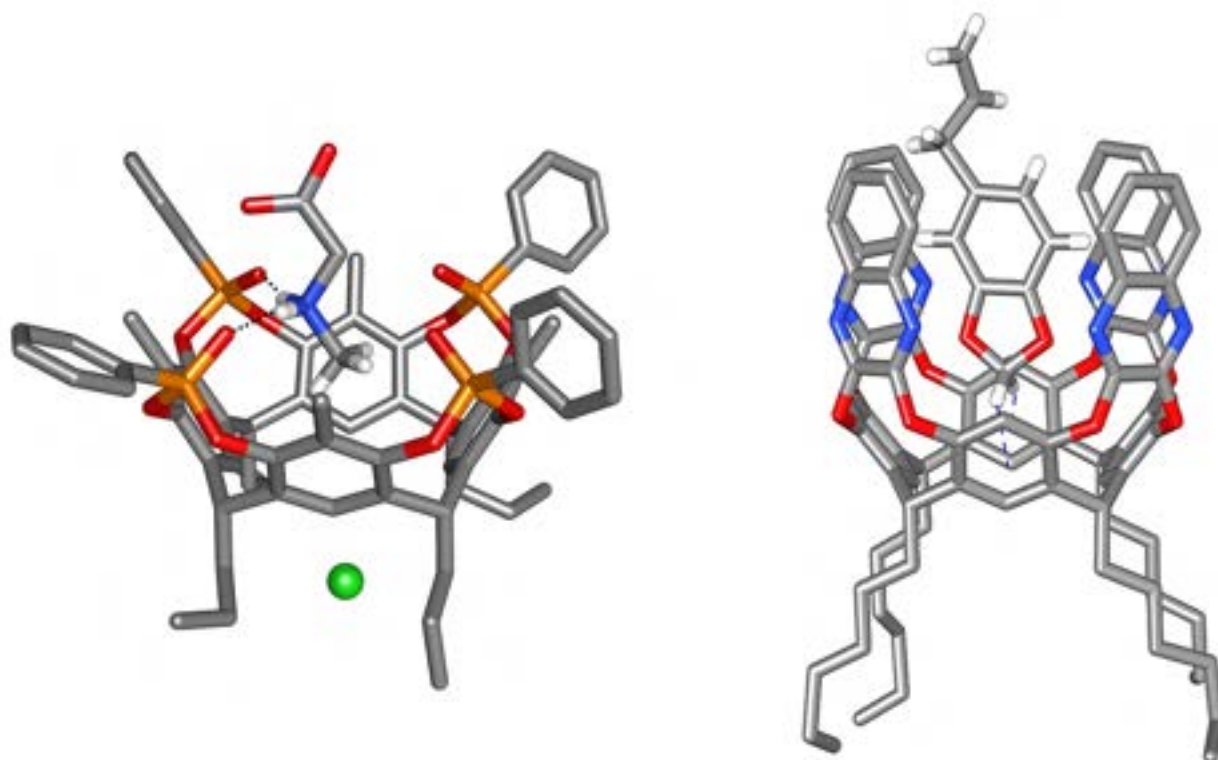
The many lives of resorcinarene-based cavitands

Chiara Massera



Since their first appearance on the chemistry scene 30 years ago (Cram, 1983), resorcinarene-based cavitands have been exploited as receptors for molecular recognition, as recently reported in *Acta Cryst. E* (Biavardi, 2019; Pinalli, 2019), as building blocks for crystal engineering (Pinalli et al., 2016), and in self-folding and self-assembly processes.

Their versatility primarily stems from the ability to choose different bridging groups to connect the phenolic hydroxyls of the resorcinarene scaffold. This allows the tuning of the depth, shape, dimension and complexation properties of the cavity, which can thus interact with neutral and charged molecules not simply because of shape complementarity but also through hydrogen bonding, π - π stacking, cation- and CH- π interactions. The study of the host-guest complexes in the solid state through X-ray diffraction on single crystals is hence fundamental for understanding and tailoring the weak interactions operating on functional surfaces that are responsible for the desired performance. The group of Professor Dalcanale from the University of Parma, Italy, has been particularly active in this field and has reported many examples in which cavitands have been effectively used in sensing devices for the recognition of different types of analytes, spanning from illicit drugs in the forms of hydrochloride salts (cocaine, mephedrone and amphetamines), sarcosine (a prostate cancer marker), peptides, alcohols and the volatile BTEX family (benzene, toluene, ethylbenzene and xylenes).



Functionalisation at the lower rim has allowed them to be grafted onto different surfaces like gold, silicon, carbon nanotubes and magnetic (based on iron oxides) nanoparticles. The molecular recognition has been translated into a signal mainly through two different types of devices, namely quartz crystal microbalances (QCM), where they are deposited as a thin film by spin-coating or electropolymerisation, and microcantilevers, by covalent grafting. Moreover, cavitands have also been successfully employed in solid-phase microextraction (SPME) analysis by functionalisation of the SPME fibres through sol-gel techniques.

Finally, cavitands can also form coordinative bonds with soft and hard metal centres to create discrete complexes, cages or extended polymeric networks. This allows the shape and property of the cavity to be changed to create biomimetic models or to produce species with catalytic properties.

The examples presented here demonstrate the many innovative applications that cavitands offer in many different fields, spanning from materials science to biology. The creativity of the researchers active in the field will bring cavitand research to the next level.

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FEATURE ARTICLE

More fun with quartz crystals!

Shigeru Ohba



An article in the last issue of the *IUCr Newsletter* written by the Editor, Mike Glazer, entitled "[Some musings on crystals of quartz](#)" attracted my attention and has prompted me to add some more information on the subject of quartz and its handedness. I sent Mike an email to say that, according to the current literature, it is not the *s*-face but the *x*-face that is normally used to tell us about the handedness, and that the handedness of as-grown quartz crystals can be judged by observing the so-called Airy's spiral. To begin with, there is so much confusion about the definition of right quartz. As pointed out in Glazer's article, the history of the description of quartz is replete with errors. Traditionally, dextrorotatory quartz has been called right-handed quartz. Sometimes right-handed quartz has been mistakenly described in space group $P3_121$ rather than in $P3_221$. In order to clarify this confusion, I wrote recently a short note in the *Journal of the Crystallographic Society of Japan* reviewing studies on the optical properties of quartz throughout history and on the determination of the absolute structure. The conclusion is that the definition of right quartz should be unified as dextrorotatory quartz, with citation of the article "Confusion over the description of the quartz structure yet again" (Glazer, 2018). Surprisingly, I realized later that the article "A new view of conoscopic illumination of optically active crystals" (Geday & Glazer, 2002) had also been cited in my accounts on the use of Airy's spiral (Ohba, 2009, 2014). Here, I will describe the use of Airy's spiral as a way to discriminate between left and right quartz crystals.

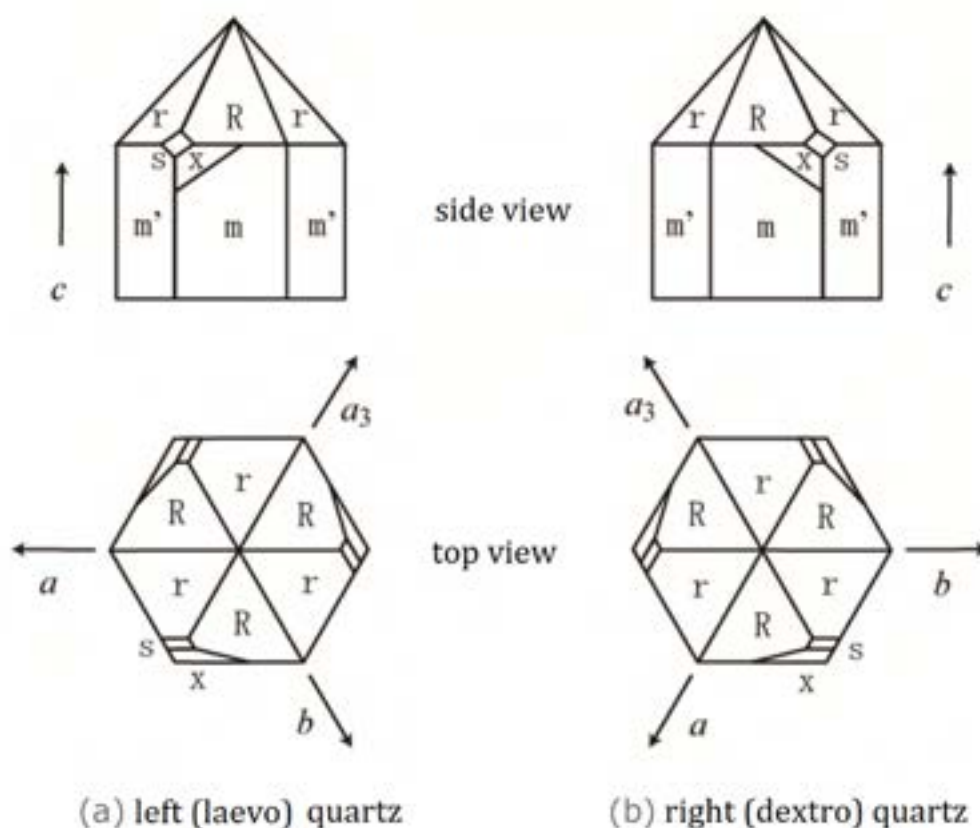


Figure 1. Habit of (a) left- and (b) right-handed quartz crystals. The conventional labels for the faces and the hexagonal axes are indicated.

Fig. 1 shows an idealized habit of the quartz crystals in the low-temperature phase, where the labels of the crystal faces and crystallographic hexagonal axes are indicated. The *s* face is inclined to the neighboring *m* and *m'* faces at the same angle, 45.7° , calculated from the Miller indices and lattice constants at 293 K. The conclusive evidence for handedness has historically been given by the *x* face, which lays nearly parallel to the *m* face, at an angle of 12.0° . As seen from Fig. 1, three sets of *x* and *s* faces are arranged around the *c* axis as mirror images between left-handed and right-handed quartz. In practice, however, it is very rare to see the *x* face even by looking at the crystal edges with a magnifying glass.



Figure 2. Left- and right-handed smoky quartz crystals ca 2 cm in length (Val Guiv, Switzerland) with unusually large x faces (highlighted).

Fortunately, eight years ago I obtained smoky quartz crystals with apparent x faces (Fig. 2) from the owner of a shop for minerals and fossils, Yoshihisa Yamamoto, who invented several tools to observe Airy's spiral in quartz including the use of a point prism described below.

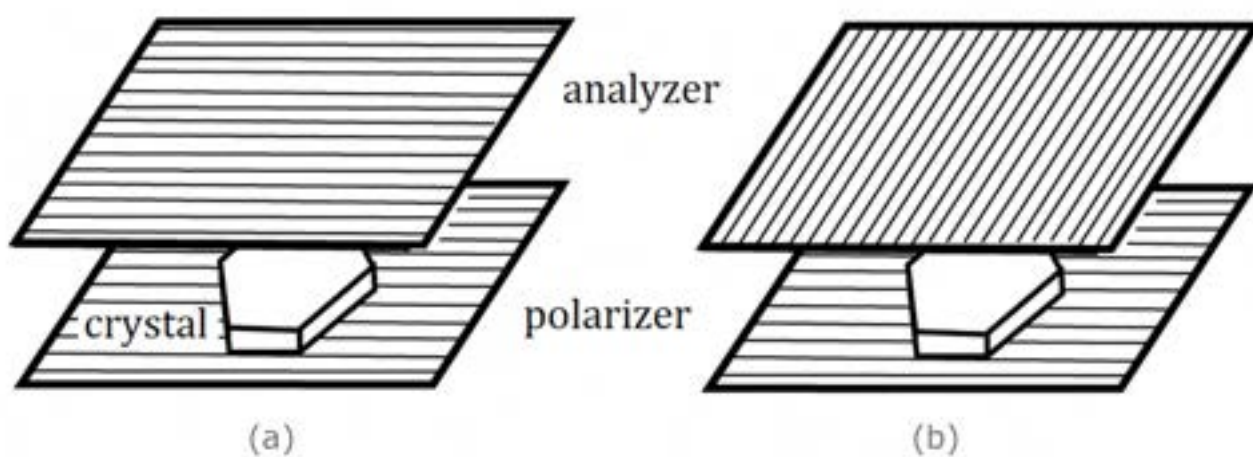


Figure 3. A quartz plate (perpendicular to the c axis) between linear polarized plates (a) parallel (b) crossed.

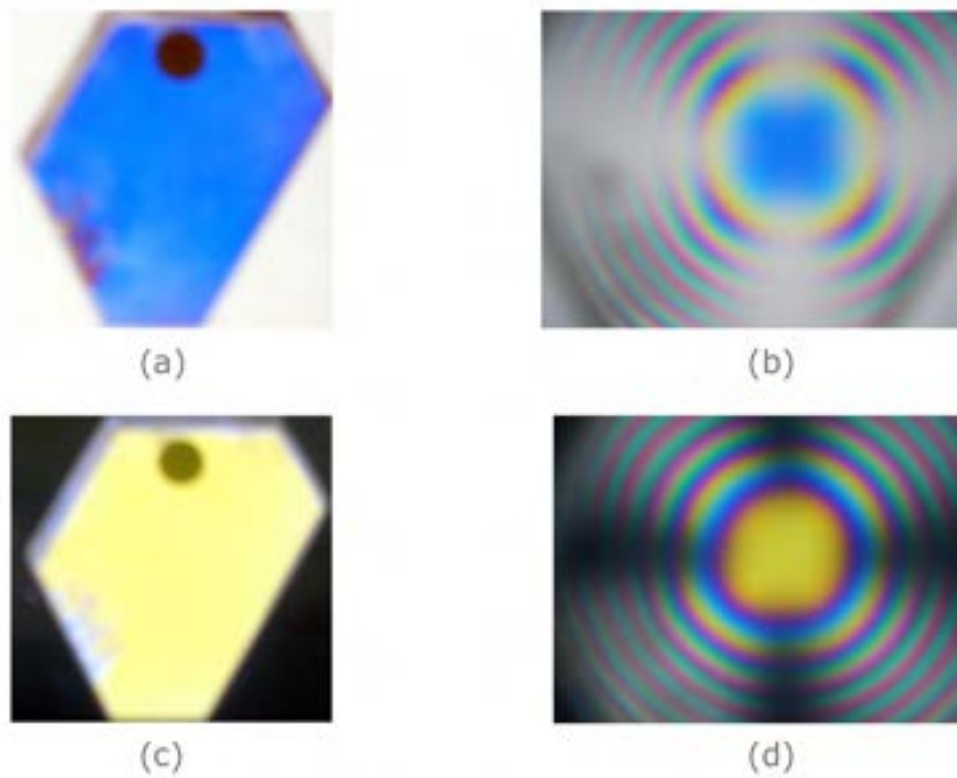


Figure 4. Images of a quartz plate 4 mm in thickness. (a) Parallel polars (b) corresponding conoscopic image (c) crossed polars (d) corresponding conoscopic image.

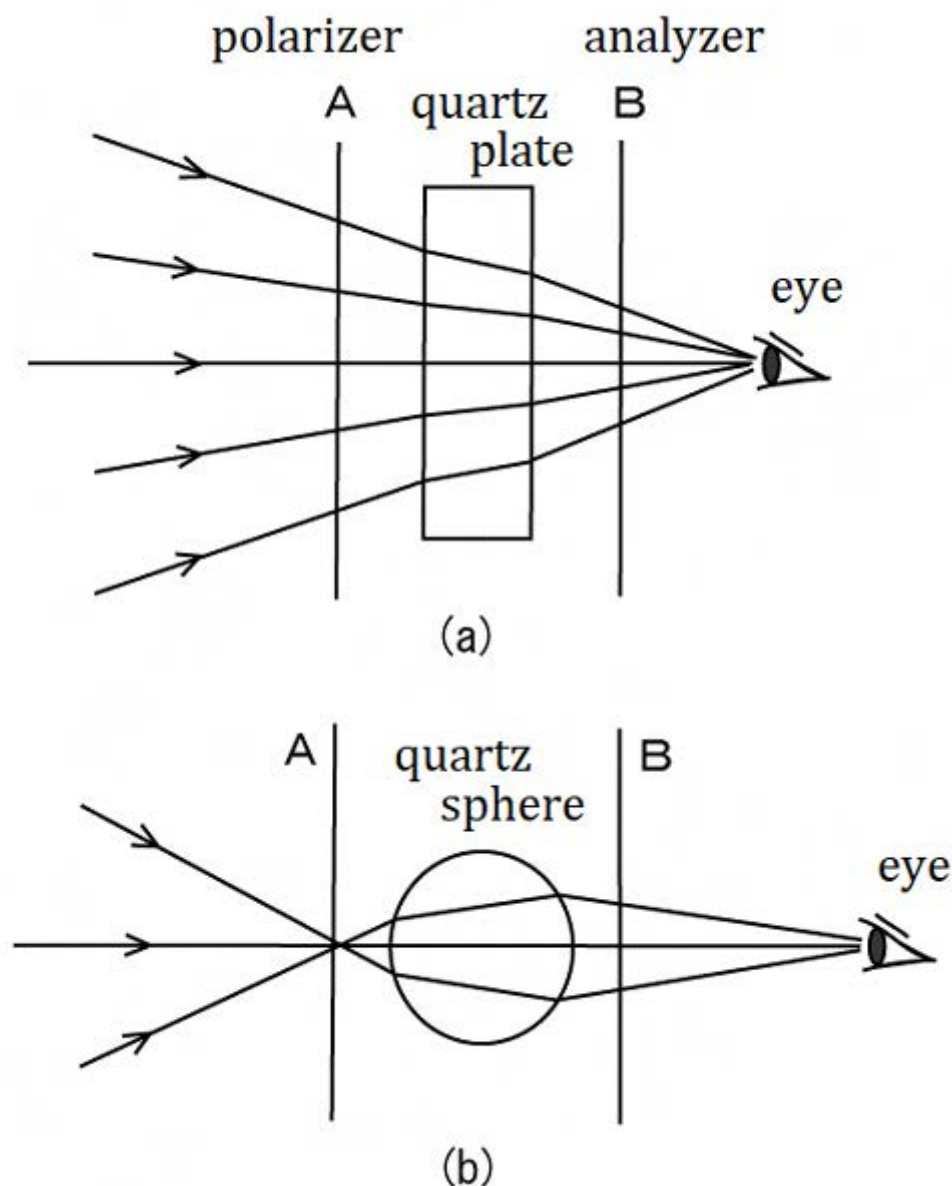


Figure 5. Observation of a conoscopic image by refraction of light through (a) a quartz plate and (b) a quartz sphere.

Quartz is an optically uniaxial material, and the crystallographic c axis is the optical axis. This means that the velocity of light propagating along c in the crystal is independent from its polarization direction. If the quartz crystal is cut into slices perpendicular to the c axis, and a piece is placed between two polarizing plates (Fig. 3), an image of the crystal will appear in a single color (Fig. 4). The color may depend on both the thickness of the crystal plate and the relative orientation of the polarizers. This is due to the wavelength dependence of the specific rotation of quartz, which is optically active in the c direction. The oscillation direction of the polarized light rotates on passing through the quartz crystal, and if the total rotation angle is 90° it will be interrupted by the 2nd polarizer (analyzer) when the polarizers are in parallel, but pass through in the crossed setting. Therefore, different colors appear according to the orientation of the analyzer. When your eye or camera lens comes very close to the analyzer, fringes may appear because farther from the center of the view the light wave has passed through the crystal at a larger inclination angle to the c axis (Fig. 5). The interference occurs because of the birefringence, *i.e.* light of the same wavelength will split into two components with different velocities depending on the direction of oscillation in the crystal, and they will interfere with each other. Furthermore, if the analyzer is changed from a linear to a circular polarizer, the circular fringes become a double spiral known as Airy's spiral after G. B. Airy, a famous astronomer in the UK (Fig. 6). The chirality

of the spiral is related to the optical rotatory power of quartz. One thing to note is that both the right and left circular polarizers are available, but if the analyzer is replaced with the other type, the handedness of the Airy's spiral remains the same although the bright and the dark regions of the interference image are exchanged. For a quartz sphere, Airy's spiral can also be observed when the c axis is directed parallel to the line between the light source and the observer's eye (Fig. 7). Remember that the definition of left and right is important. For Airy's spiral, start at the center, and then trace a curved line of the same color towards the outside. A clockwise Airy's spiral corresponds to right-handed quartz, and an anti-clockwise spiral to left-handed quartz.

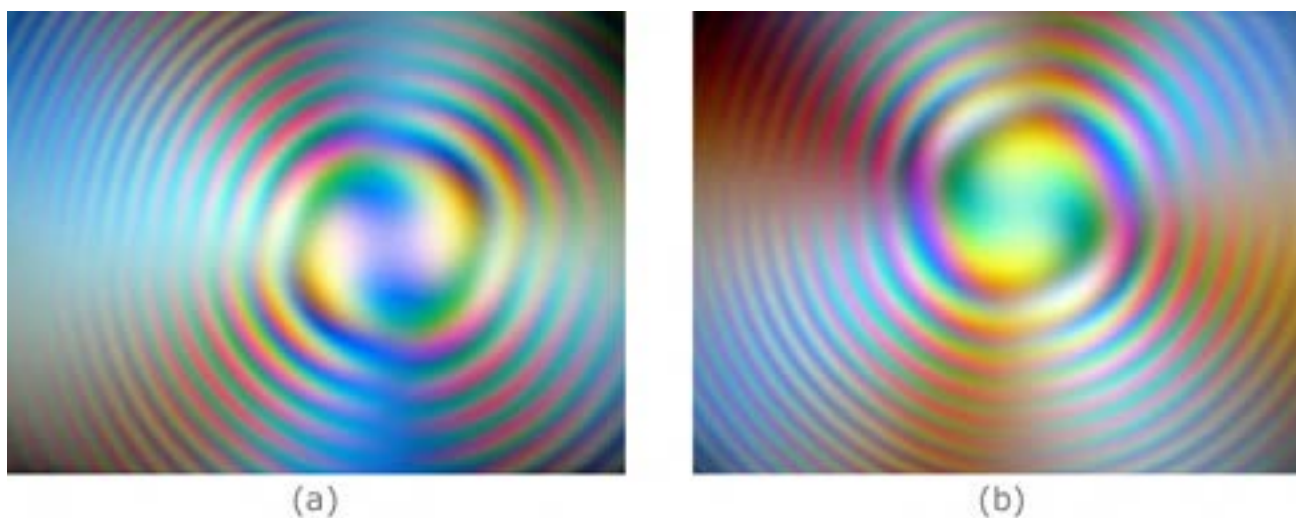


Figure 6. Conoscopic images of a (a) left-handed (b) right-handed quartz plate 4 mm thick using a circular polarizer as the analyzer.

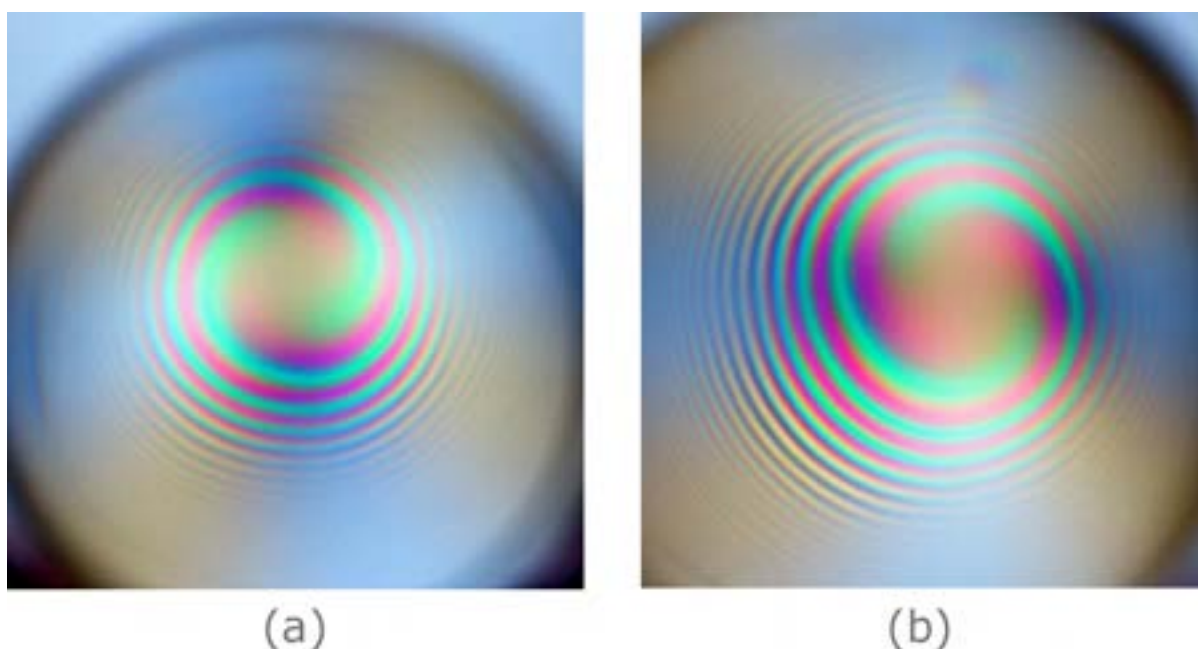


Figure 7. Airy's spiral for a (a) left-handed (b) right-handed quartz sphere 15 mm in diameter.

For an as-grown crystal, its Airy's spiral can be looked at if the specimen is optically clear and the bottom is flat by cutting perpendicularly to the c axis. Mr Yamamoto has developed a neat tool called a point prism (Fig. 8). A circular polarizer and a triangular prism are glued onto a glass pedestal. On the inclined (R or r) face of the quartz crystal, the point prism is placed in contact with a small amount of water, and

polarized white light enters from the bottom of the crystal. Then through the point prism you can see Airy's spiral or part of it for each R and r face, a total of six faces (Fig. 9). The larger the quartz crystal, the sharper the fringes of the spiral. The normal direction of the inclined (R or r) face to the c axis is 51.8° , which is almost compensated by the angle of the prism (45°). The clever trick is that the refractive index of the optical glass is nearly the same as that of quartz, and the light passes almost equally through them. The water at the plane of contact helps to avoid any scattering of light. As shown in Fig. 10, the paths of the waves propagating in a direction inclined by α to the c axis differ from each other. However, the effect of the path difference due to birefringence is the same for small differences in α . This is the reason why Airy's spiral is observed as a circular shape without apparent distortion. Interestingly, if the spiral is observed only for one of the inclined faces, this tells you that the crystal has been cut and polished from a larger crystal to look like a natural crystal of quartz without reference to the axes. I came across such a specimen and learned why it was so cheap for such a huge size!

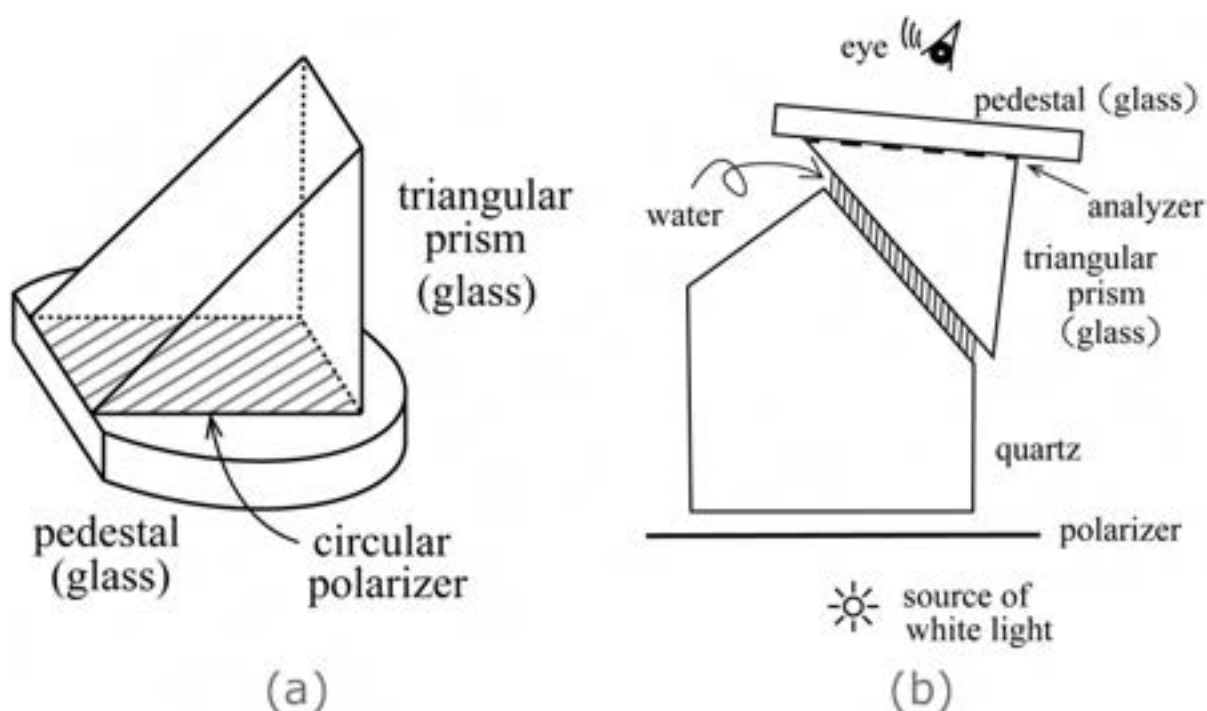


Figure 8. (a) Point prism consisting of an isosceles right triangular prism 3 cm in length and width and a glass pedestal 8 mm thick, and (b) how to use it.

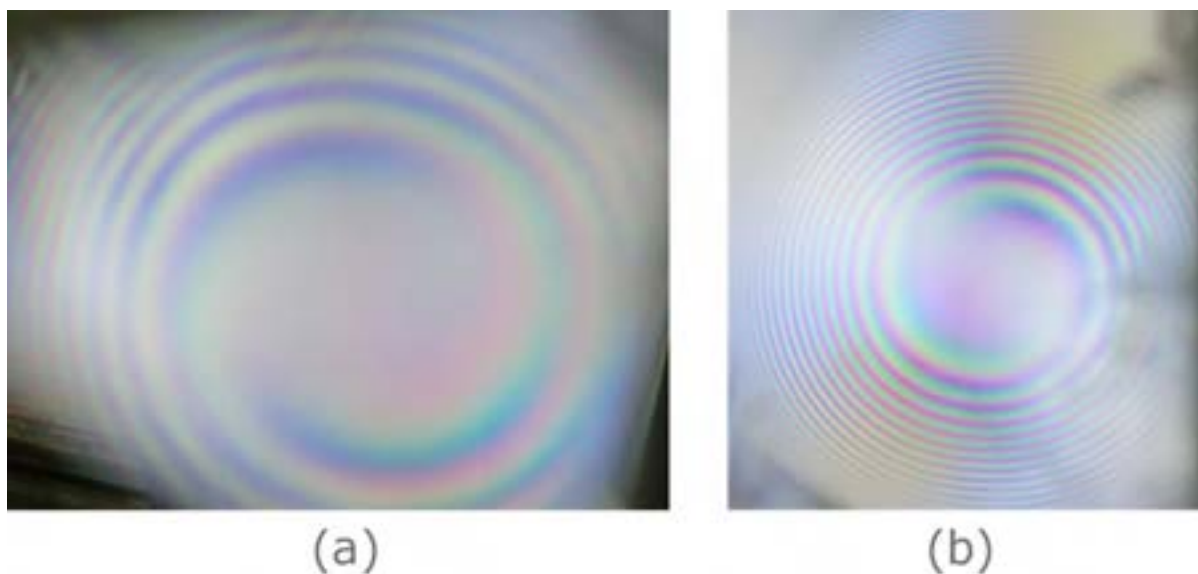


Figure 9. Airy's spiral for (a) left-handed and (b) right-handed as-grown quartz crystals, the bottoms of which are flat perpendicular to the c axis. Sizes are (a) $2 \times 2 \times 3$ cm and (b) $3 \times 4 \times 4$ cm. Photographs taken with a camera lens attached to the point prism.

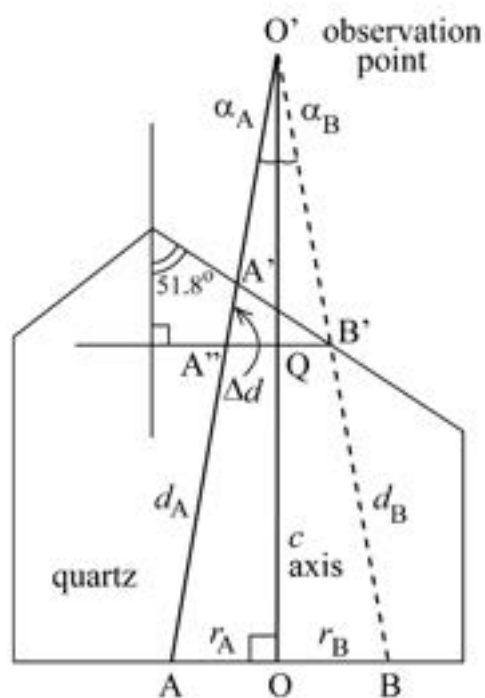


Figure 10. Path differences for light propagating from the bottom of a quartz crystal to an inclined R or r face at the top. When the semi-apex angles α_A and α_B are the same, the path $A-A'$ in quartz is longer than $B-B'$ by Δd .

Lastly, I would like to thank Mr Yamamoto who provided me with the point prisms, and Mike Glazer for encouragement and advice on this manuscript.

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FEATURE ARTICLE

Some humble side-notes on quartz, handedness and possible evolution of the human mind

Wulf Depmeier



Almost the whole of my scientific life I have spent time doing things that other crystallographers do: growing crystals, performing diffraction studies at various temperatures and pressures, determining structures, analysing and interpreting the results, publishing in scientific journals and teaching students. Some 20 years ago, sparked by private relationships, I started to devote a small part of my time and interests to more transcendental aspects of crystals, such as their roles in paintings, sculptures, literature or architecture (but not cinema, I am afraid, and certainly excluding esoterism). In doing so I was lucky to contribute to a small number of expositions. I also gave non-technical public lectures and occasionally wrote short essays. A recent example of such writing can be found in a book devoted to the paintings of Stefanie Kettel (<https://www.stefaniekettel.com/>). Her book has the rather enigmatic title *als wenn sich nach langem warten alle erkenntnisse im kopf zu einer einzigen frage zusammengefügt hätten* (ISBN 978-3-9817475-1-5, © 2017 Trademark Publishing and author). My own contribution to the book, entitled “Kristall und Mensch – Mensch und Kristall”, represents a personal view on the artist’s oeuvre and is an attempt to understand the role of crystalline forms in her paintings and sculptures. For the present short note I have borrowed a few ideas from that essay. Alongside the German version the book contains also an English translation: “Crystal and humans – humans and crystal”.

The last issue of the *IUCr Newsletter* presents a number of very interesting and well-written contributions. Personally I was most attracted by Mike Glazer's Feature Article "[Some musings on crystals of quartz](#)", John Helliwell's interview with Juanma García-Ruiz: "[Wrestling with questions at the edge of science methods](#)", the [Editor's comment on this interview](#) and, of course, Juanma's thoughtful, inspiring as well as provocative essay "2001: The Crystal Monolith", which is available [here](#).

Mike Glazer's Feature Article outlines very nicely some of the most mind-boggling intricacies of quartz, especially the handedness of its structure and optical properties. I always recall with pleasure some of Mike's splendid lectures, especially when he explained the senses of rotation of helical structural motifs of quartz (as shown nicely in his article) and its optical activity by the example of certain helix-shaped pasta. Since then I seem to have developed a mild mental problem, because when eating this food I am always stuck with the question, if the specific noodle turns left or right, and if all the others on the dish do the same. This is maybe the reason why nowadays I prefer long and thin noodles – or rather turn to a much more radical solution such as having pizza instead of pasta, or even mashed potatoes.

In the context of handedness I feel it also appropriate to commemorate the late Howard Flack who liked to puzzle his audience by skilfully dissecting an apple into two homochiral halves [*la coupe du roi*, see *IUCr Newsletter* (2016). **24**(4)]. The mysteries of "left" and "right" have fascinated many people, certainly scientists, but also laypeople and artists, including the Austrian poet Ernst Jandl (1925-2000), who expressed this in a famous poem as follows (ernst jandl: lechts und rinks – gedichte statements peppermints. Deutscher Taschenbuch Verlag, München, 1997):

"Lichtung":

"manche meinen
lechts und rinks
kann man nicht velwechsern
werch ein illtum"

Here each "r" is replaced by "l" and *vice versa*, thus the German "rechts" (English "right") becomes "lechts" and so forth. Wordplays like this are very hard to transfer, let alone to translate, into other languages. The translator of my text in the above-mentioned book offered this version:

"many say
reft and light
cannot be focused
whas a mittake"

Obviously there were not enough fitting words with "r" and "l" to come closer to the German version. Another artist's appealing view of the mysteries of crystals in general and of quartz in particular is Max Ernst's (1891-1976) "Ein Kristall, seine Witwe und sein Kind" (A crystal, its widow and child). A reproduction of his painting can be found on the internet.

As reported by himself, Juanma's article "2001: The Crystal Monolith" was also inspired by an artwork, namely by the movie "2001: A Space Odyssey", directed by Stanley Kubrick. Juanma describes how the basic idea of a crystal served as a metaphor for the general message of the film and how this idea developed during the process of making the film. From this film Juanma seems to have developed his idea that careful visual inspection of the morphology of a special crystal species – here quartz – and the haptic experience of its smooth faces, sharp edges and corners might have triggered the abstract thinking in early human's brains. I certainly agree with Juanma that the discovery, inspection, collection and keeping of certain crystals, particularly quartz, may have played an important role in the cultural evolution of early mankind. However, further below I would like to offer another possible explanation of why in particular quartz crystals could have attracted the earliest human's attention.

First let me slightly object to the argument that “... the world of these early humans was one in which everything visible around them was dominated by curves and irregularities” (from the Editor’s comment). While this is generally true, it is not the whole truth, as Juanma also states in one of his footnotes. Living on the shores of the Baltic Sea at the fjord of Kiel I know from my own daily observation that the horizon separating water and sky appears essentially as a straight line, provided that the state of the sea is not too rough. Likewise, the surface of a dormant lake appears essentially flat. Of course, I gladly admit that a well-shaped crystal is much more than just one straight line or one flat surface.

I fully agree with Juanma that most crystals differ sharply from other natural things as most of them are harder than animal or vegetable tissue and are heavier than water; many crystals are transparent, reflect light, some are fissile and separate along smooth surfaces, some are beautifully coloured. One may note that rotational and reflection symmetry of crystals are not unique to crystals, because many flowers and also animals (see “The Tyger” by William Blake) show symmetry as well.

Altogether, it is the combination of all these characteristics that makes crystals unique among natural things. As an extension rather than a contradiction to Juanma’s arguments based on morphology I would like to offer a slightly different approach for consideration: apart from their special morphology, it is in my opinion the optical properties that make some crystals so special. In particular the reflection of light from smooth surfaces is a very characteristic property of crystals. Qualitatively, mineralogists distinguish minerals by their lustre. Quartz, for example, has glass-like lustre. The lustre of other minerals may be metallic for example, or fatty or silky. In some favourable cases, a given crystal can be cut, polished and thus be made into a gemstone. The lustre, the gleam or especially brilliance give such a gemstone an aura that reaches far beyond its physical reality. In a sense, this interplay of crystal, light and human sense of vision creates something new that, to a certain extent, can be called dematerialised material. Whoever at the opera or a ball has caught sight of the flashing of cut diamonds will agree with this opinion. The relatively cheap glass prisms hanging from a chandelier serve a similar purpose as the precious jewels decorating wealthy ladies or gentlemen. Quartz is a very common mineral, but well-formed jewel-like crystals are less common. At certain locations of the world, perfectly shaped, centimetre-sized, highly reflecting quartz crystals can be found buried in some soft matrix, such as clay or marl, where they have resisted abrasion that otherwise would have transformed them into a rounded pebble if transported in a brook or stream. In some places such crystals can even be found on farmland, preferentially in early spring after ploughing and before vegetation has started to grow. Then after a rain-shower followed by sunshine, these little objects can be spotted from far away by their reflectivity and picked. Often such quartz crystals are then called “diamonds”, specified by the location, *e.g.* “Schaumburger Diamanten” or “Herkimer Diamonds” and the like, and are much sought-after by mineral-collectors. Again, the combination of crystal, sunlight and observer results in an aura and allows the actual crystal to be spotted from quite a distance. Note, the flash effect changes with the angle of sight, *i.e.* with the movement of the observer. Coming back to the early humans, in my opinion, it might be quite possible that the first attraction to quartz crystals was due to their reflectivity, perhaps followed by closer inspection of their morphology. It may well be that the lucky finder might have considered such a crystal as a treasure, he might have believed that its aura gave the owner supernatural power, youth, health or whatever. Perhaps here lies the reason why gemstones in general were so important in many religions or early civilisations.

If the above arguments are accepted then John Helliwell’s question concerning calcite finds an easy answer. Calcite is a quite common mineral too, not much rarer than quartz, and it often occurs as nicely shaped crystals. However, calcite is much softer than quartz and as such it is easily scratched by other crystals, in particular by quartz, or even by ordinary rocks. One could therefore suppose that in pre-scientific times this could have been regarded as an indication of some kind of inferiority with respect to quartz, and therefore the latter would have been assigned a higher status in the transcendental sense. In addition, contrary to quartz, calcite breaks easily and separates into small rhombohedra when dropped on the ground. Some believe that the observation of this cleavage was the starting point for Haüy’s

theory of *molécules intégrantes*. More important in the present context is the fact that while fresh cleavage planes of calcite have a lustre quite similar to that of quartz, the faces of naturally grown calcite crystals often present a dull surface, such that the reflectivity is low and the aura vanishes. This is probably due to the relatively high susceptibility of calcite to water and thus to humidity. Quartz is much more resistant in this respect.

I thank Mike Glazer, Juanma García-Ruiz and John Helliwell for their contributions, which gave me the necessary impetus to write these lines.

OPINION

Open access open for business

Massimo Nespolo



Publication of scientific research results requires a validation process, without which articles would not be more trustworthy than blog posts. Although certainly imperfect, like any human activity, the best validation model we have been able to develop so far is the peer-review process, in which a panel of (at least two) anonymous reviewers (“referees”), solicited by an editor, critically analyse a manuscript submitted for publication. The reviewers' task is to find any possible flaw, mistake or overlooked material in the manuscript that may have gone unnoticed by the authors. It is a well-known fact that authors are often blind to their own mistakes; the good practice of putting a manuscript asleep for a couple of weeks before submission and reading it once again after this rest period helps in seeing that which has escaped at the editing stage. Unfortunately, in the world of “publish or perish”, delaying a submission has become a luxurious practice seldom adopted, especially when working in a highly competitive field.

Publication of reviewed manuscripts was in the hands of scientific not-for-profit societies until commercial publishers understood that it represented a lucrative market and joined the business; this change brought in a revolution in terms of technical handling and customer-oriented approach, but handling of manuscripts was still the responsibility of renowned experts in the field. Access to published manuscripts required one to pay a physical visit to a library. Later on, on-demand copy services were introduced, which eased somewhat the task of getting one's hands on the articles. With the exponential increase in published articles, libraries started to have space problems and had to move older issues of their journals to storage facilities, or to microfilm them. At the same time, the cost of subscription to the ever-increasing number of journals skyrocketed, and the profits of commercial publishers kept on growing. The sustainability of the model began to be questioned. An ever-increasing proportion of the

results of research, funded in most cases by tax-payers' money, finished in the hands of commercial publishers and researchers had to use further tax-payers' money to access these results. Choosing not-for-profit scientific societies like the IUCr would have limited these costs; unfortunately, a vicious circle arose (or rather, was put in place): evaluation of research results and decision of what research to fund moved into the hands of non-specialist politicians who require “objective” criteria in some numerical, easy-to-read form: the journal impact factor is the most visible and best known indicator. Commercial publishers, especially large companies, have enough market power to promote their journals and obtain more visible (“quotable”) articles; once a high-index profile has been established, it is easier to keep on attracting submissions on “hot topics” that preserve the high-index profile. Competition is not easy for not-for-profit scientific societies, although some of them, like the IUCr, RSC and ACS – just to mention a few – do a remarkable job.

With the move to electronic-only publication, the printing costs have been cut down, together with the publication delay. At the same time, the proportion of the job done by the authors themselves has increased. Unlike the IUCr, some commercial publishers do not assure a high-level technical editing process but require files almost ready for electronic archiving. The high costs of the subscription to electronic-only journals that are commercially published are therefore even less justifiable.

This approach has been challenged by the Open Access initiative (formulated in 2002 in the [Budapest Open Access Initiative](#)), which in principle tends to move the costs of scientific publishing from the reader (subscription) to the author. Well before the term “open access” came into use, computer scientists started the practice of self-archiving in anonymous ftp archives; later, physicists followed the same path by using [arXiv](#), a repository of electronic preprints that are accessible to the general public after moderation. This approach has at least two drawbacks: for the community, because “moderation” is by no means a guarantee of quality comparable to peer-review (an extreme example can be seen at the address <https://arxiv.org/pdf/0906.1358>); and for the authors, because a “moderated” (non-peer-reviewed) manuscript is not recognized as a research result. These drawbacks are overcome by the possibility of publishing open-access articles in existing journals, where both classical (subscription or pay-per-article) access and open access coexist, although this practice requires the payment of open-access fees. IUCr journals have been among the pioneers along this route, the first open-access article being published in 2004, with approximately 30,000 open-access articles published up to the end of 2018. In addition to seven hybrid journals, the IUCr today publishes three entirely open-access journals: *Acta Cryst. E*, the high-profile journal **IUCrJ**, as well as *IUCrData*.

The current situation is particularly complex and financially challenging because of the co-existence of the two models (subscription and open access). Libraries still have to pay for highly expensive subscription packages, which represent a very important source of revenue especially for large commercial publishers. At the same time, an increasing number of journals are moving towards an open-access-only submission. Considering the increased number of views that an open-access article receives with respect to a traditional one, and the fact that some high-impact journals have adopted this model, the pressure on researchers to publish in open-access journals is increasing, sometimes to the point of jeopardizing the (constantly shrinking) recurrent research budget (for those institutions that still provide some budget besides the grants for which one has to apply). One may therefore imagine that the solution would be to move to a fully open-access model: the budget currently devoted to library subscriptions would be transferred to paying the open-access fees, possibly saving on the global expenses. Such a simple position does not take into account a serious threat that has arisen with the open-access initiative: predatory publishers.

[Wikipedia](#) has a precise definition for this phenomenon. “Predatory open-access publishing is an exploitative open-access academic publishing business model that involves charging publication fees to authors without providing the editorial and publishing services associated with legitimate journals”. The “editorial and publishing services” mentioned in this definition concern not only the quality of technical editing – which is limited or absent in predatory journals – but especially the peer-review process. The

source of revenue being the open-access fees paid by the authors, each manuscript rejected represents a loss of revenue. Moreover, each manuscript that is delayed because of extensive revisions requested by the referees represents a delay in the payment, aggravated by the risk that the manuscript be withdrawn if the authors realize that they cannot comply with the requested revisions. The temptation to loosen the review process is constantly in the grip of less scrupulous publishers, which, brought to its extreme consequences, leads to by-passing it completely. The lucrative market of academic publishing has therefore been polluted by predatory publishers that accept whatever manuscript is submitted provided that the open-access fees are paid. Such a perverse phenomenon has reached extreme proportions today with the ease of starting an online journal through ready-to-use software packages. One may spend a few hours in browsing the websites of open-access journals and look at the editorial board, often composed of totally unknown people who have no serious publication history in the field, or even at all.

Jeffrey Beall, a librarian of the University of Colorado, set forth criteria for categorizing publications as predatory and maintained a list of predatory journals. He was forced to take his list offline in January 2017, owing to serious legal threats by publishers appearing in his list. The list, however, has been taken up again and is now maintained “by an independent group which wishes to remain anonymous in order to avoid the harassment suffered by the creator/maintainer”: it is available at the address <https://predatoryjournals.com/publishers/>. Other initiatives to keep track of predatory publishers exist as well, like the [Flaky Academic Journals](#) website. Unfortunately, not only are these lists not (yet?) officially considered as a reference by the academic authorities, but the most dangerous predatory publishers succeed, with a clever strategy, in remaining borderline outside the list, as we are going to see: I will call them “insidious publishers” hereafter, for the sake of brevity. I will not try to mention any of these explicitly to avoid enduring what Jeffrey Beall had to suffer, but I am confident that most readers will easily recognise the targets. Before going more into depth, however, it is interesting to point out that several researchers have attempted, and sometimes have succeeded, in trapping predatory publishers by submitting completely nonsensical or even hoax manuscripts, that were accepted without any review process. A famous example is that of the Star Wars Hoax Paper, where mitochondria were called “midichlorians”: extensive quotations from George Lucas movies were included in the manuscript, and a large number of fake references were provided as “literature”, attributed to non-existing authors whose names are simply characters from the galactic saga. Hard enough to believe, the hoax manuscript was published in four journals. It has since been taken off-line but I could download a copy before it disappeared: for those who are curious enough to see how huge the hoax was, the file, with the Star Wars references highlighted, is now available at the address <https://frama.link/dq1A1WGQ>.

An opposite approach with respect to the predatory publisher list has been adopted by the DOAJ ([Directory of Open Access Journals](#)), which defines itself as “a community-curated online directory that indexes and provides access to high-quality, open access, peer-reviewed journals”. However, as clearly stated in the top page of the directory, “All funding is via donations, 40% of which comes from sponsors and 60% from members and publisher members”. Among the sponsors one can see institutions and publishers that are above any possible suspicion; but there are also a number of insidious publishers. As Henry Louis Menken wrote, “It is a sin to believe evil of others, but it is seldom a mistake”. Initiatives like DOAJ should be encouraged, but one needs to ensure that they remain completely independent in their assessments of journals.

Let us finally analyse how the insidious publishers succeed in sneaking into the market and what are the potential long-term consequences of their practice. The strategy of remaining outside the blacklists exploits a fundamental defect of the scientific mind: most scientists are fundamentally too trusting, inclined to think that their environment, colleagues and co-workers are basically honest and motivated by intellectual curiosity and rigour, which unfortunately is not always the case. The attitude “innocent until proven guilty” that we more or less unconsciously adopt as a *forma mentis* is being exploited by

dishonest commercial practices, against which the opposite attitude “guilty until proven innocent” should be mandatory.

An editorial board composed of upright scientists would mean a high rate of rejection of low-quality manuscripts, and therefore a limitation on the source of open-access fees. An editorial board composed of unscrupulous characters playing a fictional role would mean that every manuscript submitted goes online and provides a source of revenue to the publisher, but at the same time would also be a short-cut to the blacklist of predatory publishers. Insidious publishers smartly exploit a mix of the two to maximize the economic benefits while remaining borderline outside the blacklists. Concretely, the strategy adopted can be described as follows. The editorial board is composed of three types of editors:

1. confirmed scientists, who seldom if ever receive manuscripts: their role is to bestow a certain degree of prestige to the journal; they are victims of the “innocent until proven guilty” syndrome;
2. young scientists, who see their role as an opportunity to boost their CV; these are fundamentally honest people who, however, lack the necessary experience for a critical handling of manuscripts and are unable to resist the pressure by the publisher to let dubious manuscripts go through the review process, even when the reviewers’ reports are less than positive;
3. non-entities on the publisher’s payrolls, who just play a role.

This is, however, not sufficient to grab a significant part of market: some degree of recognition is necessary, in particular to obtain a more than negligible impact factor. To reach this target a simple but effective strategy is put in place: special issues in the hands of guest editors. Some of these special issues are entrusted to well-known scientists, who are unaware of the flaws of the journal. For other special issues, young and less-known scientists are recruited, exploiting the same psychobiological mechanism used for the editorial board: flattery and the chance of CV-boosting. As for every special issue, editors are responsible for finding contributing authors. Invitations coming from well-known colleagues are a gauge of seriousness; waiving of open-access fees is even offered in some cases: the lack of revenue from those manuscripts is a sacrifice to build a reputation whose return on investment eventually pays off. When the invitation comes from unknown names with minimal publication records in the field, suspicion should be mandatory; the “innocent until proven guilty” flaw acts more than one would expect, but not enough to allow a complete success of the strategy. As a result, several special issues of these journals are closed with a ridiculously small number of contributions: sometimes not even a single manuscript appears after the deadline. If you keep an eye on the list of special issues, you will realize that those which failed to attract any contribution at all suddenly disappear, as if they never existed.

In some cases, experienced guest editors, who had seriously done their job, discover that manuscripts they had rejected have actually been published. Some authors see their submitted manuscript accepted in a couple of weeks, without even getting any review report. Reviewers for other serious journals discover the manuscript they had rejected appears online for these insidious journals a few weeks later, without any change with respect to the version that had been rejected (personal experience). It goes without saying that in a journal where practically everything is accepted, one finds also good articles by serious authors who are unaware of the predatory behaviour of the publisher. These authors are, however, sometimes guilty of refusing to see the evil even when others warn them. On more than one occasion I have tried to raise colleagues’ awareness about the dangers of contributing to such a scheme, but only in a few cases have these efforts been successful. After all, if their manuscript is worth publishing, what is the problem in choosing a journal that also possibly publishes some rubbish? It is that by contributing to those journals, these authors bring them a patina of respectability that allows the publishers to remain borderline outside the blacklists, to gather more manuscripts that could and should have gone to established journals, and to inflate their market. In the long term, the consequences could be much more serious. Somebody might think that the following analysis is simply a dystopian illusion; they are unwitting victims of their naive syndrome.

Public research is funded by tax-payers' money. Funding agencies require fulfilment of various criteria for a research project to be funded; among these, potential benefits for society, but also a guarantee of quality and reproducibility of results. Predatory publishers are seriously jeopardizing the system, with their dishonest commercial practices. Once the trust in the academic publication is lost, there will be no reason to spend tax-payers' money to pay open-access fees. This may eventually result in a collapse of the open-access system itself; or may even seriously threaten academic publication as a whole. In fact, once serious and legitimate doubts are cast onto the credibility of the results appearing in publications that have somehow gained a veneer of respectability, the whole world of scientific publication can easily be discredited. At that point, predatory publishers will simply move away from a market that is no longer lucrative and invest in some other deceptive activities. There will then not be any reason for them to maintain the infrastructure where their online journals were published. The whole database of their publication may therefore disappear into the world of paperless publications; in this case everything is lost forever, not only the huge amount of rubbish that went through, but also the legitimate publications by scientists who have been too unaware to even consider such a possibility. This could not happen with not-for-profit publishers like the IUCr, or major established publishing companies. But even if such extreme, catastrophic consequences are not reached, once the model of scientific publication as we know it today is discredited, nobody can predict what the consequences are going to be.

Before such a dystopian future becomes a dark reality, we have a moral duty to alert especially the younger generations to how to avoid the traps of predatory and insidious publishers. Without any pretence of being exhaustive, we can provide at least some simple guidelines to be taken as good-sense “rules of the thumb”:

1. Small commercial publishers, with a short history, should be carefully scrutinized before submission of manuscripts.
2. Publishers located in developing countries may not have the financial and technical solidity for sustainable business: a number of predatory publishers have their HQ in those countries.
3. Special attention should be paid to publishers whose HQ is in a developed country but whose representatives and technical staff are either in developing countries or in countries that have an established reputation of forgery.
4. Journals with a long list of editors who have no reputation in the field are particularly suspect. It is easy to check this by going to the journal's website and ask yourself: how many of these people are known to you?
5. Journals publishing a large number of special issues with very few, if any, articles, are probably issued by “insidious publishers”, if not recognized predatory publishers.
6. Being invited to join the editorial board of a journal, or act as guest editor, at the beginning of one's career, before even getting some reputation in the field, does not necessarily mean that your first publication(s) have earned the spotlight: more likely, it is the result of a robot-scan of recent journal issues. Established scientists receive multiple invitations of this kind per day and are obliged to use spam filters to get rid of them.
7. A published article normally shows the manuscript history (if it does not, the journal has to be considered as highly suspicious). A too-short interval between submission and acceptance is clearly a bad sign. With some rare exceptions, reviewing a manuscript takes time: the reviewers have to read the manuscript, possibly some of the literature cited therein, check the experimental data or the equations or the flow of reasoning, and all this while attending their normal duties (lectures, meetings, writing their own articles...). A quick report submission by one reviewer sometimes occurs; by both reviewers of the same manuscript it is rare; by both reviewers of many manuscripts it is unrealistic and should raise suspicions. An average of – say – a 10-day review process for a journal simply means that the reviews are either non-existing or superficial and untrustworthy.

Insidious publishers have also started sponsoring small meetings and schools as a way to buy some credibility. Is that philanthropy? The amount of money they spend on having their logo on the event website, and to have the right to have their leaflets exposed during the event, is often inferior to the open-access fees of a single manuscript. One submission from a participant would be enough to cover the expenses. But even if no immediate economic gain is obtained, the return on investment in terms of image is more than worth the small contribution. Organizers of these events should be aware that by accepting this type of sponsorship, they indirectly contribute to feeding the parasite that is seriously threatening the world of academic publication as we know it.

IUCr ACTIVITIES

IUCr Gender Equity and Diversity Committee



The IUCr is proud to announce the formation of a Gender Equity and Diversity Committee (GEDC). The GEDC aims to address issues and establish new practices and policies to overcome inequity in the IUCr's processes. For instance, it will endeavour to ensure that the gender balance of invited speakers at IUCr Congresses reflects the community at large and that IUCr-sponsored events are welcoming and accessible to all those who wish to attend. The Committee's full terms of reference can be found [here](#).

The Committee will consist of two members of the IUCr Executive Committee and up to 10 other members who together represent the crystallography community across career stage, scientific speciality, gender and geography. The current Committee is as follows:

Jenny Martin, Chair (IUCr Executive Committee member, Australia)

Sven Lidin (IUCr President, Sweden)

Natalie Alvarez (Uruguay)

Ruchi Anand (India)

Christine Beavers (UK)

Annalisa Guerri (member of the IUCr Calendar Committee that awards funding for crystallography conferences, Italy)

Genji Kurisu (Japan)

Helen Maynard-Casely (Australia)

Claire Murray (UK)

Bernie Santarsiero (USA)

Eddie Snell (USA)

Michele Zema (IUCr Executive Outreach Officer)

Professor Martin said she was absolutely delighted with the response to the Expression of Interest call. "Now we can really start to make things happen", she said, adding "Given the world we live in now, the time is ripe for the IUCr to lead the way, to develop best-practice inclusive actions, and to implement these across its global scientific community."

If you have any issues you wish to raise, please contact [Jenny Martin](#).

IUCr ACTIVITIES

The IUCr Online Dictionary of Crystallography

Gervais Chapuis Carolyn P. Brock



Gervais Chapuis advertising the print version of the Online Dictionary in a lecture on crystallography at the EPFL.

The main purpose of the IUCr Online Dictionary of Crystallography (ODC) is to give the most appropriate definitions of crystallographic terms and concepts that are found in the scientific literature. The Dictionary is maintained as a wiki, *i.e.* a website where individuals can create, modify and improve the content of the website directly from the browser. From the beginning it was important for the IUCr to ensure that the definitions listed in the ODC are in line with those used throughout the IUCr publications and in particular, the *International Tables for Crystallography*.

With this objective in mind, the ODC was conceived in 2005 by Professor A. Authier, head of the IUCr Commission on Crystallographic Nomenclature at the time, and placed under his direction. The aim was to ensure that the contributing authors are *bona fide* crystallographers with sufficient expertise to contribute to the ODC.

Currently, the number of definitions amounts to 307 (early 2019) covering a broad spectrum of topics including basic definitions concerning crystals and crystalline structures, symmetry, diffraction, diffraction methods, twinning and more. There are, however, a number of domains for which more definitions are needed. For example, the field of powder diffraction is under represented. Active fields

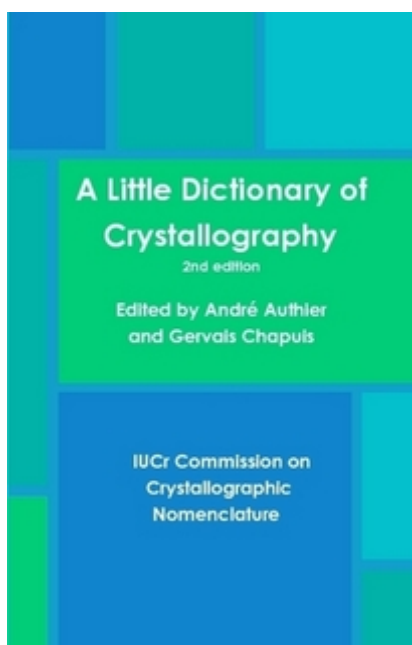
subject to new developments, e.g. synchrotron radiation, diffuse scattering, X-ray spectroscopy and electron diffraction, need to be better covered!

Evolution of definitions

The advantage of the wiki is that definitions can always be improved or changed depending on new discoveries or publications related to a specific topic. In addition, different authors can have different points of view on the same definition and here the arbitration of the Commission on Nomenclature can play a role. For example, a recurring point of discussion concerns the definition of a crystal. The classical definition of a crystal *i.e.* ‘a periodic array of atoms or group of atoms packed along the three space dimensions’ was accepted for nearly a century. In the 1980s, however, the discovery of aperiodic crystals (including the Nobel Prize winning discovery of quasicrystals by Dan Shechtman) resulted in a paradigm shift and required a generalization of the definition. The currently admitted definition of a crystal is that of ‘a material which exhibits essentially a sharp diffraction pattern’. Not everyone seems to be happy with this definition because a diffraction experiment has to be done on the sample before it can be declared a crystal! Could we perhaps define a crystal as a material with long-range order? As mathematicians have shown (Grimm, 2015), the problem with this proposal is that the concept of long-range order can only be dealt with by applying an autocorrelation function on some image - a request that is most probably no easier to obtain than a diffraction pattern! The example of the crystal definition is by no means an exception. The definition of “Miller indices” has also evolved lately owing to recent studies on the subject.

Another problem term is "polymorph" (or "polymorphism"). While there is agreement among experts that polymorphs must have the same composition, there is disagreement about how different the structures must be. One group of crystallographers believes that a different cell means a different polymorph. Another group would exclude pairs of structures that are related by a T- or P-driven phase transition during which the crystal remains single. At the time of writing, the definition in the ODC is sufficiently general to encompass both viewpoints.

The printed version of the ODC



It is now possible to obtain at a very modest price a pocket-size paper edition of the ODC, published by the IUCr. This edition gives the list of all crystallographic definitions at the time of the printing. It can be obtained [here](#).

New contributing authors

We would like to use the opportunity offered by this *Newsletter* to persuade potential authors to increase the number of definitions covered by the ODC. They should not refrain from proposing new definitions even if they feel they are not authorities in the field. The basic principle of a wiki will play its role as other authors will make amendments, improve the definitions or even start a public discussion in the forum associated with the wiki. Such a procedure can only make the ODC more attractive to a larger base of users.

The procedure for new authors is very straightforward. You simply go to the [main page of the ODC](#) and create a personal account in order to create new definitions. You have to of course identify yourself by a recognizable name, in the form FirstnameName. The second step is to send an email to the [Editor-in-Chief](#) in order to be given 'author' permissions within the ODC system. It is of course highly recommended that authors are also registered in the [World Directory of Crystallographers](#).

Once you are ready to create or upload a new definition, just add the new terms as headwords in the alphabetical list under the corresponding capital letter in the main page. The system will create a new page named according to the headword; you may then edit this newly created page to introduce the definition of the new term. The wiki editor is quite powerful. Equations can be introduced in Latex format in the form latex equation , figures can also be included. All the editing tools to create URL links or refer to other articles in the ODC can be easily accessed. The best way to start editing would be to get inspiration from already existing definitions.

More specific instructions for authors, a lightweight style guide and a sandbox for experimentation can be found [here](#).

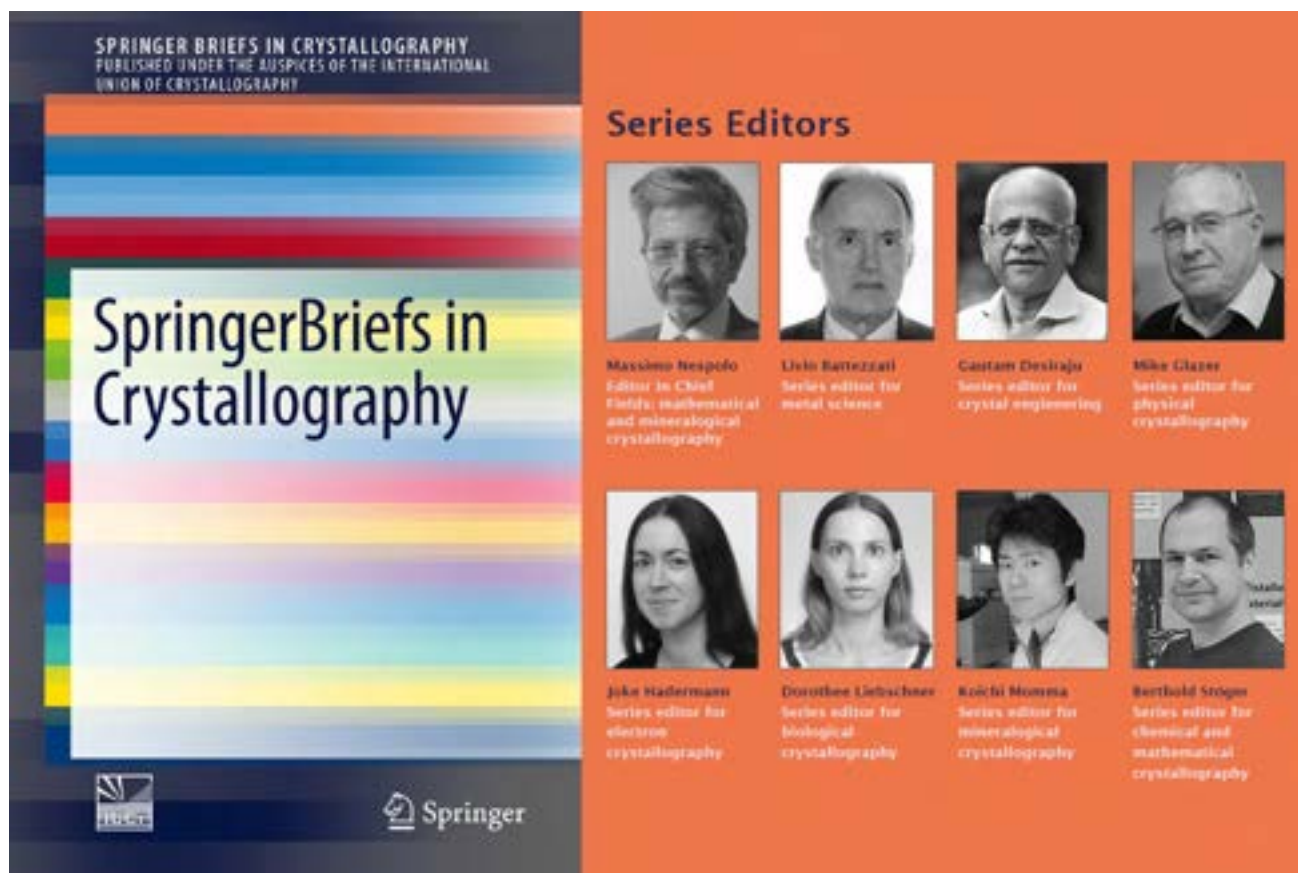
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IUCR ACTIVITIES

SpringerBriefs in Crystallography

Massimo Nespolo



It is my pleasure to announce the launch of a new series of crystallography monographs under the title *SpringerBriefs in Crystallography*. They cover a new discipline within the *SpringerBriefs* series, which publishes concise monographs with an intermediate scope. *SpringerBriefs* already covers 84 fields, spanning a wide range from natural sciences to law, social sciences and more; crystallography is now the 85th field.

The new series is published under the auspices of the IUCr and all the manuscripts will be peer-reviewed by the series editors, as well as external reviewers when necessary. It fills the gap between articles published by the IUCr journals and full monographs.

The IUCr publishes several types of articles in its [journals](#):

- Research Papers, which are full-length manuscripts that normally do not exceed 15 journal pages (about 15 000 words)
- Short Communications, for the presentation of topics of limited scope or for preliminary announcements of novel research findings
- Lead Articles, authoritative, comprehensive and forward-looking reviews of major areas of research interest (by invitation)
- Feature Articles, focused surveys covering recent advances in an area of current research, which do not aim to be comprehensive, and are generally about ten journal pages (10 000 words)

- Topical Reviews, which aim to capture the current trends of a field and are expected to be relatively short (about 6000 words and a maximum of 50 references, with half of those having been published in the last three years)
- Letters to the Editor, which may deal with non-technical aspects of crystallography, its role, its propagation, the proper function of its Societies etc.
- Scientific Commentaries, which discuss articles of particular importance for the readership of the journal.

Full monographs spanning hundreds of pages are published in the IUCr/OUP monographs, and textbooks in the IUCr/OUP texts (<https://www.iucr.org/publications/iucr-oup>).

SpringerBriefs in Crystallography aims at publishing shorter monographs, typically between 50 and 125 pages, where specific topics are dealt with more in detail with respect to what one could do in a Lead Article or Topical Review, in particular with a more pronounced accent on the background. Also, more space is given to some fundamentals, which would not find a place in a Lead Article or Topical Review, with the aim of providing the reader with a more pedagogical introduction (whenever suitable) without the need to look for it in a separate text. Publications in this series help support the [IUCr Outreach and Education Fund](#).

The website of the new series is available [here](#), where you can find more details as well as the responsible editor contact information who, upon request, can provide you with a proposal form. On submission, the responsible editor will then forward it to the series editors for discussion and approval.

Please feel free to forward this information to your colleagues who may be interested in publishing a monograph in this series.

IUCR CONGRESS

25th General Assembly and Congress of the International Union of Crystallography

Radomír KuželIvana Kutá Smatanová



IUCr2020 core organising team during the exhibition at ECM31 in Oviedo, Spain, in 2018. From the left: Ivana Kutá Smatanová (IPC Chair), Radomír Kužel (Congress Chair), Martin Haloun (PCO Auletris) and Pavlína Řezáčová (Chair of the Local Organising Committee).

About the Congress

Modern crystallography is an interdisciplinary subject covering structural biology, pharmacy and chemistry as well as physics and materials science. It includes the study of protein structures and also the crystal structures and microstructures of minerals, new functional materials, nanoparticles, bulk materials, thin films *etc.* It is interested also in the relationship between the structure and function of materials. Development of instrumental techniques including large facilities – XFELs, synchrotrons and neutron sources – as well as continuous improvement of laboratory equipment allow the investigation of structural changes under extreme conditions such as high and low temperatures, high pressures, time-resolved studies, different *in situ* experiments in external fields (magnetic, electric) or chemical reactions. The core methods of modern crystallography are X-ray and neutron scattering, but in recent years electron diffraction and microscopy, NMR and different spectroscopies have become of increasing interest.

The 25th anniversary IUCr Congress will complete one era of these Congresses, which started in 1948.

About the Programme

The Congress programme is prepared by the International Programme Committee (IPC) representing mainly the [IUCr Commissions](#), which are also the main focus of the Congress.

All the organisers and the IPC will do their best to set up an attractive programme covering the latest advances in crystallography and related sciences to attract both young and senior scientists as well as companies.

The IPC meeting will take place on 15-16 May 2019 in Prague and will be introduced by a one-day workshop entitled "Current Trends and Future of Crystallography". The decision to organise such a meeting came about for several reasons. This will be an anniversary congress and it is worthwhile creating some summary on this occasion. All the IUCr Commissions were asked to submit a text with highlights in their fields and possible considerations for the future. This will be presented in the workshop as short talks by Commission representatives in the IPC. This should also help the IPC members to understand crystallography in a broader sense and not just confine themselves to their own topics at the IPC meeting.

The inauguration of the Congress will take place on the evening of 22 August 2020 followed by seven full days of scientific sessions, at most 8-9 in parallel. The closing ceremony will take place on the evening of 29 August 2020. Workshops (half and full day) can be held on 21-22 August and also on 30 August, after the Congress. There are two equivalent web sites: www.iucr2020.org and www.iucr25.org where more information, links and photos can be found.



About the Organisers

The main organiser of the Congress is the [Czech and Slovak Crystallographic Association \(CSCA\)](#). This association publishes its own crystallographic journal *Materials Structure* and organises annual meetings. The CSCA has organised several international conferences in the past. It began a series of Size-Strain meetings in 1995, and organised the European Crystallographic Meeting (ECM-18 in 1998, with 1200

participants), the European Powder Diffraction Conference (EPDIC-IX in 2004, 330 participants), XTOP - the X-ray topography and high-resolution conference (2004 in Prague, 2016 in Brno, 150 participants), Aperiodic 2015 (Prague, 130 participants) and the International Conference on Crystallization of Biological Macromolecules (ICCBM-16 in 2016, 200 participants). During these meetings, we succeeded in putting together an organising team of enthusiastic colleagues and volunteers, who now have invaluable experience. Because of its size, the Congress is being organised in close cooperation with PCO [Auletris](#).

About Prague and the Prague Congress Centre

We are inviting crystallographers from all over the world to Prague, the capital of the Czech Republic and one of the principal European cities with a long history. Its original medieval monuments are attractive to visitors from any part of the world and its modern infrastructure makes it easily accessible and friendly. The Congress will take place in the modern and well-equipped [Prague Congress Centre](#), which has already hosted several large congresses, the largest of which were the NATO Summit in 2002 (8000 participants), the Annual Meeting of the International Monetary Fund and World Bank Group (17,000 participants) and some international medical conferences. The Centre has five halls for 400-3000 people and 8 rooms with a capacity of about 100 people. The total number of meeting rooms is 50 and the exhibition space covers 13,000 m². The conference centre is located within walking distance of the city centre and offers a magnificent view of the historical part of the city, including Prague Castle.



A view of the Prague Congress Centre showing the poster area on the left and the exhibition area looking over Prague on the right.

Prague has an accommodation capacity of about 100,000 visitors. There are almost 800 guest rooms in 4 or 5 star hotels in the immediate vicinity of the congress centre. Many other hotels and dormitories in all categories and prices from 20 to 200 EUR per day are easily accessible *via* public transport in less than 30 minutes. Our frequently running and comfortable Metro ensures very fast transport from any part of Prague.

Crystallography has a long and rich tradition in the region of the former Czechoslovakia. It was cultivated under the auspices of two principal Czech scientific organizations, Charles University (founded in 1348) and the Academy of Sciences (formerly the Academy of Sciences and Arts, founded in 1770). During his stay in Prague (1600-1612), the famous astronomer Johannes Kepler wrote a paper *On hexagonal snowflakes*. This work is the oldest written document of the new era of crystallography and deals with the outer symmetry seen in the morphology of crystals as a reflection of the inner symmetry of matter, without any idea about the nature of the building elements at that time. Ivan Puluž developed an X-ray emitting device in Prague as early as 1881, and it was in Prague that Friedrich Reinitzer discovered liquid crystals.

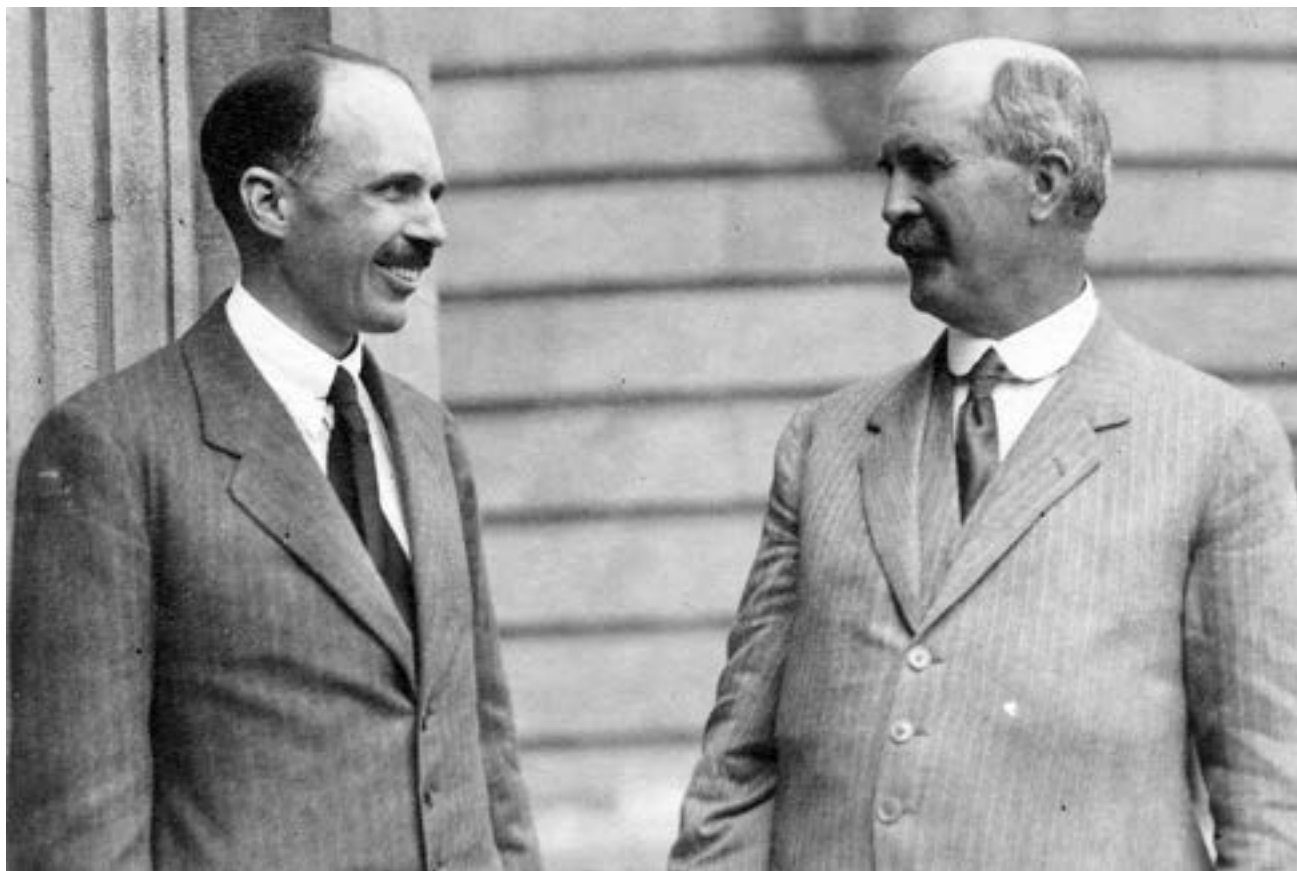
We look forward to welcoming you to Prague in 2020!



A view from the Prague Congress Centre.

AWARDS AND PRIZES

W. H. & W. L. Bragg Prize



William Lawrence Bragg (left) and William Henry Bragg. Credit: Smithsonian Institution Archives. [Image # SIA2007-0340](#).

In 2017 the IUCr established a prize in the name of the father and son team William Henry and William Lawrence Bragg, who pioneered the scientific discipline of X-ray crystallography, and shared the Nobel Prize for Physics in 1915. W. L. Bragg was only 25 at that time and he remains the youngest Nobel Prize recipient in any scientific discipline.

Although most scientific awards are made to well-established scientists, the W. H. & W. L. Bragg Prize will be awarded to up to two promising early-career crystallographers. This is very much in line with the characters of the two Braggs, who actively encouraged young scientists, both women and men without discrimination, to pursue a career in crystallography. Their encouragement resulted in many young crystallographers achieving considerable distinction, including the Nobel Prize winners Dorothy Hodgkin, Max Perutz, John Kendrew, Francis Crick and James Watson.

The W. H. & W. L. Bragg Prize will be awarded at IUCr Congresses, the first in [2020 in Prague](#), Czech Republic. The awardee(s) will receive a certificate and a financial reward, and will be invited to make a presentation at the Congress on a topic related to the prize citation.

Research achievement relative to opportunity will define the eligibility of candidates for this award. For this purpose an “early-career researcher” is defined as one who received their PhD no more than 10 years before the closing date for nominations. Academic interruptions, including periods of parental leave, will be taken into account if clearly indicated in the letter of support accompanying the nomination. A current Curriculum Vitae and relevant details of the nominee’s research publications should also accompany the nomination. The Selection Committee is as follows:

Elena Boldyreva, Chair (Russia)

Susan Bourne (South Africa)

Kenneth Harris (UK)

Cora Lind (USA)

Mark Spackman (Australia)

Michiyoshi Tanaka (Japan)

Manfred Weiss (Germany)

More information about making a nomination for the First W. H. & W. L. Bragg Prize will be available on the IUCr website or from the [IUCr Executive Secretary](#).

OUTREACH

Winners of the 2018 IUCr Crystal Growing Competition



A team from Wellspring High School, Hanoi (Vietnam) who won the bronze medal in the 15-18 year old category for their video “DNA of Rosalind Franklin”.

Continuing the success of the crystal growing competition that launched during IYCr2014, we are delighted to announce the winners of the 2018 IUCr Crystal Growing Competition.

Schoolchildren were invited to convey their experiences of growing crystals through a video. The entries were judged on their creativity, aesthetic value, description of the working plan and experimental work, clarity of explanation, scientific background, and safety by an international panel. The winners, who will receive a certificate and medal, are as follows:

Category: 15-18 - GOLD: Wellspring High School, Hanoi (Vietnam); SILVER: Colegio de Jesús, Salta (Argentina); BRONZE: Wellspring High School, Hanoi (Vietnam)

Category: 11-15 - GOLD: IES Antonio de Mendoza, Alcalá la Real, Jaén (Spain); SILVER: Sint-Barbaracollege, Gent (Belgium); BRONZE: Wellspring Secondary School, Hanoi (Vietnam)

Honorary mention for 12-18 year old pupils: Colegio Santa Ana, Zaragoza (Spain)

Honorary mention for the best use of Personal Protective Equipment: Centro de Estudios para Sordos, Valparaíso (Chile)

and the winning videos can be watched [here](#).



The [2019 IUCr Crystal Growing Competition](#) is now open. The deadline for submission of videos is **17 November 2019**. Please note that videos submitted to local competitions during 2019 may also be submitted to the IUCr competition.

MEETING REPORT

FEBS practical crystallization course "Advanced methods in macromolecular crystallization VIII"

Pavína Řezáčová Ivana Kutá Smatanová



Group photo in front of the course venue.

The [FEBS practical crystallization course "Advanced methods in macromolecular crystallization VIII"](#) was held from 10 to 16 June 2018 and attended by 38 participants from European laboratories and 30 outstanding lecturers and tutors from Europe and North America. This course is becoming a tradition: it has been organized biennially since 2004 at the Academic and University Center in Nove Hrad, a small town in the southern part of the Czech Republic, a few kilometers from the Austrian border. The venue is a historical and stylish chateau surrounded by parkland and housing many lecture halls, festive poster halls and laboratories, which provide a unique opportunity to organize all of the course activities such as lectures, discussions, lab exercises, the social program and accommodation under one roof.



In the lab: seeding experiments under the supervision of Terese Bergfors.

The course was organized by Ivana Kuta Smatanova (University of South Bohemia) and Pavlina Rezacova (Czech Academy of Sciences) under the main sponsorship of the Federation of European Biochemical Societies (FEBS). Participants, mostly students and postdocs, were introduced not only to the theory but also to the practical aspects of standard and advanced methods of protein crystallization: morning lectures were supplemented by afternoon practical sessions. The majority of the students performed experiments on their own proteins. Evenings were filled with discussions, poster sessions and networking. Three poster prizes were awarded, the [IUCr Journals Poster Prize](#) being awarded to [Michal Busa](#) (Institute of Organic Chemistry and Biochemistry, Prague, Czech Republic).



Organizers Ivana Kuta Smatanova (right) and Pavlina Rezacova (left) with the IUBMB speaker Petra Fromme.

Based on the feedback, the majority of the participants were very satisfied. The course was very successful for four students who were able to find initial crystallization conditions and grew crystals during the practical sessions. Five months after the course, the organizers received great news: diffraction data had been taken from one of the crystals grown during the course and the structure solved and refined to a resolution of 2.5 Å!

MEETING REPORT (IUCR SUPPORTED)

XXV Conference of the Serbian Crystallographic Society

Sladjana Novaković



SRPSKO KRISTALOGRAFSKO DRUŠTVO
SERBIAN CRYSTALLOGRAPHIC SOCIETY



The XXV Conference of the Serbian Crystallographic Society was held from 21 to 23 June 2018 in Bajina Bašta, a small town located at the edge of Tara National Park in western Serbia. The conference was organised by the Serbian Crystallographic Society (SCS) and the Vinča Institute of Nuclear Sciences, University of Belgrade, under the patronage of the Ministry of Education, Science and Technological Development of the Republic of Serbia. The conference was attended by 70 participants from 14 countries. The [programme](#) was composed of welcome addresses, invited lectures (45 min), short oral presentations (15 min) and an extended poster session. The IUCr supported the conference by providing Visiting Professorships and a fund of USD2500 to assist young scientists to attend. The invitation to attend the conference as Visiting Professors (VPs) and plenary lecturers was kindly accepted by Vaclav Petříček (Academy of Sciences of the Czech Republic), Ivana Radosavljević Evans (Durham University, UK) and Christoph Janiak (Heinrich-Heine-Universität Düsseldorf, Germany). The SCS also had a pleasure of hosting three other eminent scientists: Anne Spasojevic-de Biré (CentraleSupélec, France), Piero Macchi (University of Bern, Switzerland) and Kittipong Chainok (Thammasat University, Thailand).

The IUCr fund for young scientists was used to support the travel and accommodation expenses for 16 young participants. These young scientists could choose to present their latest results through an oral or a poster presentation or both. The workshop “Crystallographic methods, tools and possibilities” was organised in the form of a two-day extended poster session. During this session, the young scientists were encouraged to present the challenging problems of their current research and to exchange ideas

about problem solving with our international guests and other participants. The poster session was very well attended, with 33 posters being available for the whole duration of the conference. Two young scientists – Ivana Marjanović (University of Novi Sad, Serbia) and Predrag Dabić (University of Belgrade, Serbia) – were honoured with the [IUCr Journals Poster Prizes](#) for the best posters in the categories of Structural Chemistry and Materials, respectively, judged by Professors Spasojevic-de Biré, Chainok and Tamara Todorović (University of Belgrade, Serbia). An additional Poster Prize was provided by the SCS, which considered the best poster in all categories. The VPs prepared a special award for the best oral presentation given by the IUCr-supported young scientists, which was won by Marko Rodić (University of Novi Sad, Serbia) for his talk "Preliminary Results of Experimental Charge Density Determination of $[\text{Ni}(\text{L})\text{py}]$ (H_2L = benzoylacetone *S*-methylisothiosemicarbazone)".



Marko Rodić (left) receives his VP Prize, a copy of the IUCr/OUP book *Fundamentals of Crystallography* by Giacovazzo *et al.*, from VP Ivana Radosavljević Evans.

In general, the conference covered a wide range of topics: single-crystal and powder diffraction, chemical crystallography, crystal engineering, charge density, quantum-chemical and database studies, and materials science. The event passed in an informal and friendly atmosphere with stimulating discussions during the sessions as well as in the coffee breaks. We hope that the conference helped our

young colleagues to get better acquainted with the possibilities of contemporary crystallographic research and to recognize appropriate methods for further improvement of their work. On the last day of the conference, all participants were invited on a guided excursion to the beautiful Tara Mountain, River Drina and Perućac Lake. The General Assembly of SCS evaluated the conference as very successful and the generous support from the IUCr was gratefully acknowledged. The presence of the excellent lecturers and the IUCr support for young scientists certainly contributed to the increased number of conference participants compared with the SCS conferences held in previous years.

MEETING REPORT (IUCR SUPPORTED)

Introduction to Crystallographic Techniques

Jorge Efrén Silva Yumi



To promote the development of research as well as constant training, the Escuela Superior Politécnica de Chimborazo and the Department of Chemistry of the Faculty of Sciences organized the First International Congress of Chemistry Ecuador 2018 (I-CIQ-Ec-18) and the Pre-Congress Course "Introduction to Crystallographic Techniques" in Riobamba, Ecuador, with the collaboration of the IUCr, the Latin American Crystallographic Association (LACA) and the International Center for Diffraction Data (ICDD).

Pre-Congress Course (27-30 July 2018)

The Course was attended by students, teachers and researchers from different universities, mainly from the central region of the country, including the Central University of Ecuador, the University of the Armed Forces (ESPE), the University Yachay Tech, the Technical University of Ambato and the Escuela Superior Politécnica de Chimborazo. The participants came from different areas: chemistry, biotechnology, environmental biotechnology, geology and mines, mechanics, biochemistry, nanotechnology, chemical engineering and polymer engineering.

The Course was aimed at introducing crystallography and crystallographic techniques to promote the development of crystallography in Ecuador as well as satisfying the need for specialized training in the area of analysis by crystallographic techniques. Its objectives were as follows:

- to transmit the principles of crystallography and the qualitative and quantitative applications of powder diffraction
- to introduce the principles of the analysis of powder and monocrystalline samples by X-ray diffraction
- to interpret the procedures for refining and determining crystalline structures using the Rietveld method.

The trainers were IUCr Visiting Professors Diego Lamas (Universidad Nacional de San Martín, Argentina) and Graciela Díaz del Delgado (Universidad de Los Andes, Mérida, Venezuela), and Miguel Delgado (Universidad de Los Andes, Mérida, Venezuela).

First International Congress of Chemistry (31 July-2 August 2018)

The Congress was held to promote scientific research at the national level through the dissemination of research results in the area of chemistry, proposing the following objectives:

- to invite recognized national and international researchers in the field of chemistry
- to present to the academic community the testimony and experiences of one of the winners of the 2009 Nobel Prize in Chemistry, [Ada Yonath](#)
- to exchange research results in the area of chemistry
- to promote the structuring of research networks.

This event also included the participation of Professors Lamas and Díaz de Delgado, who gave the keynote lectures “The History and Current Impact of Crystallography” and “Characterization of Drugs and Medications by X-ray Diffraction in Polycrystalline and Mono-Crystal Samples”, respectively.



Principal guest Ada Yonath (fourth from left) with organizers and speakers.

Professors Lamas, Díaz de Delgado and Delgado also participated in the event recognizing the Nobel Laureate Ada Yonath, which took place in the municipality of the city of Riobamba, and in a meeting with teachers and researchers from the Faculty of Sciences to establish networks and contacts for future projects.

Both the Pre-Congress Course and the Congress were received very well, exceeding expectations. There was interest in crystallography as well as analytical techniques, raising the possibility of working towards the development of an OpenLab in Ecuador.

The Escuela Superior Politécnica de Chimborazo, the Faculty of Sciences, Chemistry Department and the Organizing Committee of the I-CIQ-Ec-18 thank the IUCr, LACA and the ICDD for their support in developing both the Pre-Congress Course as well as for the participation of their representatives as keynote speakers in the Congress.

MEETING REPORT

Neutron Macromolecular Crystallography Workshop at ECM31

Matthew Blakeley John R. Helliwell, Zoë Fisher Tobias Schrader



Palacio de Exposiciones y Congresos, Oviedo, Spain.

To the best of our knowledge, this was the first [workshop on neutron macromolecular crystallography](#) (nMX) held outside a specific neutron facility. Spread over a day and a half (21-22 August 2018), the talks were naturally grouped into facilities, deuteration, crystallization, software, and methods and applications. Some talks of course bridged two or more of these categories. In addition, software and validation of models before deposition in the PDB and checking files after release of PDB depositions emerged as a keen theme. Overviews were provided by Matthew Blakeley at the start and John Helliwell at the end of the workshop.

Within the facilities theme there were talks from Matthew Blakeley [Institut Laue-Langevin (ILL), France], Tobias Schrader [Heinz Maier-Leibnitz Zentrum (MLZ), Germany] and Flora Meilleur [Oak Ridge National Lab (ORNL), USA]. For crystallization there were talks from Monika Spano (IBS, France), José Gavira (CSIR-UGR, Spain) and Zoë Fisher (ESS, Sweden). Deuteration of proteins was described by Juliette Devos (ILL, France) and Zoë Fisher. Software and validation was described by Pavel Afonine (*PHENIX*; Lawrence Berkeley Laboratory, USA). A talk by Ashley Jordan of the ILL described magnetically aligned protein microcrystals for neutron diffraction studies.

There were a wide variety of application case studies described, each illustrating how they had previously investigated their chosen system using X-rays and/or spectroscopy and then came to use

neutrons to resolve key questions regarding protonation, hydrogen bonding and hydration for their particular biological macromolecule of interest. Derek Logan (Lund, Sweden) presented an analysis of protein, ligand and water hydrogen bonding in galectin-3 by neutron crystallography to guide drug design. Motoyasu Adachi (Quantum Science and Technology, Japan) described the first neutron structural analysis of human casein kinase II. Katarina Koruza (Lund, Sweden) talked on how sweet to 'see' hydrogen atoms with neutrons: an explanation for carbonic anhydrase IX selective inhibition by saccharin and a derivative. Andrey Kovalevsky (ORNL, USA) described the unexpected protonation states and hydrogen bonding revealed by neutron crystallography in enzymes and nucleic acids. Irene Schaffner (Vienna, Austria) combined X-ray/neutron crystallography to investigate structure-function relationships of chlorite dismutase. Flora Meilleur showed the advantages of neutron macromolecular crystallography to elucidate the mechanisms of industrial and biomedical enzymes. Andreas Heine (Marburg, Germany) described the ligand protonation and changes of the water inventory determined by high-resolution neutron structures upon trypsin complex formation. Peter Moody (Leicester, UK) reviewed the secrets of heme peroxidases uncovered by neutron crystallography. Marvin Seibert (Uppsala, Sweden) described his progress thus far with a new project for neutrons on the carbon dioxide fixing enzyme rubisco.

In conclusion, it was very satisfying to see so many application projects from the five nMX instruments worldwide and the vigorous way in which those facilities envisaged further development and flexibilities in their provision for users. One would highlight dynamic nuclear polarisation for near elimination of hydrogen incoherent background being investigated in detail at ORNL. The workshop participants supported the call for a repeat of this excellent event two years on from ECM31. The support of the ECM31 local organisers was heartily acknowledged, as was the core of financial support from the ILL for which we were also very grateful.

MEETING REPORT (IUCR SUPPORTED)

2018 Kuo Symposium on 3D-EM of Macromolecules and Cells/11th K. H. Kuo Summer School of Electron Microscopy & Crystallography



The 2018 Kuo Symposium on 3D-EM of Macromolecules and Cells and the 11th K. H. Kuo Summer School of Electron Microscopy & Crystallography was held at Zhejiang University, Hangzhou, China, from 24 to 29 August 2018. The University houses a newly established state-of-the-art cryo-electron microscopy (cryo-EM) facility for structural studies of macromolecules and cells.

The summer school covered practical sessions of single-particle cryo-EM, electron tomography (ET) and hands-on experience in image-processing programs. Both basic principles of these techniques and their latest applications to biological systems was taught at the school. The IUCr supported the attendance of nine young scientists (four from China, two from Germany and three from Japan).



The IUCr-supported students proudly show their certificates.

The symposium invited 40 leading scientists to share their latest research, including Prof. Joachim Frank, who won the 2017 Nobel Prize in Chemistry. Almost 400 students/scientists attended the symposium. The major topics were advances in cryo-EM sample preparation and data acquisition, cryo-EM image analysis and reconstruction, cryo-ET and *in situ* structural biology, and correlative and hybrid methods for cellular structural analysis.

The cryo-EM meeting and workshop series is named after K. H. Kuo (1923–2006), a prominent Chinese scientist who is among the pioneers who discovered several types of quasicrystals in the 1980s. Dr Kuo was also an important educator and mentor who had fostered a generation of electron microscopists in China, Asia and across the world. Since 2008, the Kuo Summer School of Electron Microscopy has provided numerous opportunities for a new generation of scientists to learn the technique of cryo-EM through close interactions with many leading scientists in the field during the workshop and symposium.

MEETING REPORT (IUCR SUPPORTED)

Students from 21 countries gathered for the AIC International Crystallography School 2018

Serena C. Tarantino



Participants at the AIC International Crystallography School 2018.

The Italian Crystallographic Association (AIC) International Crystallography School 2018 (AICS2018) on 'Powder diffraction: Theory, Software and Applications' was held in Bari, Italy, from 29 August to 2 September 2018. The school was organised by the AIC Commission on Crystallographic Teaching (Serena C. Tarantino, coordinator; Paolo Lotti; Chiara Massera; Paolo P. Mazzeo) in collaboration with the Institute of Crystallography of the Italian Research Council (CNR-IC) and the Department of Earth and Geo-environmental Sciences of the University of Bari (DSTG-UniBA). The Programme Committee was chaired by Angela Altomare (CNR-IC) and Emanuela Schingaro (DSTG-UniBA), while the Organising Committee was chaired by Anna Moliterni (CNR-IC) and Gennaro Ventruti (DSTG-UniBA).

The School had a strong international character. It was in fact attended by 69 students from 21 countries (Italy, Albania, Algeria, Belgium, China, Croatia, Czech Republic, Denmark, Egypt, France, Germany, India, Ireland, Malaysia, Morocco, Norway, Poland, Romania, Russia, Sweden and Tunisia; over 60% from outside Italy) and different scientific backgrounds (chemistry, mineralogy, material sciences, pharmaceutical sciences), and by 19 invited lecturers and organisers. Four representatives of the supporting institutions and sponsors (IUCr, Dectris, ICDD, Assing) were also present.



IUCr Executive Outreach Officer Michele Zema (left) congratulates Paolo Mazzeo on becoming an IUCr Individual Associate during AICS2018. Paolo's contribution will help the IUCr to continue to sponsor such schools, bringing crystallographic training to all parts of the world.

The IUCr was represented by its Executive Outreach Officer, Michele Zema. In his speech at the opening ceremony, in the presence of Antonio Felice Uricchio, Rector of the University of Bari; Michele Saviano, Director of the CNR-IC; and Pierfrancesco Dellino, Director of the DSTG-UniBA, he emphasised the importance of international cooperation in science, well addressed by the AICS2018. Michele also staffed the IUCr stand, giving information about publishing with the [IUCr Journals](#) and promoting the new [IUCr Associates Programme](#).

The AICS series has a long-standing tradition dating back to 1972, and schools are held on an annual basis in a different venue in Italy (some venues, like Perugia and Camerino, have hosted several editions) and on a different topic. There is a strong financial effort of the association, in line with its mission of promoting education and the diffusion of crystallography.

For AICS2018, in addition to the important financial contribution of AIC, the other partner institutions, DSTG-UniBA and CNR-IC, have supported the School economically. The School has also received generous support from the IUCr and numerous commercial companies (ICDD; Dectris; Malvern Panalytical; GNR; Crystal Impact; Anton Paar; *Crystals*; Assing-Rigaku; Bruker AXS; Sanofi) that participated as sponsors. Thanks to the contributions of organising institutions and sponsors, 44 scholarships were granted for partial or total coverage of the registration fee.

The scientific programme of AICS2018 has addressed the different aspects of the structural study by powder diffraction methods. The school days were divided into sessions dedicated to the different phases of structural analysis: phase recognition; pattern indexing; space-group determination; structural solution in real and reciprocal space; Rietveld refinement; microstructural and textural study through profile analysis; applications in different scientific and industrial fields.

The school programme included 20 hours of lectures and 13 hours of practical sessions. The following specialists presented lectures at the school: Gilberto Artioli (University of Padua, Italy); Radovan Černý (University of Geneva, Switzerland); Nicola Corriero (IC-CNR Bari, Italy); Giuseppe Cruciani (University of Ferrara, Italy); Corrado Cuocci (IC-CNR Bari, Italy); Aurelia Falcicchio (IC-CNR Bari, Italy); Andrew N. Fitch (ESRF, Grenoble, France); Elena Kabova (University of Reading, UK); Bruno Lanson (ISTerre, Université Grenoble Alpes, Grenoble, France); Matteo Leoni (University of Trento, Italy); Paolo P. Mazzeo (University of Parma, Italy); Ernesto Mesto (University of Bari, Italy); Anna Moliterni (IC-CNR Bari, Italy); Jasminka Popović (Ruđer Bošković Institute, Zagreb, Croatia); Rosanna Rizzi (IC-CNR Bari, Italy); Juan Rodríguez-Carvajal (Institute Laue Langevin, Grenoble, France); Dubravka Šišak Jung (DECTRIS Ltd, Baden-Daettwil, Switzerland); Željko Skoko (University of Zagreb, Croatia); Gennaro Venturini (University of Bari, Italy).

During the closing ceremony, several prizes were awarded to students, including the IUCr Young Scientist Awards to 11 students, who were offered partial coverage of travel and subsistence expenses. Other awards were provided by ICDD, Bruker and Malvern Panalytical.

An anonymous evaluation form was provided for the students to give their own opinions on different aspects of the school. The large majority of comments were positive and some helpful remarks were given that will help in the organisation of future schools.

The teaching method, based on lectures and tutorials on the use of pertinent software, is a hallmark of AIC schools. We have experienced that the distribution of a Lecture Notes booklet, where students can take notes directly on the slides of the lectures, is a helpful strategy to assist in their understanding. A teacher/student ratio of at least 1:5 allows profitable interaction and encourages students to relate and have discussions with teachers. When hands-on sessions are involved, students are invited to bring their own laptop and are provided with installation and working files before the school starts, so that they are ready for the tutorials beforehand and go on practising even after the school.

The AIC School is now adjourned to the 2019 edition in Naples on 30 August to 4 September 2019 for the [Crystallographic Information Fiesta](#), an intensive course in Crystallographic Information, covering the extraction, dissemination and use of scientific knowledge from the structure determination experiment to database-driven discovery.

MEETING REPORT (IUCR SUPPORTED)

Second European Symposium on Chemical Bonding

A. Martín Pendás



The [2nd European Symposium on Chemical Bonding](#) (ESCB2) was held in Oviedo, Spain, from 3 to 7 September 2018 at the Conference Palace "Ciudad de Oviedo". It was preceded by a practical School on Quantum Chemical Topology (QCT), which took place in the Faculty of Chemistry of the University of Oviedo from 2 to 3 September.

Following the spirit of the ESCB1, which took place in Rouen, France, in 2016, the conference was devoted to showing new developments as well as relevant applications in the field of chemical bonding. Besides a set of invited lectures by leaders in the field, we gathered a considerable number of younger researchers, who offered shorter oral communications. The meeting was a satellite of the 31st European Crystallographic Meeting, which took place in Oviedo a week before.

We believe that the conference was a great success, gathering 118 people from all over the world, from Japan to the US, including India and most of the European countries. The school included 26 young students. Social activities included an excursion to the "Tito Bustillo" rock caves (World Heritage) followed by a traditional "espicha" get-together party, and a banquet dinner.

The nine plenary lecturers included Peter Gill, Paul Ayers, Alexander Boldyrev, Manuel Yáñez and Gernot Frenking. Three sessions with 10-minute flash presentations for young researchers were also included. Finally, a bond-slam session in which several aspects of energy partitions were openly discussed was

conducted by Bernard Silvi; it will be repeated in the next edition. Around 100 posters were presented during the official poster session.

During the conference, the first meeting of the new European Chemical Bonding (ECB) society was held and its several committees elected. We hope that this initiative will help the chemical bonding community reach a minimum critical mass in the next few years that will foster cooperation and access to European funds.

We received financial support from the IUCr, which helped 10 young scientists to attend. In addition, we were able to raise funds from several local organizations and companies, including SCM and the Royal Society of Chemistry, that funded three poster prizes to young poster presenters.

MEETING REPORT (IUCR SUPPORTED)

XTOP 2018: 14th Biennial Conference on High-Resolution X-Ray Diffraction and Imaging



Originally, the main topics of the XTOP conference series were X-ray topography, double- and triple-crystal diffractometry, reflectometry and standing waves techniques, later extended by small-angle scattering and a broad portfolio of imaging techniques. Today, XTOP brings together scientists from the fields of X-ray diffractometry, reflectometry, standing waves, coherent and conventional X-ray diffraction and imaging and topography. XTOP concerns methods and instrumentation with both laboratory and synchrotron sources.

The XTOP 2018 conference, held in Bari, Italy, from 3 to 7 September 2018, was attended by 157 researchers and students from 23 countries. The conference started with a one-day companion school presenting tutorials reviewing the current state of the art of X-ray diffraction and imaging using both laboratory sources and synchrotron radiation: (1) X-ray diffraction in nanoscience (Ullrich Pietsch), (2) Full field imaging methods (Tilo Baumbach), (3) Scanning imaging methods (Oliver Bunk), (4) Recent synchrotron radiation sources (Gerardina Carbone), (5) X-ray surface science methods (Gilles Renaud) and (6) X-ray scattering from imperfect crystals (Vladimir Kaganer).

The scientific program that followed was composed of 10 sessions, each being introduced by one or more keynote speakers (in total 12):

- (1) Imaging I/Full field microscopy (Peter Cloetens)
- (2) Imaging II/Microscopy in scanning mode (Marianne Liebi)

- (3) Probing matter with coherent X-rays (Ana Diaz)
- (4) New generation sources (Pantaleo Raimondi)
- (5) Theory: high throughput computing, phase retrieval, statistical approaches (Stefano Marchesini)
- (6) X-ray scattering from imperfect crystals (Andrei Benediktovitch)
- (7) Strain analysis and mechanical properties (Henning Friis Poulsen)
- (8) Industrial applications with X-ray diffraction (Maxim Myronov; Erik Mejdal Lauridsen; Raj Suryanarayanan)
- (9) *In situ* and *operando* experiments I (Marie Ingrid Richard)
- (10) *In situ* and *operando* experiments II (Tao Zhou).

followed by oral presentations highlighting experimental results. In total, more than 50 talks were presented leading to interesting questions and discussions.

In addition, the poster sessions with more than 100 contributions were heavily attended. The two best poster prizes were awarded to Lacub Fam and Christina Boemer.

XTOP 2020 will probably take place in Minsk (Belarus).

MEETING REPORT (IUCR SUPPORTED)

Hot Topics in Contemporary Crystallography 3 - HTCC3

Ana Šantić



The third [Hot Topics in Contemporary Crystallography](#) workshop (HTCC3), held in Bol, Croatia, from 23 to 27 September 2018, was organized by the Croatian Association of Crystallographers, as were its second (HTCC2, Poreč, 22-26 April 2017) and first (HTCC1, Šibenik, 10-15 May 2014) editions. The main sponsor of the workshop was Bruker AXS Inc. and it was also supported by DECTRIS, *Crystals*, PLIVA and the Ministry of Science and Education of the Republic of Croatia. With the ambition to tackle the most fascinating achievements in experimental methods and theoretical approaches in modern crystallography, HTCC3 put the focus on the three carefully selected "hot topics": (i) crystallography under extreme conditions (HT1), (ii) total scattering and PDF analysis of complex materials (HT2) and (iii) dynamical crystallography (HT3). Each of these topics was presented and discussed through an intensive full-day programme of lectures and hands-on sessions conducted by the leading experts in the field:

HT1 (24 September): Elena Boldyreva (Institute of Solid State Chemistry and Mechanochemistry SB RAS, University of Novosibirsk, Russia), Simon Parsons (Centre for Science at Extreme Conditions, University of Edinburgh, UK), Michael Probert (University of Newcastle, UK).

HT2 (25 September): Simon Billinge (Brookhaven National Laboratory, Columbia University, USA), Emil Božin (Brookhaven National Laboratory, USA), Matthew Tucker (Oak Ridge National Laboratory, USA).

HT3 (26 September): Christian Bressler (European XFEL Unit, Hamburg, Germany), Michael Först (Max Planck Institute for the Structure and Dynamics of Matter CFEL, Germany).

In addition, two tutors for the hands-on sessions, Boris Zakharov (Novosibirsk State University, Russia) and Marshall McDonnell (Oak Ridge National Laboratory, USA) were involved in HT1 and HT2.

HTCC3 in numbers

Altogether, HTCC3 had 48 participants: 31 students, 8 lecturers, 6 organizers, 2 tutors and 1 sponsor representative. The participants came from 11 countries: Croatia (21), Germany (5), UK (4), USA (4), Russia (4), Poland (2), Czech Republic (2), Slovenia (1), Canada (1), Israel (1) and Ireland (1). The overall gender distribution of the participants was 65% male and 35% female.

Best poster awards



Best poster winners: Matic Lozinšek (left), Eugenia V. Peresyphkina (middle) and Giulia Novelli (right).

The poster session contained 18 presentations, which were displayed throughout the duration of the workshop. The presented posters covered diverse research topics within the field of crystallography. The best poster award was given for three categories:

- 1) The DECTRIS best poster award, which focused on an innovative approach to solving problems, collaborative spirit and knowledge sharing, was given to Matic Lozinšek (Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia) for his research on "Novel Krypton Compounds", authored by M. Lozinšek, H. P. A. Mercier and G. J. Schrobilgen. The award winner received 100 Euros and an opportunity to promote his work in the form of a short article on the DECTRIS website.
- 2) The IUCr Journals best poster award, consisting of a certificate and a copy of *Symmetry Aspects of M. C. Escher's Periodic Drawings*, was given to Eugenia V. Peresyphkina (Institute of Inorganic Chemistry, University of Regensburg, Germany) for her research in the field of coordination chemistry presented under the title "Supramolecular Zoo", authored by E. V. Peresyphkina, A. V. Virovets and M. Scheer.
- 3) The *Crystals* best poster award focused on excellence in research, clarity of presentation, and personal knowledge and understanding of the matter. The award was given to Giulia Novelli (School of Chemistry and Centre for Science at Extreme Conditions, University of Edinburgh, UK) for her work on "Carbon Molecules in Space: a Thermal Equation of State Study of Solid Hexamethylenetetramine", authored by G. Novelli, H. Maynard-Casely, K. Kamenev, W. G. Marshall, G. McIntyre and S. Parsons.

IUCr sponsorship

The IUCr generously supported HTCC3, enabling the Organizing Committee to allocate eight bursaries to the utterly motivated students. All of them expressed their appreciation to the IUCr Young Scientist

Award and stated their benefits from attending HTCC3. Some of their personal statements are given below:

Jelena Vukašinović (PhD student, University of Belgrade, Serbia)

The HTCC3 workshop has been completed successfully. It was a great honor to participate and listen to the lectures of all of the experts in the field of crystallography. Thanks to the bursary of the IUCr I had the opportunity to learn a lot about the role of crystallography, which was almost completely unfamiliar to me, and - moreover - to get to know how to process the data through the newest software. In my previous work I didn't know how to use some of the necessary programs or I didn't have access to them. Now, I am familiar with many of them and that will for sure help me in my future work, especially for the detailed study of crystalline structures. Also, the lectures gave me ideas on how to expand my work and maybe even follow some new directions. During the workshop I became friends with many new colleagues with whom I exchanged opinions and ideas and I hope that in the future we will have successful collaborations.

Nico Giordano (PhD student, University of Edinburgh, UK)

I attended the HTCC3 workshop in Bol as a final-year PhD student. I found the school informative and useful in consolidating my knowledge in my field of study: high-pressure crystallography. It was also great to learn about the use of other techniques including the hot new topic of free-electron lasers. I think the three topics covered provided a lot of opportunity for me to think and discuss the options I have as I take the next steps in my career. Without the bursary I would not have been able to attend the school and I am extremely thankful to the organisers, lecturers and sponsors of HTCC3. Thank you.

Anna Gaydamaka (Master student, Novosibirsk State University, Russia)

Dear Organizers of HTCC3: I would like to thank you for this perfect event. My participation would not have been possible without the bursary (IUCr award for young scientists). I appreciate it. The HTCC3 was a great experience for me to get familiar with the advanced methods of contemporary crystallography from the experts in these fields. Hot topics 2 and 3 were absolutely new for me, so it was very interesting and useful (Hot topic 1 was of course also very interesting). One more thing: most of the lecturers not only use the methods but also create and develop special software and hardware. I think, the choice of topics and lecturers was effective. Moreover, the operative work of all organization team should be noted. Thank you very much again.

Robert Katava (PhD student, University of Zagreb, Croatia)

I would like to express gratitude to the IUCr and the organizers for giving me a bursary and enabling my participation at HTCC3. All three hot topics, lectures and hands-on sessions from experts gave me a valuable insight into the latest developments in the fields of crystallography, material physics and structural chemistry. Currently, I am a third-year student of Doctoral studies in the field of Inorganic and Structural Chemistry. For me, most useful were the lectures and hands-on sessions regarding extreme conditions. Investigations of intermolecular and intramolecular interactions of organic and complex compounds represent an important part of my research. Investigating such interactions under non-ambient conditions could help me expand my knowledge and prove extremely valuable in the continuation of my scientific career.

Irina Konyaeva (PhD student, National Research Tomsk Polytechnic University, Russia)

Dear Organizers: Thank you for your kind invitation and of course the bursary. I was a beginner in crystallography but due to this unique opportunity, I have learned a lot about this method. My only criticism would be that in the practicals, there was no difference between beginners and advanced scientists. In my opinion, this bursary is a good chance for students to up their skill in crystallography.

Nikola Ilić (PhD student, University of Belgrade, Serbia)

At the end of the HTCC3, I would like to point out once again how pleased I am for having the opportunity to attend this workshop with the financial support of the IUCr. All the organized lectures were of very high quality. They did not exactly match my field of expertise and current scientific work as I mostly

study ceramic materials but they gave me a great insight into the field of monocrystals and organic crystals, some ideas for future work and an excellent introduction into work with the most popular software for data processing and simulations. I have also used the chance to meet several new people from all over Europe and we spent all our free time exploring the island of Bol together and discussing our scientific work.”

In conclusion, HTCC3 was a successful workshop with highly motivated participants, enthusiastic lecturers, a vibrant atmosphere and good organization.

MEETING REPORT (IUCR SUPPORTED)

XIV Annual Meeting and X School of the Argentinean Association of Crystallography

Daniel Vega



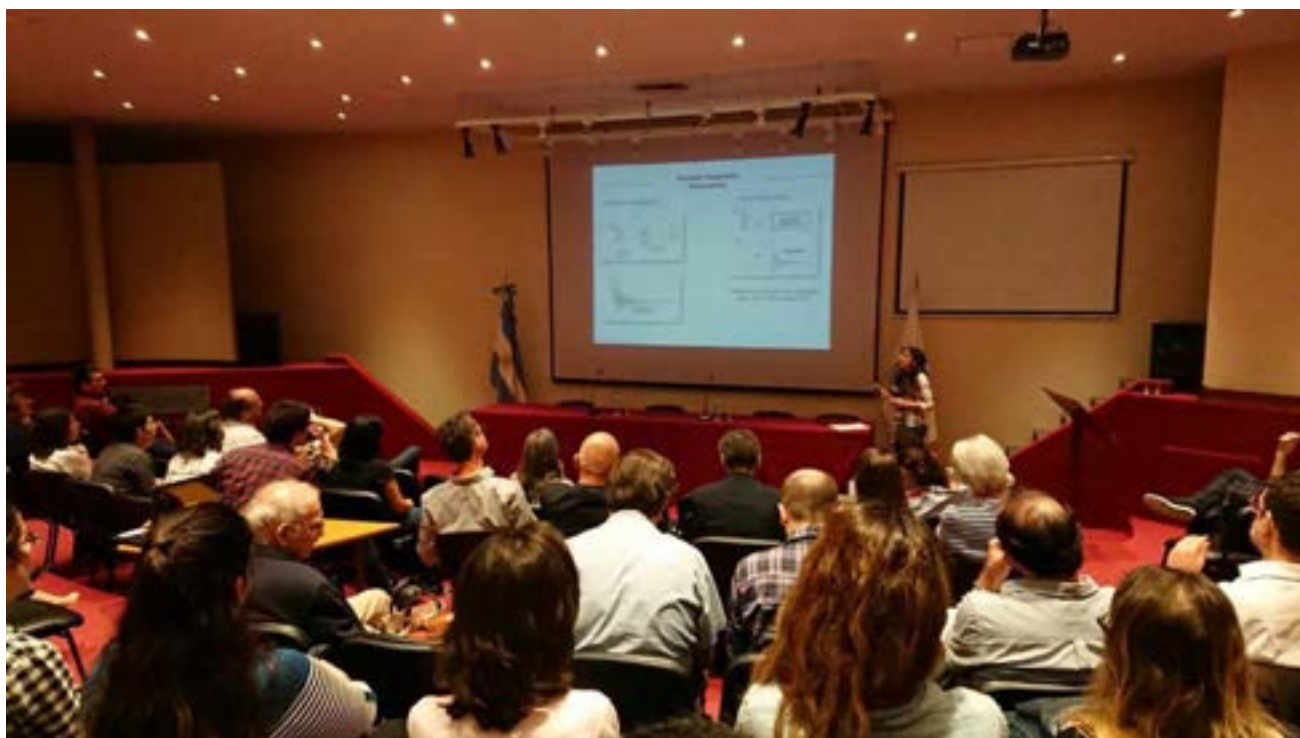
Professors, tutors and participants at the X School of the AACr, “X-ray diffraction in the study of phase transitions”.

The XIV Annual Meeting of the Argentinean Association of Crystallography (AACr) was held from 31 October to 2 November 2018 at the Centro Atómico Constituyentes, Comisión Nacional de Energía Atómica (CNEA, Atomic National Commission) Buenos Aires, Argentina. There were 148 registered participants from Argentina and several Latin American countries. The plenary lectures were presented by Mario Amzel (Johns Hopkins University, USA), María Lidia Herrera (UNSAM, Argentina), Gastón Garbarino (ESRF, France), Florean Meneau (LNLS, Brazil) and Mike Glazer (Oxford University, UK). Moreover, 11 semi-plenary talks, 18 oral contributions and 57 posters completed the event. Those participants in the poster session had the opportunity to give a 2 minute talk in a “Rapid Fire” session, which gave young scientists the opportunity to invite every participant to attend their poster. The topics addressed were very broad, including structure determination of organic, inorganic and coordination compounds; crystal architecture and design; phase transitions; solid solutions; structure-property relationships; synergy of diffraction and complementary techniques; and history. The meeting was a space to promote academic activity, allowing the discussion of scientific research, knowledge exchange and the generation of new collaborations. At the close of the meeting, a tribute was paid to Dr Bonfiglioli,

a recently deceased crystallographer, who developed a large part of his work in this CNEA. The tribute was given by Aldo Craievich.



Participants at the XIV Annual Meeting of the AACr.



A semi-plenary talk during the XIV Annual Meeting of the AACr.

Following the Meeting, the X School of the AACr was held at the same location from 5 to 9 November. On this occasion, the School addressed “X-ray diffraction in the study of phase transitions” and 30 students had the opportunity to attend lectures by Professor Glazer, an expert on the subject, financed by the IUCr Visiting Professorship scheme. In addition, Leopoldo Suescun (from Uruguay) was in charge of the introduction to symmetry and space groups.



Mike Glazer during a lecture.

The Local Organizing Committee obtained financial support from the IUCr, Bioanalytica-Rigaku, Jenck-Shimadzu and the local funding agency: Ministerio de Ciencia y Tecnología. The event brought together 30 participants (postdocs, PhD, MSc and undergraduate students) from different countries: Argentina (17), Bolivia (1), Colombia (5), Cuba (1), Ecuador (1), Guatemala (1), Venezuela (2) and Uruguay (2). They all had the chance to learn the fundamentals of phase transitions and the use of X-ray diffraction techniques as an invaluable tool for the study of the associated structural details. For the practical aspects of the school the participants made use of a Bruker D8 Quest Eco diffractometer, installed in 2018, and APEX3 software and an Oxford Cryostream 800 Plus system. Thus, the participants experienced all the processes of single-crystal X-ray diffraction, from crystal selection and mounting, with practice samples and data. The students also had the opportunity to follow a temperature-driven phase transition using a Malvern Panalytical Empyrean diffractometer with a PIXcel^{3D} detector and an Anton Paar hot stage.



Liliana Mogni at the experimental tutorial session.

The school program consisted of a 40 hour schedule (24 hours of lectures, 14 for experimental and practical tutorial sessions and 2 for a final exam). A second questionnaire was given to the students, to be worked on at home and returned one week after the School had finished. This two-step exam was taken by 28 participants, who will receive academic credit for their participation in the School.

The students were asked for their opinions on different aspects of the School in an anonymous survey. The large majority of comments were positive, many of them including helpful remarks that will be a valuable help in the organization of future schools.

MEETING REPORT

International Data Week and the CODATA General Assembly 2018

John R. Helliwell



Gaborone International Convention Centre, venue for the 2018 International Data Week in Botswana.

Traditionally the IUCr has had a strong presence at CODATA meetings (see [previous reports](#) on the IUCr web site), and it was a particular pleasure to see the main international CODATA conference SciDataCon (now part of the International Data Week) return to Africa for the first time since 2010. The meeting took place in Gaborone, Botswana; International Data Week 2018 ran from 5 to 8 November, and was followed by the CODATA General Assembly (9-10 November).

The meeting theme of IDW2018 (<http://www.internationaldataweek.org/programme-overview>) was **The Digital Frontiers of Global Science**. It attracted 820 participants from 66 countries with 60% of the attendees being from Africa.

A major role IUCr had within this conference was its organisation with IUPAC of a double session entitled *Data interoperability in chemistry, biology, and crystallography: Enabling multidisciplinary solutions to societal challenges*. The session organisers were Ian Bruno (Cambridge Crystallographic Data Centre), Jeremy Frey (University of Southampton), Richard Hartshorn (IUPAC), John Helliwell (IUCr) and Leah McEwen (Cornell University).

Through IDW2018 there were two plenary sessions. This commenced with the Opening Event, attended by the President of Botswana. The Plenary themes were: Science and Data in Africa; Data and Health;

Science Policy and the Future of Science; Pan African Infrastructure; CODATA and WDS (World Data System) Initiatives; Data Science; Data and Scholarly Communications.

There were multiple parallel sessions on data topics and themes. I attended: Journals and Data FAIR; African Health Data; Libraries and Research Data Management; the European Open Science Cloud; FAIR and Interoperability; Supporting FAIR Data; Data citation; Chemistry Research Data; Data Interoperability; and Data and Scholarly Communications.



Big data in astronomy (the Square Kilometre Array). MeerKAT, SKA-1 and SKA-2 are different stages of development of the project concept, and are expected to attain measurement data rates of 20, 300 and 7500 Gbps, respectively. For comparison, CERN currently generates 40 Gbps of data, while the total video streaming output from Google is 2.2 Gbps.

Within these, of direct interest to crystallographers was the citing of the CODATA-ICSTI [Data Citation Standards and Practices Report](#), which was very warmly commended in the sessions and in which IUCr had been a participant (Brian McMahon, IUCr Chester). It was well received by the scientific communities and was testimony that scientific data can be properly cited and that recognition of quality scientific data can thereby be gained. Of general interest I highlight the presentation on the radio astronomy Square Kilometre Array, the largest data-generating scientific project, which was very interesting and provided a comparison of measured data rates with some other 'big science' projects.



Keynote address by Fosca Giannotti, Director of Research at the Information Science and Technology Institute "A. Faedo" of the National Research Council, Pisa, Italy.

The merger of the International Council of Scientific Unions and the International Council for the Social Sciences into the International Council for Science made its presence felt in the IDW2018 programme. Of especial note I felt was the Keynote Lecture of Professor Dr Fosca Giannotti (Italy) in which she stressed the need for data to be both “FACT and FAIR”. The Public would expect no less, *i.e.* reproducibility, not irreproducibility, of her studies, she said. She is the coordinator of SoBigData, the European research infrastructure on Big Data Analytics and Social Mining, an ecosystem of ten cutting-edge European research centres providing an open platform for interdisciplinary data science and data-driven innovation (<http://www.sobigdata.eu>).

CODATA General Assembly

At the General Assembly there were miscellaneous topics of specific interest to IUCr. I highlight three items.

1. Crystallography’s track record with preservation of its data and metadata along with its publications is frequently referred to as an exemplar for all science disciplines. A [CODATA Task Group on Data Standards](#) has been established to effect improvement in all science areas towards the ideal of IUCr. Lesley Wyborn, Adjunct Fellow at the National Computational Infrastructure Facility and The Research School of Earth Sciences in Australia (lesley.wyborn@anu.edu.au), Deputy Chair, along with the CODATA President, reaffirmed to me as IUCr Representative the strong role that IUCr has in this effort.
2. The [CODATA VAMAS Nanomaterials Uniform Description project](#), in which IUCr was a participant (represented by John R. Helliwell, Reinhard Neder and Daniel Chateigner), was very warmly commended as being both well received by the science communities and testimony that scientific data integration towards a common good is possible. The common good in this case is society’s

need for guidance on the safety of nanomaterials and, first and foremost, a clear set of descriptors for them.

3. The CODATA strategic initiative on Integration of Standards with the launch Workshop in Paris (JRH as participant) has led to several subsequent Workshops and the identification of three important themes for CODATA and the International Council for Science to focus on: (i) Infectious diseases, (ii) Resilient cities and (iii) Disaster risks reduction. See <http://www.codata.org/strategic-initiatives/commission-on-standards>.

MEETING REPORT (IUCR SUPPORTED)

6th International School on Fundamental Crystallography

Mario MacíasElizabeth Jimenéz



Participants at the ISFC2018 school in Bogotá, Colombia.

The sixth edition of the International School on Fundamental Crystallography (ISFC2018) was held at the Universidad de Los Andes, Bogotá, Colombia, from 26 November to 1 December 2018. The School was locally organized by Elizabeth Jimenéz, Mario Macías, Edgar Vargas, Wolfram Baumann and Andreas Reiber from the Department of Chemistry. The event was sponsored by the IUCr, Malvern-Panalytical, Facultad de Ciencias of Universidad de Los Andes and the Consejo Profesional de Química Colombia (CPQCOL).

The school was attended by 39 students from Argentina, Brazil, Colombia, Costa Rica, Ecuador, México, Perú, Switzerland and Uruguay with backgrounds in chemistry, physics, materials chemistry and biochemistry. The school was preceded by a preparatory session covering fundamental mathematics including matrix algebra and Fourier series led by Professor Leopoldo Suescun, which helped students to be prepared for the following sessions.

During the week, lectures were given by Massimo Nespolo (Université de Lorraine, France), Mois I. Aroyo (Universidad del País Vasco, Spain), Leopoldo Suescun (Universidad de la República, Uruguay) and Arbelio Penton Madrigal (Universidad de la Habana, Cuba). On the last day, Mike Glazer (University of Oxford and University of Warwick, UK) presented a workshop on the applications of group theory in the study of phase transitions. In general, the program covered the fundamentals of crystallography helping

students to immerse themselves in the world of crystal lattices and structures, group theory, space groups, Fourier transforms, reciprocal space, diffraction equations and the use of the Bilbao Crystallographic Server to solve structural problems.

Students presented posters of their respective research projects with sessions devoted to the open discussion of the application of crystallography in their own research. During the closing ceremony, two poster prizes were awarded. The first place was granted to Bastien Francesco Grosso from ETH Zurich with the poster titled “Stabilization of a new antiferroelectric phase in oxide heterostructure with (La,Bi)FeO₃” and the second place to Natasha Di Benedetto and Joaquin Grassi from Universidad de la República, Uruguay, for the poster titled “Synthesis and characterization of perovskite ceramics for catalysis and SOFC applications”. An anonymous evaluation form was given to the students. In response, comments were globally positive with a general impression considering the course as very intense.

The international organizing committee is actively working in the preparation of the next ISFC2020 in Latin America. Chile and Perú are strong candidates to host the School.

More information is available on the [MaThCryst Commission website](#) or the [local portal for the ISFC2018](#). More pictures are available in the [photo gallery on the IUCr website](#).

MEETING REPORT (IUCR SUPPORTED)

The Second Pan African Conference on Crystallography

Compiled by Delia Haynes with contributions from Benjamin Agyei-Tuffour, Richard Garratt, Simon Coles, Claude Lecomte



George Okyere Dwapanyin presenting his research to a delegate (photo: George Okyere Dwapanyin).

The second Pan African Conference on Crystallography (PCCr2) was held from 28 January to 2 February 2019 in Accra, Ghana. The theme of the conference was 'Crystallography, a tool for sustainable development in Africa', and there were over 200 participants representing around 35 countries from Africa, Europe, North America, Asia and Australia. Activities included workshops, symposia, an exhibition, poster presentations and a varied social programme. The meeting was held jointly with the second African Light Source meeting (AfLS), highlighting the synergy between these two communities.

PCCr2 took place at the well-equipped Bank of Ghana conference centre on the lovely campus of the University of Ghana in Legon-Accra. Activities kicked off with a day of pre-conference workshops. The first of these, the Biostruct Africa workshop, was coordinated by Emmanuel Nji, a postdoctoral fellow at Stockholm University, Sweden. It covered protein crystallography, and included a remote session on beamline I04 at Diamond (UK). There was also an introductory crystallography workshop presented by Gilberto Artioli (University of Padova, Italy) and Claude Lecomte (Université de Lorraine, CRM², Nancy, France), among others. This workshop included an OpenLab where participants could carry out analysis on their own samples using a benchtop instrument provided by Bruker. This instrument remained on site throughout the conference. During the conference a further well-attended workshop was organised by

the Cambridge Crystallographic Data Centre (CCDC), UK, which was led by Amy Sarjeant and Suzanna Ward.



A cross-section of participants at the opening ceremony in the Bank of Ghana Hall.

Ghana is an astonishingly friendly country (I have never encountered such a welcome from customs officials!) and this generous nature was particularly apparent at the official start of the meeting on Tuesday morning, where participants were met by Ghanaian music and dance from the Ghana Dance Ensemble Troupe of the University of Ghana. The opening ceremony was chaired by Robert Kingsford-Adaboh, Dean of the School of Physical and Mathematical Sciences and Chair of the Local Organizing Committee, and had many dignitaries in attendance, including the Pro-Vice Chancellor of the University of Ghana, Kwame Offei; the Provost of the College of Basic and Applied Sciences, Daniel Asiedu; Ivan Addai Mensah; His Excellency Özlem Ergün Ulueren (Ambassador, Embassy of Turkey); His Excellency Timothy Mwaba Walamba (High Commissioner, Zambian High Commission); and Richard Catlow (Foreign Secretary of the Royal Society, UK).



A performance by the Ghana Dance Ensemble at the opening ceremony.

His Excellency the President of the Republic of Ghana's keynote address was delivered by Kwabena Frimpong Boateng, Minister of Environment, Science, Technology and Innovation, on the theme 'Accelerating Africa's Economic Growth and Industrial Competitiveness: the role of cutting-edge science, technology and its application'. His Excellency the President, Nana Addo Dankwa Akufo-Addo, described how science and technology have played a major role in the rapid advancement of developed countries and this fact cannot be lost on Africans. He indicated that it was imperative for African governments who desire to undertake a transformative agenda and eradicate poverty to allow science and technology to play a leading role in economic transformation. This clearly stated support of science and technology on the part of Ghana's government was apparent throughout the meeting. The opening ceremony also included addresses from the chair of the International Organizing Committee, Professor Artioli; the chair of the African Light Source project, Simon Connell (University of Johannesburg, South Africa); and Michele Zema, IUCr Executive Outreach Officer (UK).

The conference consisted of three plenary lectures, as well as parallel sessions organised by both PCCR2 and AfLS. The first plenary was presented by Sir Tom Blundell (University of Cambridge, UK), who gave an inspirational lecture on structure-guided fragment-based drug discovery. A tour-de-force of remarkable science was presented with true modesty, resulting in a lecture all participants will remember. By describing ultrafast out-of-equilibrium transformation with time-resolved techniques at synchrotron and X-FEL facilities, Eric Collet (University of Rennes 1, France) convinced all delegates, with his usual enthusiasm, that the dynamics and thermodynamics of crystals can now be described at the femtosecond scale. Gavin Vaughan (ESRF, France) delivered an exciting plenary on 'Advanced diffraction techniques for *operando* and *ex situ* studies of real systems'.

The PCCR2 parallel sessions covered a wide variety of topics. The session on Biological Macromolecular Crystallography, chaired by Richard Garratt (University of São Paulo, Brazil) and Wolf-Dieter Schubert (University of Pretoria, South Africa), was composed of six speakers including Africans active on the continent (Wolf-Dieter Schubert), Africans currently working abroad [Daouda Traore (Monash University,

Australia), Emmanuel Nji and Mike Lawrence (Walter and Eliza Hall Institute, Parkville, Australia)] and non-Africans who have shown interest in the development of the field in the region [Silvia Onesti (Elettra Sincrotrone Trieste, Italy) and Menico Rizzi (University of Piemonte Orientale, Novara, Italy)]. The talks were very diverse in their subject matter, revealing the richness of the work being undertaken, and it was universally agreed that all were of very high quality. Topics raised ranged from techniques for the crystallization of membrane proteins to targets for drug development against diseases relevant to Africa and how information from structural studies on snail insulins could be used for improving the bioavailability of current therapies. The issue of alternative funding opportunities for Africans *via* international institutions was also raised. Although the community of biological crystallographers in Africa is still small, the session generated enthusiastic discussion among the participants.

The session on Molecular Materials and Large Facilities [chaired by Claude Lecomte and Jules Tenon (Université Félix Houphouët-Boigny de Cocody, Abidjan, Côte d'Ivoire)] introduced the audience to some applications of synchrotron and neutron science to crystallography research. Pierre Fertey (Soleil, France), El-Eulmi Bendeif (Université de Lorraine, CRM², Nancy, France) and Jason Benedict (SUNY Buffalo, USA) showed the necessity of using synchrotron X-rays to precisely detail structural phase transitions, molecular movements and PDF (pair distribution function) analysis of molecular materials. Bolivard Voufack (University of Dschang, Cameroon) presented the spin-resolved electron density of YTiO₃ perovskite using an original combined synchrotron and polarized neutron refinement method. Patrice Kenfack (University of Dschang, Cameroon), discussed his research on hydrates.

The broad topic of Crystal Engineering and Structural Chemistry was addressed in a session organised by Delia Haynes (Stellenbosch University, South Africa), C. Malla Reddy (IISER Kolkata, India) and Magatte Camara (Ziguinchor University, Senegal). The session began with two keynote lectures: Alessia Bacchi (University of Parma, Italy), past president of the European Crystallographic Association (ECA), gave an accessible and inspiring presentation on using crystal engineering to produce crystalline forms of active ingredients for various applications, and Aurora Cruz-Cabeza (University of Manchester, UK) delivered an excellent lecture on polymorphism and its relevance in crystal engineering. Jules Tenon then updated the audience on progress with the diffractometer centre in Abidjan. Christelle Dzesse Tekouo (University of Buea, Cameroon) presented her work on metal-organic frameworks, and Dominik Schaniel (Université de Lorraine, CRM², Nancy, France) discussed using a combination of photocrystallography and infrared spectroscopy to study linkage isomers. The session ended with an excellent and energetic presentation from Mamoudou Diallo (Ziguinchor University, Senegal) on lanthanide-based materials.



Speakers and chairs in the sessions on Biological Macromolecules (left) and Crystal Engineering and Structural Chemistry.

The Wednesday session on Chemical Databases was very well attended – perhaps due to the workshop run by CCDC on the previous day acting as a great ‘warm up’! Ms Ward and Dr Sarjeant started the session with two talks, firstly on the content and approach of the Cambridge Structural Database (CSD) and then on the new kinds of research that it can empower. Tom Blanton from the International Center

for Diffraction Data (ICDD) then followed by giving a very insightful talk about how the Powder Diffraction File can be used in tandem with experimental work for investigating advanced materials. In a change from the programme, Philip Rodenbough, a science communicator from NYU Abu Dhabi, described his new approaches to education development that he is designing whilst based in Kenya and the Democratic Republic of Congo. The session was completed by a talk from Samuel Tetteh (University of Cape Coast, Ghana) who discussed insights into some first-row transition metal complexes that were provided by a combined CSD and computational DFT study.



Simon Connell describing the calling stick to participants (photo: George Okyere Dwapanyin).

PCCr2 also included sessions on inorganic materials, diffraction physics and phase transitions. Speakers in the plenary sessions and the AfLS sessions were handed a traditional Ashanti speaking stick by session chairs before they could begin their presentation. At Ashanti tribal meetings, the chief used a calling stick to announce a meeting, and gave such a speaking stick to speakers, and the echoing of this tradition gave a wonderful local flair to the sessions. The plenary hall was also graced by a model of vitamin B12 donated to the University of Ghana by Dorothy Hodgkin, who accepted her Nobel Prize whilst visiting Ghana.

The final day of the conference was common to both PCCr2 and AfLS, and involved presentations on large-scale facilities, and a number of productive strategy sessions around moving the plans to construct

an African synchrotron forward. The conference closed with a presentation on the progress made in forming an [African Crystallographic Association](#), and a [call for bids for the next PCCr](#).

The conference also included an exhibition, and an excellent poster session. Over 50 posters were presented by both postgraduate students and faculty, and six poster prizes, sponsored by *CrystEngComm*, IUCr and PCCr, were awarded.



Sir Tom Blundell joins the Ghana Dance Ensemble at the banquet dinner (photo: George Okyere Dwapanyin).

Conference participants were treated to a busy social programme. A tour of Accra introduced delegates to the important monuments in the city, as well as to the skills required to haggle down a price at the fascinating artists' market. A superb conference dinner involved much drumming and dancing, both by the Ghana Dance Ensemble and by the delegates. After the close of the conference, a full day tour to the central region of Ghana was organised, which included an exhilarating canopy walk in the Kakum National Park, a thought-provoking tour of Elmina castle and some crocodiles!



Conference participants enjoying the canopy walk at Kakum National Park (photo: George Okyere Dwapanyin).

PCCr2 was organised by a dedicated local organising committee, and was run with the support of an endlessly energetic group of students. The meeting was busy and productive, and all participants will have returned home with memories of collegiality and excellent science, the echoes of drums and a fondness for tilapia!

PCCr2 was a joint meeting with the second African Light Source meeting, and was held in partnership with the Ministry of Environment, Science, Technology and Innovation (MESTI) and the Ghana National Petroleum Company (GNPC). The joint meeting was under the auspices of the IUCr, the Executive Steering Committee of the African Crystallographic Association (AfCA), the United Nations Education, Scientific and Cultural Organization (UNESCO), International Atomic Energy Agency (IAEA), the Light Sources for Africa, Asia, Americas and the Middle East project (*LAAAMP*), and the African Academy of Sciences (AAS). We are grateful to all of our sponsors: MESTI, GNPC, Office of Research Innovation and Development-University of Ghana, Centre for Scientific and Industrial Research (CSIR-Ghana), Government of Benin, Bruker, UNESCO, International Centre for Theoretical Physics-*LAAAMP*, IUCr, the Royal Society of Chemistry, the Optical Society of America (OSA), Stellenbosch University, International Science Council (ISC), Elettra Sincrotrone Trieste, Diamond Light Source, Soleil synchrotron, XENOCs, Dectris, CCDC, STOE, British Crystallography Association (BCA), Italian Crystallography Association (AIC), French Crystallography Association (AFC), ECA, Société Française de Physique (SFP), ICDD, *CrystEngComm*, and the Universal Merchant Bank Ltd (UMB).

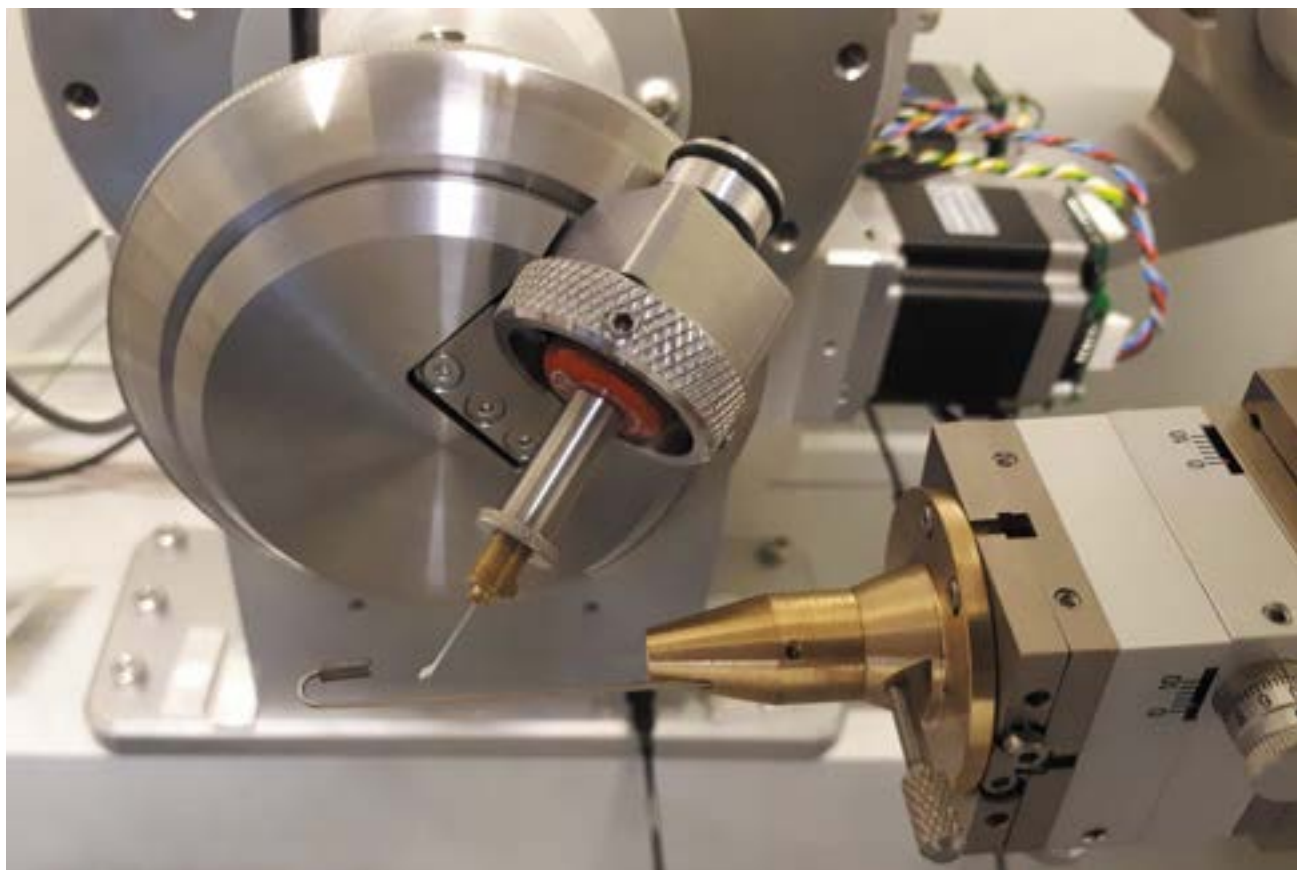


Participants at PCCr2/AfLS2, with the calling stick front centre.

ADVERTISING FEATURE

The Gandolfi Stage: A Novel Approach for the Analysis of Single Crystals and Small Volume Samples

Gregory Schmidt



Gandolfi Stage (with crystal) assembly mounted on the diffractometer.

Introduction

Accurate analysis of single crystals and/or small clusters of crystals requires the use of a single-crystal diffractometer. Conventional powder X-ray diffraction (XRD) systems are extremely limited in their capabilities for such samples. Capillary spinners are capable of accommodating such samples, but cannot accurately provide diffraction from more than a few hkl planes due to the single rotation axis. Other methods for analyzing small volumes on conventional laboratory systems require the grinding of the sample; but many samples, such as rare minerals, gemstones and newly developed materials consisting of only a few crystals, are not conducive to such alterations.

The Gandolfi Stage, developed for use in conventional powder diffractometers, enables the analysis of single-crystal or small-volume samples without the need of a dedicated single-crystal diffractometer. The stage effectively turns the diffractometer into a three-circle system, allowing for the fast analysis of samples previously unsuitable for conventional XRD systems. Combined with proper software applications, the Gandolfi Stage allows for a variety of analyses from phase identification to structure solution.

Instrument

System

The Thermo Scientific ARL EQUINOX 5000 system utilizes a unique tall vertical goniometer. Samples can be analyzed in either θ/θ or $\theta/2\theta$ geometries. Its features include a large choice of X-ray sources and higher resolution detectors. The large sample compartment accommodates a large array of sample sizes and sample handling devices such as large assemblies, auto samplers and furnaces. Software capabilities allow expansive analysis capabilities including crystal structure analysis, qualitative analysis, degree-of-crystallinity determination, phase identification and quantification, uniaxial stress, phase transition on various environments and thin-film analysis.

The ARL EQUINOX 5000 provides faster data collection when compared with other diffractometers due to its unique curved position-sensitive (CPS) detector that measures all diffraction peaks simultaneously and in real time. It is therefore well suited for both reflection and transmission measurements.



Figure 1: ARL EQUINOX 5000 X-ray diffractometer.

Stage

The stage consists of two motors and a goniometer head with a standard brass pin, which is used along with glass fibers to mount the crystal(s) (Fig. 2). Alignment is performed using the USB camera, connected to the controlling computer, and associated software on the stage holder (Fig. 3). The stage is then transferred to the diffractometer; a collimator and beam stop are added to the slit assembly to provide a more accurate analysis (Fig. 4). Then the stage is rotated during data collection to maximize the redundancy of hkl s collected.



Figure 2: Gandolfi Stage on centering station.

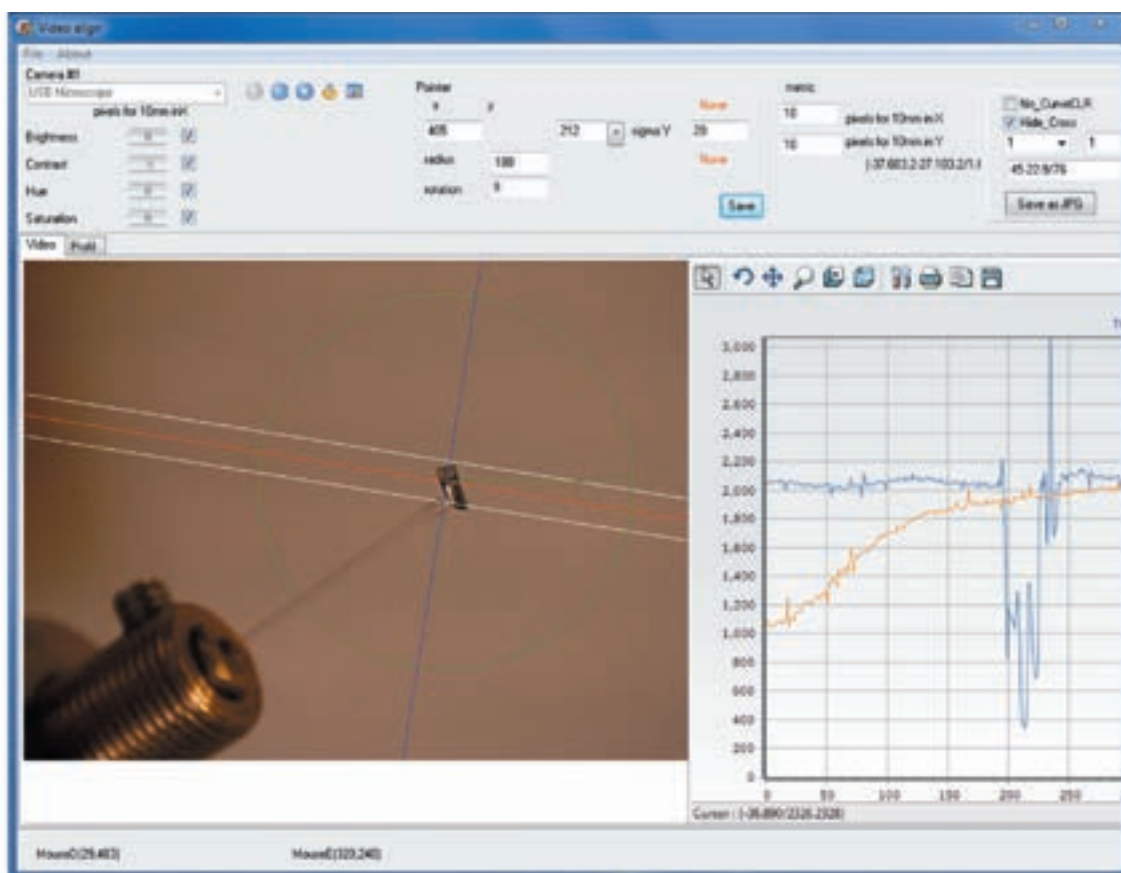


Figure 3: Crystal-centering software showing mounted crystal.

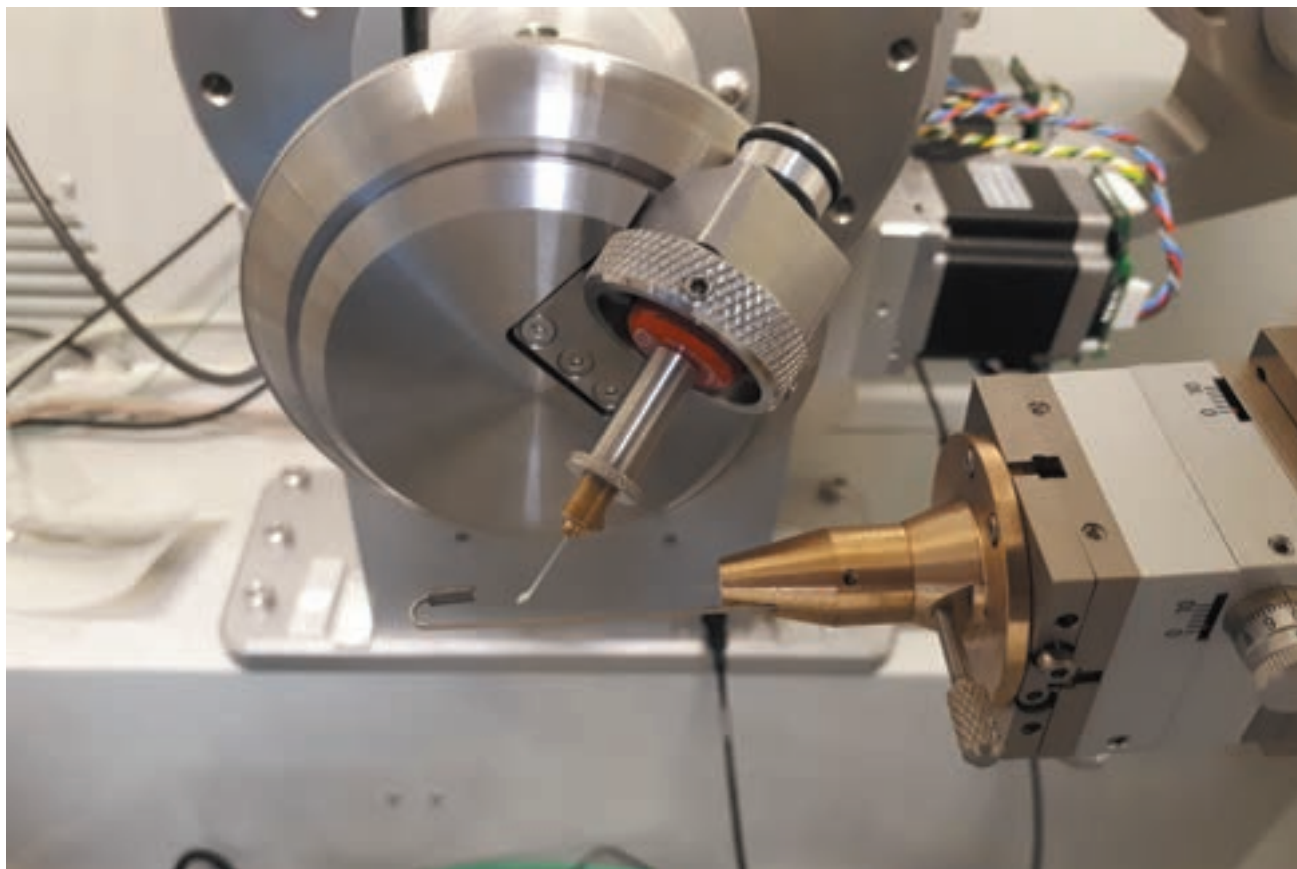


Figure 4: Gandolfi Stage (with crystal) assembly mounted on the diffractometer.

Experimental

Two different experiments were carried out. The first was a non-destructive phase determination of an unknown gemstone using MDI JADE 2010. The second experiment is the structure solution of a single crystal of acetaminophen recrystallized from IPA using GSAS-II (Toby & Von Dreele, 2013). In each case, the crystal was mounted on a glass fiber (Fig. 5) centered and placed in the instrument. Data was collected for 5 minutes and 1 hour under Cu K α radiation at 30 kV, 40 mA using a CPS 120 detector.

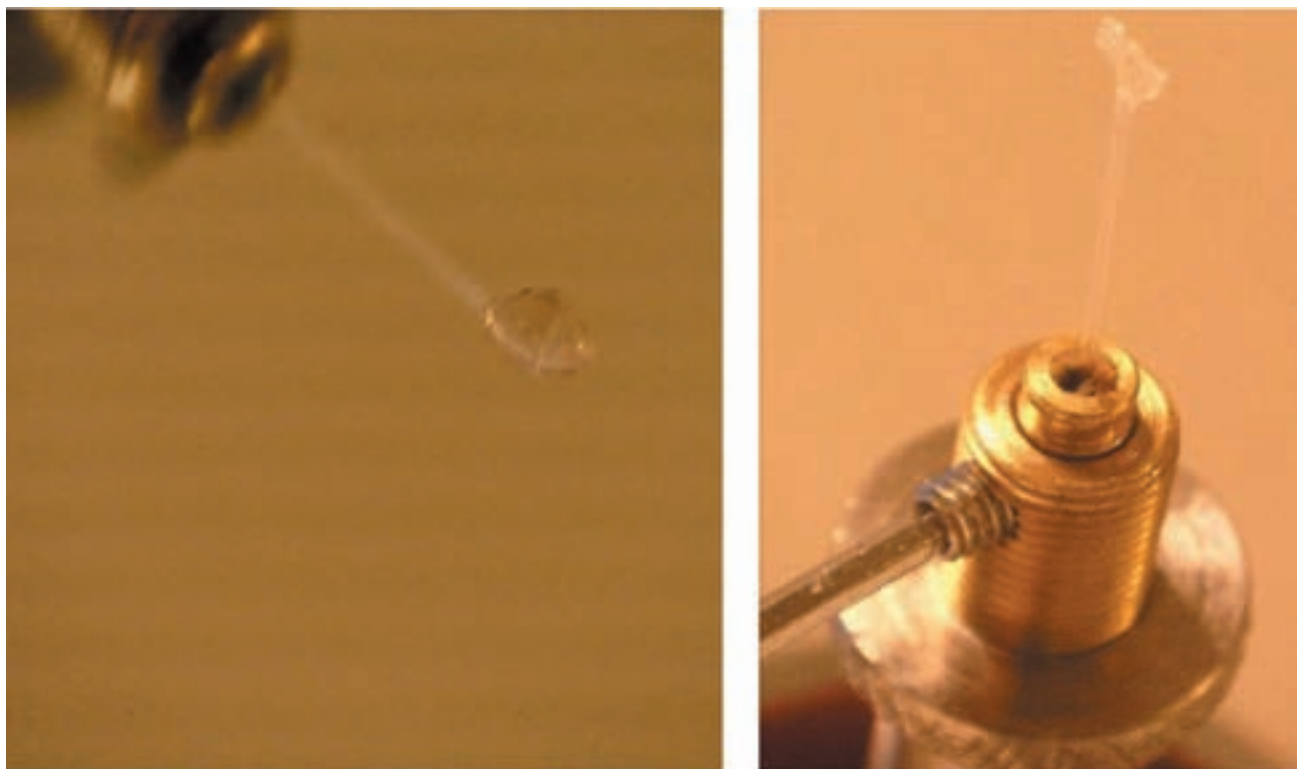


Figure 5: Gemstone (left) and Acetaminophen crystal (right) mounted on a glass fiber.

Results

Gemstone

The collected intensities were imported into MDI JADE 2010 for phase identification, where they were analyzed in the range $17\text{--}104^\circ 2\theta$. A search-match was performed using the American Mineralogist Crystal Structure Database (AMCSD) (Downs & Hall-Wallace, 2003), and the gemstone was identified as the mineral elbaite (Fig. 6). Elbaite is the most commonly used member of the tourmaline family in jewelry, ranging from dark purplish-red to colorless. After performing a whole pattern fitting Rietveld analysis, the fit had an R factor of 7.29 and a $GooF$ value of 1.08 (Fig. 7). The skewed background is due, at least in part, to the large crystal size.

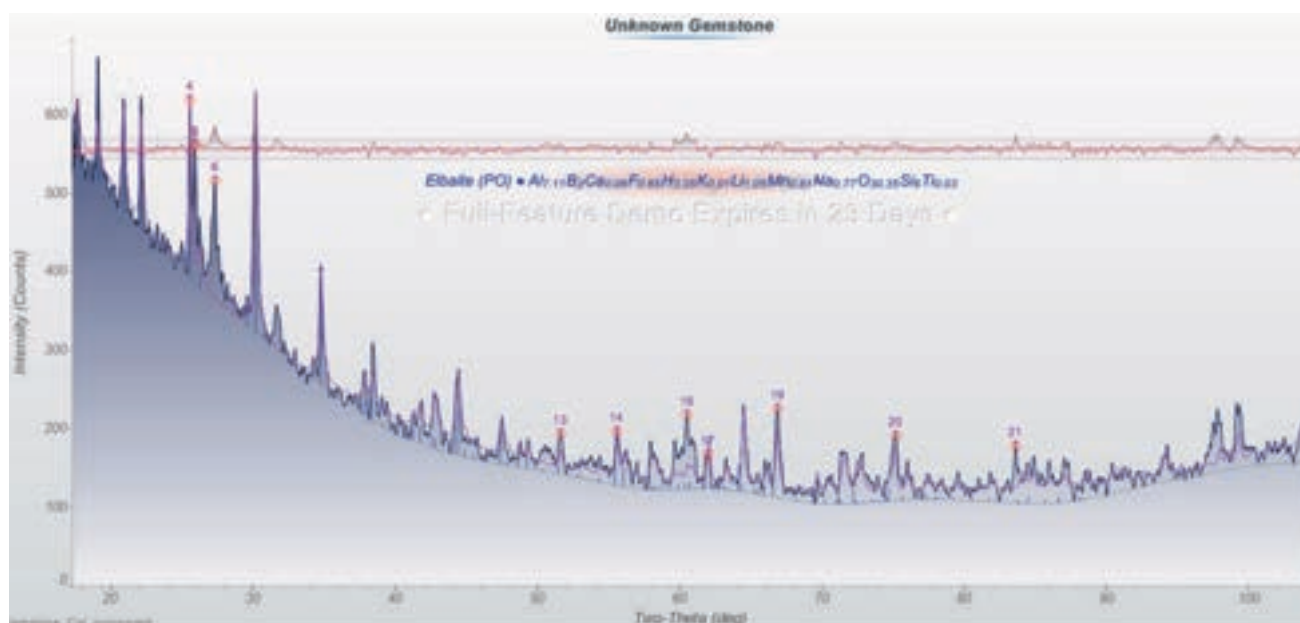


Figure 6: Unknown gemstone sample showing elbaite fit.

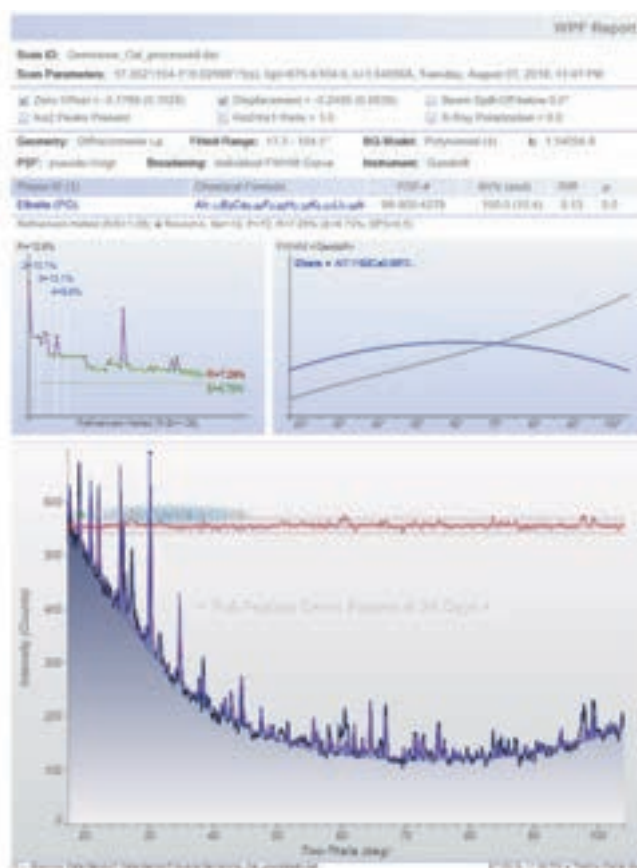


Figure 7: WPF report on unknown gemstone analysis using MDI JADE 2010.

Acetaminophen

Intensities were extracted from a 1 hour data set of acetaminophens (Fig. 8). The data were first imported into GSAS-II, where the *ab initio* structure solution was performed by applying a Pawley refinement followed by charge flipping methods to map peaks of the electron density over a range of 10–70° 2 θ . The final parameters of the solution and Rietveld refinement (Fig. 9) resulted in $R_w = 8.128$ with a unit cell of $a = 12.816(9)$, $b = 9.3254(8)$, $c = 7.0629(29)$ Å, $\beta = 115.654(9)^\circ$ and $V = 760.93(22)$ Å³ in the space group $P2_1/a$. The solved structure and atomic parameters are shown in Fig. 10 and Table 1, respectively.

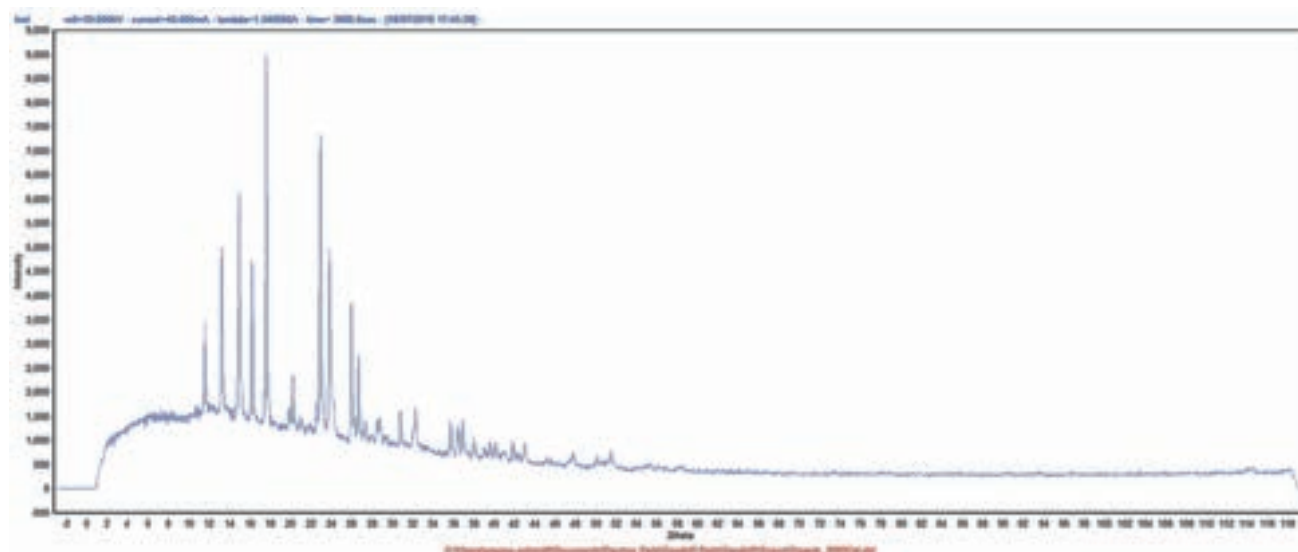


Figure 8: One-hour acetaminophen raw data.

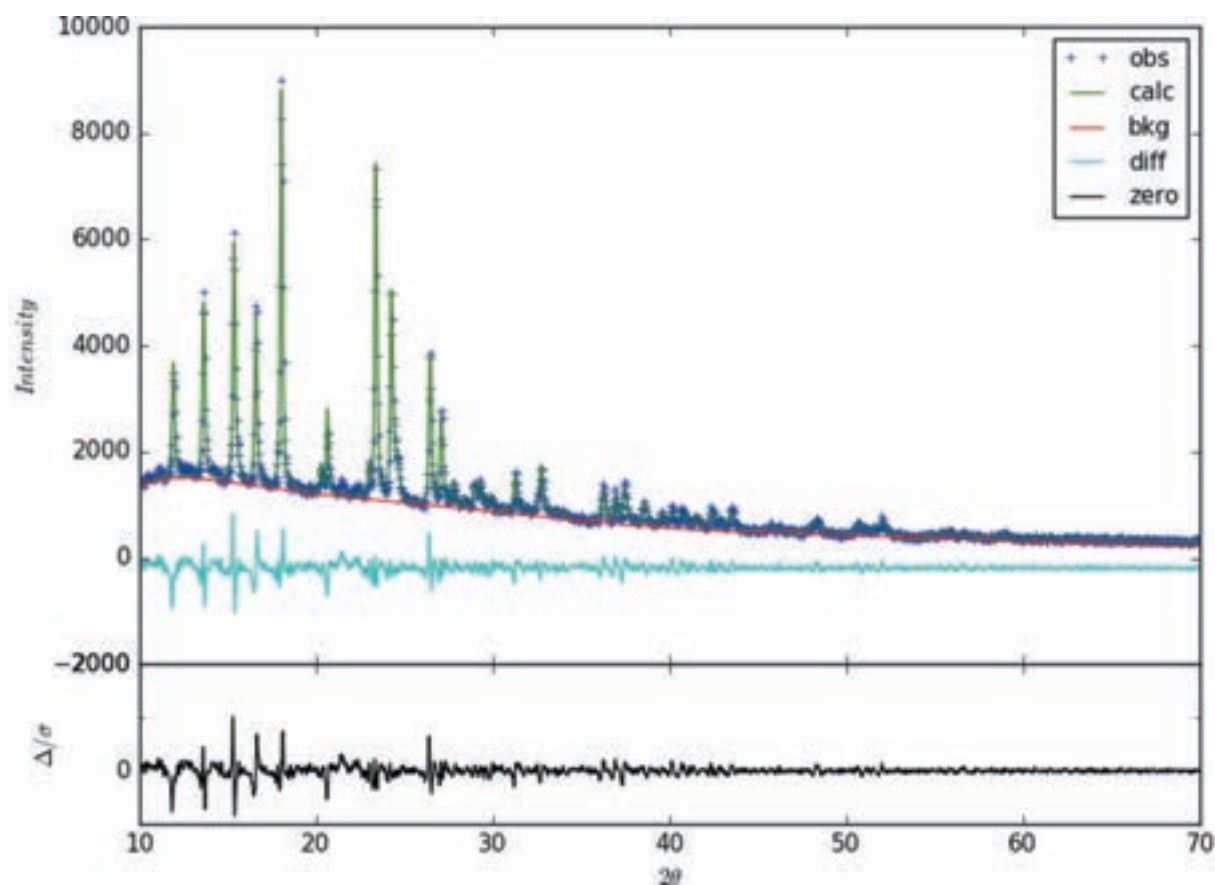


Figure 9: Final GSAS-II fit.

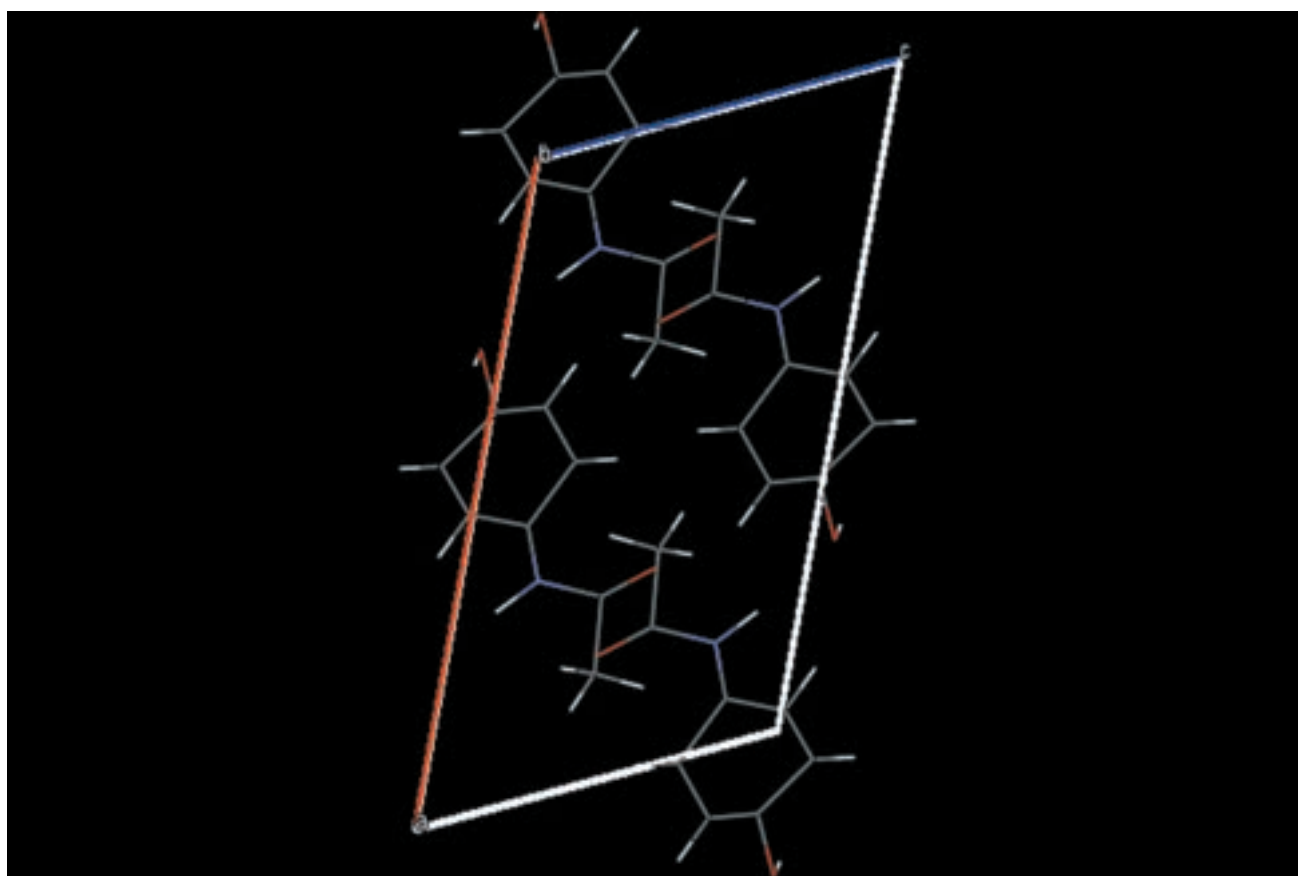


Figure 10: Final wireframe structure.

Table 1: Solved and refined atomic fractional coordinates

Atom	X _{frac}	Y _{frac}	Z _{frac}	U _{iso}
C1	0.4294	0.3701	0.8347	0.025
C2	0.5101	0.3446	0.7307	0.113
C3	0.6089	0.2557	0.8481	0.067
C4	0.6225	0.162	0.9874	0.032
C5	0.561	0.1808	1.1188	0.026
C6	0.4727	0.2653	1.0121	0.072
C7	0.2862	0.4919	0.5828	0.079
C8	0.1675	0.579	0.5613	0.039
N1	0.3377	0.4517	0.7753	0.025
O1	0.728	0.0958	1.0675	0.066
O2	0.3078	0.5038	0.4415	0.088
H1	0.7057	-0.013	1.0771	0.079
H2	0.4957	0.4101	0.6108	0.135
H3	0.6631	0.2569	0.7817	0.08
H4	0.5754	0.1153	1.2387	0.032
H5	0.4185	0.2641	1.0784	0.087
H6	0.125	0.6091	0.4118	0.047
H7	0.1199	0.5212	0.6124	0.047
H8	0.1905	0.6605	0.662	0.047
H9	0.3068	0.4621	0.8815	0.03

Conclusions

The Gandolfi Stage, developed for use in conventional powder diffractometers, enables the analysis of single-crystal or small-volume samples without the need of a dedicated single-crystal diffractometer. Combined with the speed and resolution of the ARL EQUINOX 5000, it allows for the analysis of single crystals or small clusters from phase identification through *ab initio* structure solutions and expands the capability of a single system to include routine analyses of a variety of sample types and quantities.

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Acknowledgements

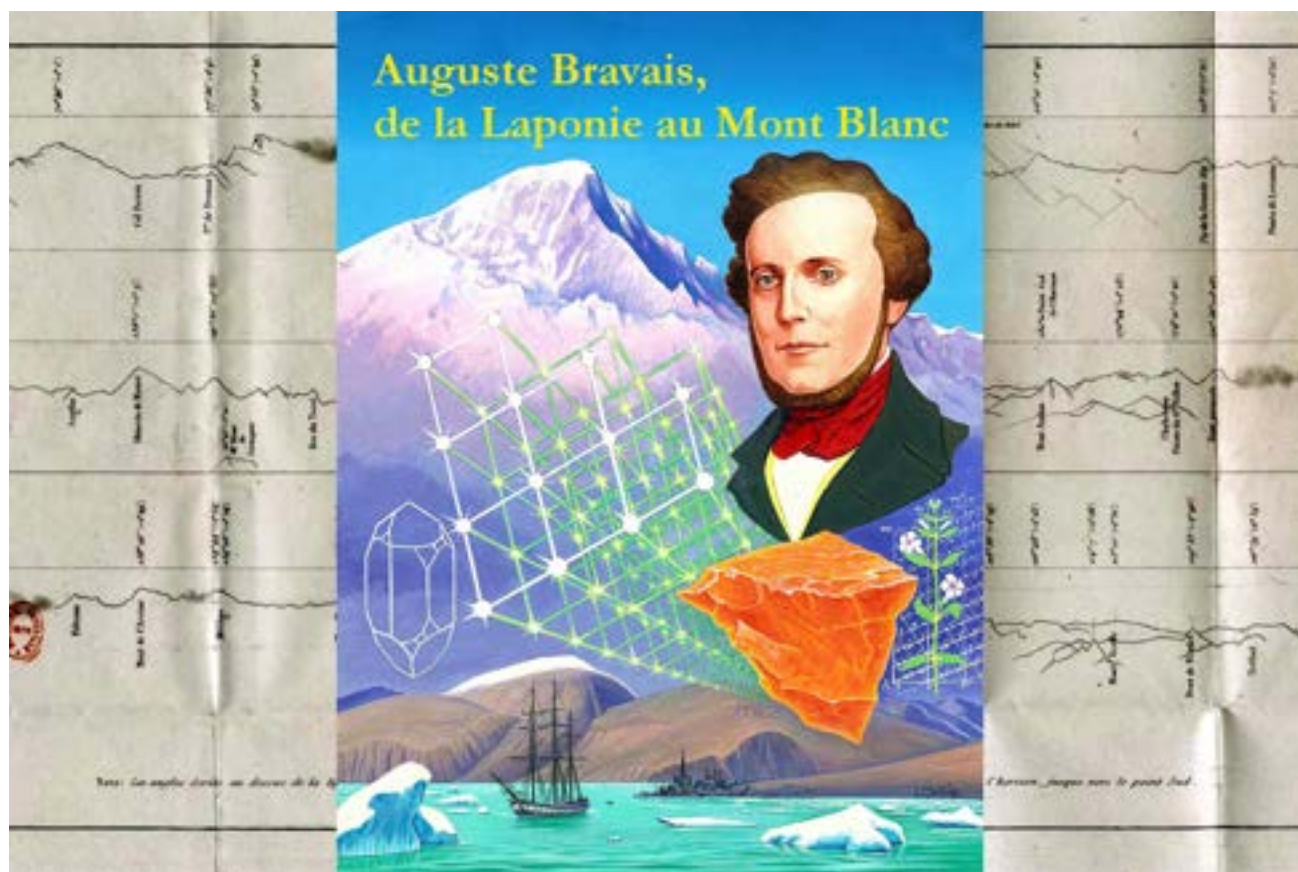
The author would like to express his thanks to Dr Henry Pilliere and Raphael Yerly for collecting the data on the provided samples used in this application note.

Gregory Schmidt is an XRD Applications Scientist at Thermo Fisher Scientific.

HISTORY OF CRYSTALLOGRAPHY

Auguste Bravais, from Lapland to Mont Blanc

Marie-Hélène Reynaud, with a Foreword by Dominique Luneau and Philippe Guionneau



Foreword

Bravais is a name known – or at least heard of – by any scientist who, directly or indirectly, is interested in crystalline matter. Clearly, crystallographers are familiar with it but mainly with the associated founding concepts. Auguste Bravais (1811-1863) played a major role in establishing the rules governing the notion of crystal structure. The first theory of the periodic structure of crystals was the result of the work of René Just Haüy (1743-1822). This theory, stated from a mathematical point of view in 1801, proposes the description of crystals from a triperiodic assembly of parallelepipedic units called constituent molecules (*molécules intégrantes*). Widely commented on and considered as the foundation of modern crystallography, this initial theory faced many problems, including the merohedry of some crystals that do not have the symmetrical elements of the constituent parallelepiped. Auguste Bravais proposed a second theory that differs relatively little from Haüy's but which includes some essential adjustments. In essence, Bravais' theory (1848-1850) uses a polyhedral constitutive unit that does not fill space but follows a triperiodic pattern of translations. This is nowadays called the Bravais network. This major advance immediately opens the way to concepts fundamental to the daily life of the crystallographer, such as nodes, reticular planes, elementary cells or crystalline systems. The originality of Bravais' work, relatively difficult in its original version – let's face it – lies in the idea of structural units separated by a void. Although obvious to us crystallographers of the 21st century, this concept

nevertheless appeared revolutionary in its context and it required the subsequent and remarkable intervention of many scientists to unravel it, improve upon it and disseminate it to all.

Thus, the 14 Bravais networks are among the first definitions given in a crystallography course – it should be noted that, although initial, these definitions nevertheless deserve particular attention because many pitfalls can mislead the novice student as well as the distracted or occasional researcher. Any worthy crystallography book includes a chapter or paragraph dedicated to Bravais' contribution. So this name is recognized by crystallographers, but is Auguste Bravais, the man, known? To answer this question, we asked a specialist, not of Bravais' scientific contribution but of the man, to enlighten us as much on the eclecticism of the work as on the hectic aspects of his life, which unfortunately ended in drama.

Marie-Hélène Reynaud, a Doctor of Letters, has devoted part of her time to studying the life of Auguste Bravais. In 1991, she published *Auguste Bravais, de la Laponie au Mont-Blanc*, a book prefaced by André Guinier, member of the Académie des Sciences (France). Marie-Hélène Reynaud is very active in promoting science, particularly in the city of Annonay located in the south-east part of France, where Auguste Bravais was born. The following article is the result of a conference given in his name at the National Congress of the Association Française de Cristallographie (AFC), which took place in July 2018 in Lyon. We believe that, in addition to the many pieces of information given about our scientist, many paths are being explored to further understand this extraordinary period in the 19th century for European science, particularly under the impetus of outstanding scientists. It should be noted in this regard that although René Just Haüy is included in the list of scientists honoured by France whose names are engraved on the first floor of the Eiffel Tower, Auguste Bravais is not. May Marie-Hélène Reynaud's article help to correct this omission!

Dominique Luneau (University of Lyon, France), Chair of AFC2018

Philippe Guionneau (University of Bordeaux, France), AFC President

The original article written by Marie-Hélène Reynaud is in French – we have attempted to translate it, making the choice to let some sentences such as the titles of the Bravais' memoirs remain in their original language.

Beginnings



As crystallographers you all know Bravais and his famous 14 crystal lattice types. The scientific work of Auguste Bravais (this was his full name) goes well beyond crystallography and may surprise us by its diversity, in these times of strong specialization. He was also a naturalist, a botanist, a geographer, a meteorologist, an optician etc. In all these fields, by his sagacious observations, he isolated and described phenomena or new facts; often, he was able to find a rational explanation. One must beware of the naïve idea that at that time discovery was easy because there was so little known. In fact, it was precisely because we started from a very low base and reliable documentation was very rare that even modest gains were of value. In this regard, the seminal work of Auguste Bravais in crystallography is astounding because of how, by simple means, he had found a property of the structures of crystals that then turned out to be a mathematical fact.^[1]

Auguste Bravais was born on 23 August 1811 in Annonay, a city located south of Lyon in southern France, the same city as the Montgolfier brothers and Marc Seguin. He was the ninth child of Victor Bravais, a medical doctor and renowned botanist. Dr Victor Bravais had correspondence with several naturalists who sent him seeds and minerals. It was in his garden that the first French dahlias were grown, as vegetables. Auguste Bravais was one of those great scientists of the 19th century who were discovered, thanks to the French Revolution, and to which the development of science in France owes a great deal. In the first place was the creation of the Ecole Polytechnique, which he entered in 1829. The Polytechnique, or X as it was eventually called, combined research and high-level teaching; this was then totally novel. Could the young Bravais have made his innate gifts flourish, if he had not found at the Polytechnique such a scientific environment of unmatched level in the world at this time? Not only was Auguste Bravais educated in scientific culture there, but he could also be initiated in research by contact with the best people of the time.

Early career

Auguste Bravais graduated from the Polytechnique in 1831 and he decided then to make a career in the navy. Assigned to the brig “Le Loiret”, he went on campaigns on the coast of what was then the regency

of Algiers. The crew's mission was to ensure the communication services between Algiers, Bône (Annaba) and Oran, while the population was hostile to the French occupation. Several other officers aboard "Le Loiret" were also scientists with a mission to identify the details of the Algerian coastline. At each stop, Auguste Bravais went in search of unknown insects, crustaceans, fish and plants not found in Europe. He sent them to Annonay, where his father and his brother Camille classified them. Some specimens were sent to the Ecole Polytechnique and to various scientists. The long days of sailing and night watching were opportunities for Auguste Bravais to engage in reflection and to write summaries of his discoveries.

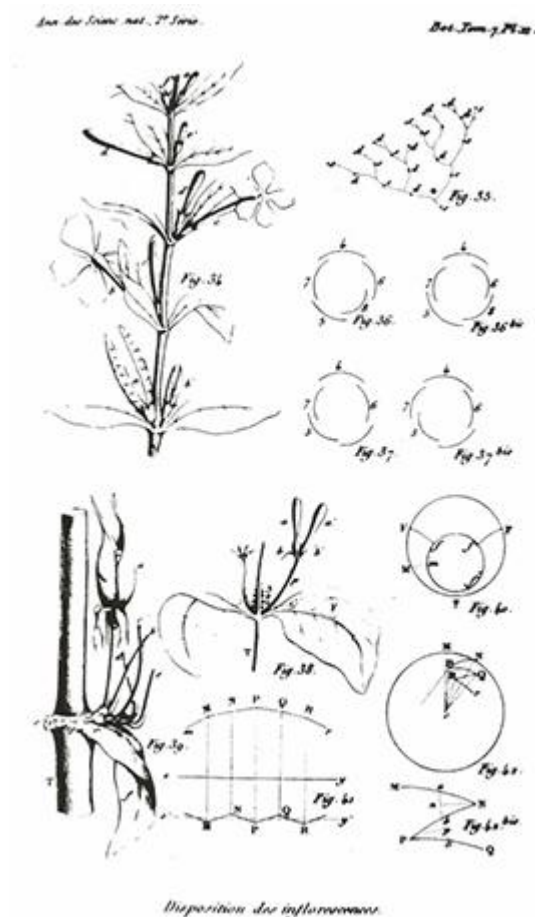


Figure 1. Page extracted from the work on the symmetry of plant leaves by the Bravais brothers (1835).

His collaboration with his brother Louis was perfect. Together, they carried out an in-depth study of the constitution and the shape of plants, and in 1835 they presented to the Academy of Sciences a dissertation entitled "Essai géométrique sur la symétrie des feuilles curvisériées et rectisériées". They both studied the symmetry relations that can be presented, at various points of the stem, the insertions of the leaves and the organs that derive from them (Fig. 1). This work did not go unnoticed by the scientific community. A Swiss botanist from Candolle dedicated to the Bravais brothers a new member of the Bignoniaceae family that he called *Bravisia*. Bravais also engaged in mathematics and wrote two memoirs. In the first one, entitled *Sur les méthodes employées dans les levés sous voiles*, he drew attention to certain errors appearing on a nautical chart when sailing using the segmentation method, caused by a possible inaccuracy in the position of the three principal points, by omitting to correct the azimuthal bearing or by an error in angular observations. The second memoir was entitled *Sur l'équilibre des corps flottants*. These two studies formed the basis of the two PhD theses Bravais defended in 1837. His dissertation on the equilibrium of floating bodies particularly appealed to the Minister of Marine who subscribed to several copies to be deposited in libraries at ports, while at the same time the Academy placed Bravais' work into the Collection of Foreign Scholars.

Auguste Bravais was then at a turning point in his life. Aware of his value, the Minister of Marine decided to appoint him as a member of the scientific commission of the north, chaired by Mr Gaynard. On 23 April 1838, the Academy of Sciences gave its approval for an expedition aimed at finding the brig "La Lilloise", which had disappeared in 1833, and also to engage in meteorological and physiological observations in Lapland and Spitsbergen. Aboard "La Recherche" they entered Bell-Sound Bay located at latitude 77° 30' north on 24 July 1838 to winter. Why choose the western shores of Norway and not elsewhere at the same latitude? In fact, the climate is milder there than in other places because the waters of the Gulf Stream warm the coast and prevent the fjord entrances from being obstructed by ice. There the scientific commission immediately made astronomical, physical and meteorological observations and calculations on the movements and the temperature of the sea. Auguste Bravais was the first to reach a difficult to reach peak subsequently named by the commission as "Pic Bravais". He then initiated a fruitful collaboration with Dr Martins, a botanist. Together, they carried out botanical research, stored plants and wrote notes; they tried to make comparisons with the flora of the Alps and the Pyrenees. On the slopes of the mountains near Hammerfest, Bravais noticed two parallel and horizontal lines. Near Alten Fjord, similar shorelines surround a lake, well above sea level, suggesting that this lake was a bay long ago. His knowledge of botany and the presence of bladderwrack (*Fucus vesiculosus*) helped him in his determination of the height of the old banks. He quickly discovered that these lines are the traces of an old shoreline emerging as a result of a rise of the coast, the current shoreline being about 30 metres below. Bravais' observations were essentially geological. Whereas it was thought that the ocean level was dropping, Bravais proved that in fact it was the coast that had risen, demonstrating the rise of the Norwegian coast that some had suspected without being able to prove it mathematically.^[2]

«La mobilité de l'écorce solide de notre globe s'est trouvée par là pleinement démontrée. On a pu dire que l'expression "ferme comme un roc", si on la prenait dans un sens trop absolu, ne serait que l'expression d'une illusion, et conclure que ce qu'il y a de moins instable autour de nous, c'est le niveau moyen de la mer.»

During this winter, the major work of Auguste Bravais was, no doubt, his study of the aurora borealis that can only be made near the Pole. In southern Europe, the aurora borealis is rarely seen and is of very short duration. Two or three times a year, well-informed observers perceive, in a northern direction, a glow that disappears rapidly. Its hues being those of twilight, novices often associate it with the reddish reflections that linger after the setting sun. If such errors are possible in our countries, in the north such confusion disappears and the aurora borealis is superb. It is like fireworks whose hues change at every moment. No aurora borealis looks like another; they vary constantly. All clear nights have had their aurora borealis; why not think that it is only because of bad sky conditions that no others are observed? Would it not be a daily phenomenon? Such a phenomenon allowed Bravais to conduct a masterful study that earned him the congratulations of all scientists.^[2]

«Malgré les mouvements dont sont doués les arcs et les rayons de l'aurore boréale, il est évident qu'ils suivent le mouvement de rotation de la terre. L'aurore boréale est donc un phénomène atmosphérique, et non un phénomène cosmique. Canton, M. Becquerel et d'autres physiciens ont signalé la ressemblance qu'offrent les teintes rouges violacées de ce météore avec celles que déploie l'électricité en se mouvant dans le vide. Cette circonstance, jointe à l'action si souvent constatée de l'aurore boréale sur l'aiguille aimantée, a porté les physiciens à la ranger parmi les phénomènes électriques. Bravais a adopté cette opinion, dont un illustre physicien M. de la Rive a récemment vérifié l'exactitude par une magnifique expérience.»

To study the northern lights and come to this conclusion, Bravais invented new instruments adapted to his research, such as a new type of compass. These observations led physicists of the commission to these deductions: "The intensity of the horizontal force increases when dawn comes; then it diminishes and when it reaches the zenith, it is less than before the appearance of the dawn. As for the vertical

intensity, it is lower during the northern lights. It only remains to find the explanation of these phenomena."

Bravais and his friends also indulged in more human studies. Having come into contact with Norwegians, Finns and Lapps, they decided to deepen their knowledge of these peoples, objects of many legends. Their physical appearance, behaviour and life differences required precise comparisons; physicists became anthropologists measuring skulls using a cephalometer. When the end of the expedition came, Bravais and Martins decided to return to France by land to complete their botanical studies, guided by a Lapp. Auguste, among other things, conducted very specific research on the growth of Scots pine: "Our goal was to discover the growth laws of Scots pine under different latitudes, from 50° to 70° parallel. This research seemed all the more interesting to us because, in no other country, the pine reached 70 m, and we could study its development on individual trees which are looked upon as the advanced sentinels of forest vegetation. Pine is distinguished by its eminent utility; alone in these icy regions, it can be used as lumber ...". Theory is not all that there is in the studies of Bravais, as practical applications and a better use of economic resources appeared in his conclusions. By planting these pines in the Hautes-Alpes and Isère, imports from Russia and Sweden would be avoided.

Recognition/honours of major work

Returning to France, Bravais wished to devote himself to the pursuit of his research and the exploitation of hundreds of pages of notes he had accumulated. The Minister of Marine entrusted him with the writing of the report of the expedition, thus freeing him from all active service. On 15 January 1841, at the age of 29, Auguste Bravais was made Chevalier in the Order of the Légion d'honneur; on 1 February, he was appointed professor of mathematics applied to astronomy at the Faculty of Sciences of Lyon where he joined his friend and Dean of the Faculty, Henri Tabareau.

As Lyon is close to Annonay, Auguste Bravais could now consider various expeditions with his brother Louis and his friend Charles Martins. In the summer of 1841, they left for Switzerland and the Faulhorn to compare their physical conditions with those of Lapland. They engaged in numerous barometric observations that they continued during the summer of 1842. Their experiments on the propagation of sound attracted many curious people. Small explosives (boxes) were used on the Faulhorn and on the banks of Lake Brienz located 2041 metres below. From each station, one could hear the noise of the explosions. The sight of the light being almost instantaneous, a watch made it possible to measure the delay of the noise and, thus, to determine the speed of propagation of sound. They found that differences appear with temperature variation: the colder it is, the lower the speed of sound.

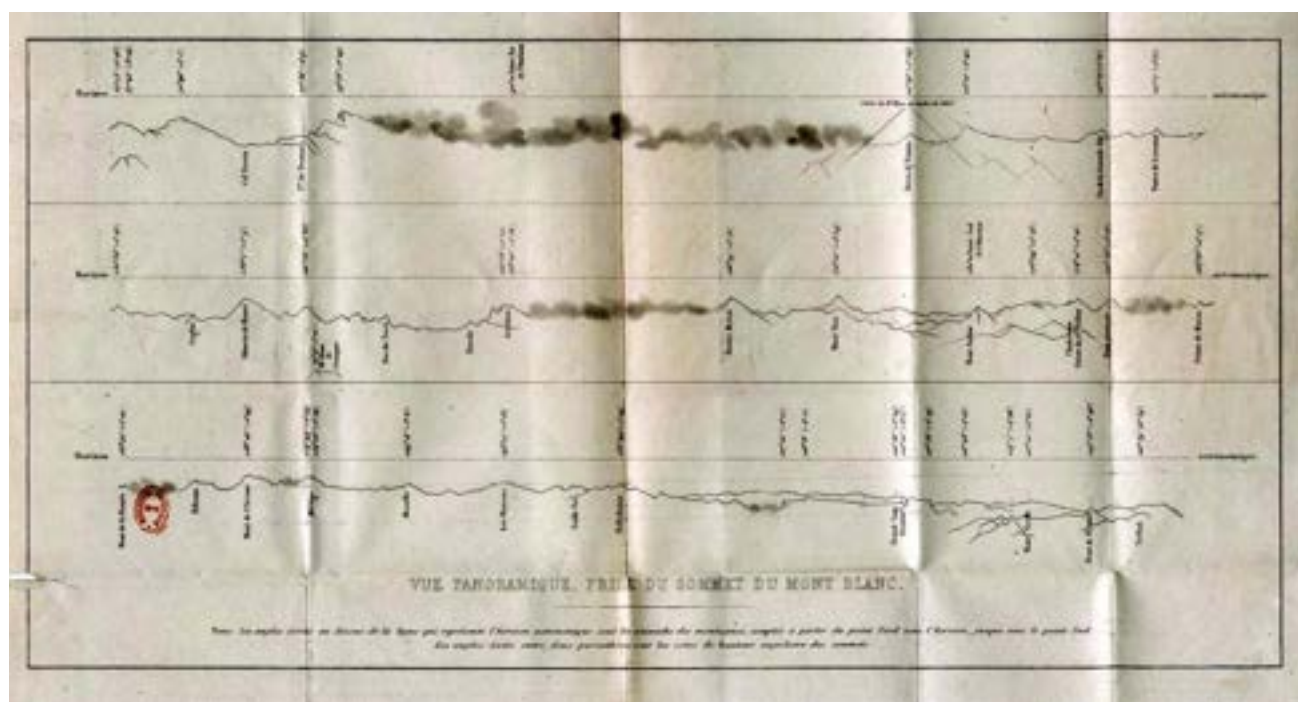
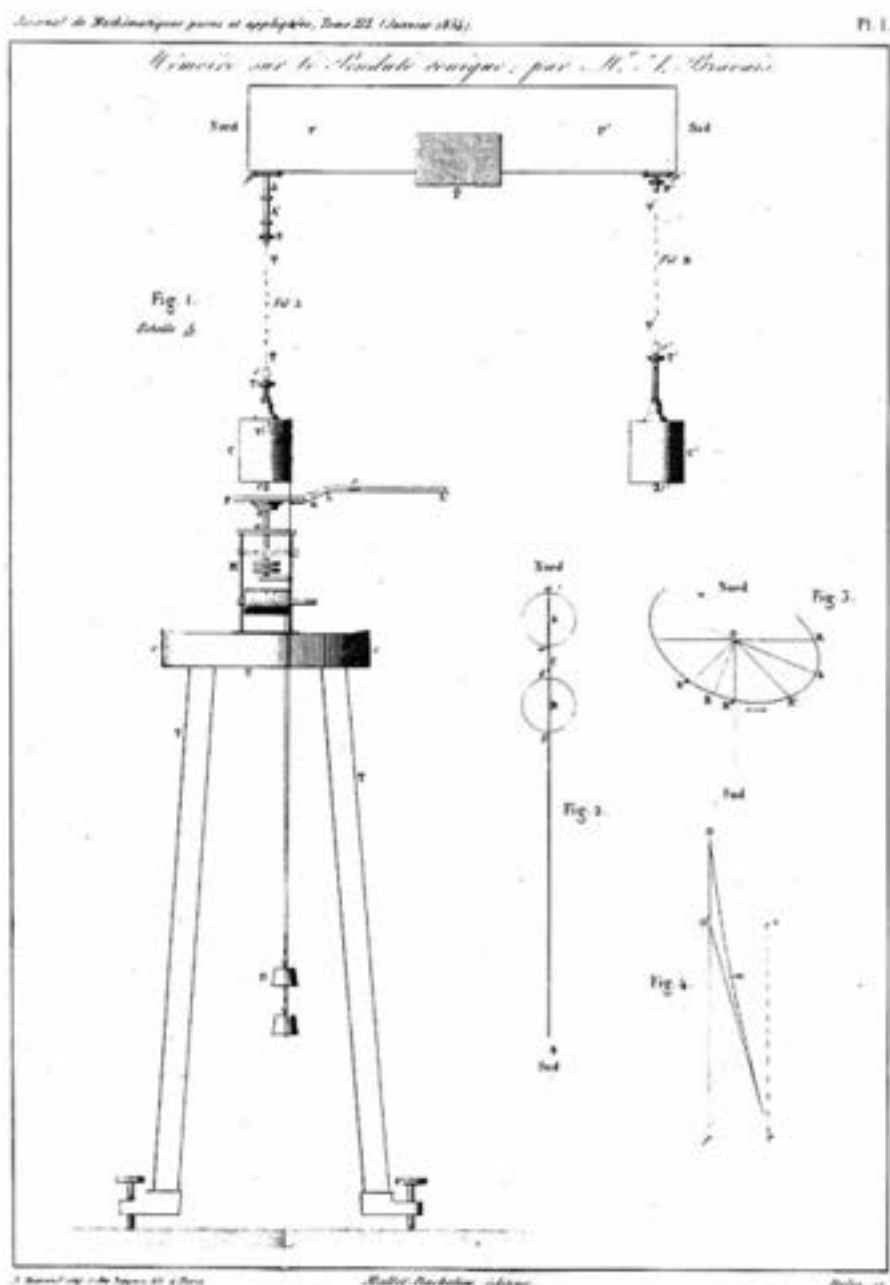


Figure 2. Drawing of the panoramic view from Mont Blanc (Alps) by Auguste Bravais.

On 1 November 1843, Bravais was promoted to the grade of lieutenant (Navy). In the Chamber of Deputies, Arago quoted him: "as one of the officers who, by their knowledge, did the most honour to our navy, even comparing him, in his improvisation, to the geometers of antiquity." In 1844, Abel Villemain, then Minister of Public Instruction, and the physicist Claude Pouillet asked Bravais to carry out a scientific expedition to Mont Blanc. Since the ascent of Benedict de Saussure, 57 years earlier, almost everything remained to be discovered. In 1844, Auguste Bravais accompanied Charles Martins and Auguste Lepileur, a medical doctor, to climb Mont Blanc to renew and complete the observations of Horace Benedict de Saussure (Fig. 2). Comparing alpine areas to boreal lands was also part of the team's goals. The instruments carried for meteorological observations were numerous: barometers, thermometers suspended in the open air or sunk in the snow at different depths, a psychrometer that measured the relative humidity of the air, a pyrliometer, an actinometer, a hygrometer, a compass, instruments for measuring the horizontal magnetic intensity, the inclination of a magnetic needle, electrical voltage, the boiling temperature of water, the hues of the sky, the transparency of the atmosphere As soon as the theodolite was installed on the summit, Auguste Bravais began to determine the angles between the mountains, in order to establish a geodesic panorama. Such measurements are important for the development of accurate geographical maps; indeed, the knowledge of the angle between two vertices, and glimpses of a third, makes it possible to build a trigonometric network, based on the map:

"A culminating peak, like that of Mont Blanc, makes it possible to directly estimate the angular distance of the two invisible mountains simultaneously from any other point on the earth's surface There is more: the angle of depression of [various] vertices below the horizontal line tangent to the summit of Mont Blanc, combined with the distance and the curvature of the earth, allowed him to calculate later in his office the relative height of these summits Like de Saussure, we were struck by the disorder of the mountains rising south of Mont Blanc; the word chain is inapplicable to them, but that of groups suits them perfectly: one recognizes very well those of the Oisans or the Pelvoux, the Rousses, the Western Alps in between the Drac and the Arve rivers, Red needles above from Chamonix, and finally from Valais"



Conical pendulum by Auguste Bravais.

The memoirs published by Auguste Bravais showed the seriousness of his research; sometimes complex for the novice, they are interesting for any scientist who has access to them. In 1845, Auguste Bravais was appointed at the Ecole Polytechnique as a Professor of physics and in the same year he received a very rare distinction as the King of Sweden raised him to the rank of Sword Knight of Sweden. Writing about his expeditions encouraged Bravais to go deeper into the discoveries made during his travels and to present condensed notes to the Académie des Sciences; the first dealt with the white rainbow (a rainbow produced by light reflected from the moon and sometimes called moonglow). For centuries, people had seen in the rainbow a sign of hope announcing better atmospheric conditions; some scientists had tried to deepen their knowledge, but were still far from completely understanding the meaning of this phenomenon. Bravais decided to unravel the mystery. Until then, no one had formulated a theory about the white rainbow. Bravais filled this gap.

"The purpose of this notice will have been achieved if I have shown in one of the most studied and best-known natural phenomena that an attentive observer can still find an ample harvest of important facts to collect. ... The rainbow is a phenomenon so well-known that it seems at first sight that it is hardly necessary to describe it To put in evidence these details, to enumerate the peculiarities rarer than the rainbow can offer accidentally, to relate them to the laws of modern optics, this is the purpose of this notice."

At the same time, Bravais presented to the Academy a memoir on the parahelion (or sun dogs) situated at the same height as the sun, and another more general one, entitled "Optical Phenomena to Frozen Clouds". The study that excited his colleagues was his presentation on halos. The name of Bravais is, alas, nowadays in the shadows; for his contemporaries, he was crowned with light, and the testimonials abound:[3]

"The halos are due to the refraction of light in the ice needles suspended in the middle of the atmosphere. A large number of physicists, among whom we must mention Huygens, Mariotte, Venturi, Cavendish, Fraunhofer, Young, Galle, Babinet etc. ... have studied the phenomenon of halos, but it is to Bravais that we owe 'the most complete study'."

In the eulogy he published on Bravais, Elie de Beaumont stated: "M. Bravais erased all doubts, by representing by the use of formulas, with the ingenious dexterity for which he had the secret, with a great simplicity, the progression of the reflected and refracted rays, and by deducing from this, the apparently most bizarre forms of the observed phenomena".

From 1845 to 1847, Auguste Bravais redoubled his activity, exploiting thousands of notes amassed during his expeditions. His fields of study shone by their variety: the physics of the globe, meteorology, terrestrial magnetism, research on the capillary action of mercury, astronomy, geometry, calculus of probabilities, and of course crystallography. The results of his research were the subject of many communications to members of the Academy or other learned societies. At times, Auguste Bravais suffered from the lack of a suitable instrument, and so he invented it, such as a polariscope.

The study of clouds with ice particles, halos and parahelions gradually led Auguste Bravais to his masterpiece: crystallography. In 1848, he presented his first memoir, *On the geometrical properties of the assemblies of points regularly distributed in space*.^[4] In a second memoir, *Crystallographic Studies*, Auguste Bravais laid out his conclusions. His two studies constitute the high point of his publications. He remarkably complemented the essays of Romé de l'Isle and the studies of R. J. Haüy. Nowadays, many of our students do not know who is really the author of the famous postulate of Bravais, namely that if we take any point A of a crystalline substance, there exists an infinite set of points in the three directions of space, points around which the atomic arrangement is the same as around A, with an identical orientation, therefore the same atomic space. Auguste Bravais imagined a very simple method that made it possible to characterize the many modes of stratification. He could now apply the notion of symmetry to a crystalline medium. This highlighted 14 types of networks grouped under all possible symmetries. Through the nodes of these networks the symmetry elements of seven of the 32 symmetry classes pass. These seven systems have the orientations: cubic, tetragonal, hexagonal, rhombohedral, orthorhombic, monoclinic and triclinic. The two memoirs of Bravais were submitted to expert committees chaired by Cauchy. They did not hide their admiration; in their report they wrote that "Auguste Bravais has given new proofs of sagacity that he had already shown in other research".

Elie de Beaumont continued: "In a second memoir entitled *Crystallographic Studies*, replacing empirical rules by theorems of geometry, M. Bravais deduces from his fundamental result all the formulas of crystallographers, with this marvelous facility which almost infallibly denotes the radical solution of the difficulties of the subject. I will confine myself to saying that in the second part of this memoir, ceasing to regard molecules as points and considering them as small bodies, which he calls atomic polyhedra, he studies and clarifies the relations existing between them and crystalline systems. He reduces to simple laws the hitherto almost mysterious phenomenon of hemihedry. M. Bravais shows that there could be 35

cases of hemihedry when only 11 had been discovered so far ... He was endowed, in fact, with an admirable facility for all kinds of intellectual work, and possessed the rare ability of being able to attend to the most varied subjects at the same time: hydrography, navigation, astronomy, atmospheric optics, physics proper, geometry, crystallography, pure analysis, natural sciences; one could almost say of him, despite the apparent opposition of words, that universality was his specialty".

Final endeavours

After these two memoirs on the assemblage of points and crystallography, Auguste Bravais continued to publish at a frantic pace; in five years, he wrote study after study; the list testifies to the diversity of studies of Bravais and their universality.^[5] In a note on his work, he recalled his aims: "I will point out that all my works, even those of pure geometry, have always been written in order to arrive either at a practical application or at the observation of a natural phenomenon, in the hope of having the good fortune to discover the explanation of its cause. These remarks will be an answer to some people who accused me of being a geometer or a too pure analyst, and of not taking enough account of observation and experiment. I answer that geometry has never been in my hands but an instrument of which I have tried to best serve myself."

But fate soon burst on Bravais. In a few months his father and his brother Jules died, and also his only son was taken by typhoid. In early 1854, at 43 years old, Auguste Bravais was elected to the Academy of Sciences, to the chair previously occupied by Admiral Roussin, in the section of geography and navigation. To try to forget his mourning, he threw himself into his work. He wrote memoirs, prepared reports for the Academy, and stayed day and night at his desk: "He had work left: he applied himself to it relentlessly. He was stimulated by the desire to respond to your kind welcome (that of the Academicians) and by the advice of his friends who urged him to try to forget his pains. He completed many memoirs; he read us important reports, and perhaps he surpassed the measure of his strength. They soon began to betray him. Sleep was running away ..."

Auguste was assiduous at the sessions of the academy; he presented many authoritative communications, but he derived no pleasure from them: "... His work was no longer successful. His memory was lacking; he could no longer find the ingenious ideas he had entrusted to memory without writing them down. He wished to put the finishing touches to a great memoir on mirages which was to complete his work on meteorological optics, and which, in his usual modesty, he called the least imperfect of his works; it caught him, it cut him off, it spoiled him and it understood ... What a new pain! The impossibility, where he was now to restore it. He felt the night overtaking that intelligence, once so bright and brilliant; he left the Ecole Polytechnique and we stopped seeing him among us."

Aware of his mental decline, Bravais could no longer teach. On 1 November 1855, the Ecole Polytechnique granted him leave. There is now no doubt that Auguste was suffering from a serious mental illness. Was this due to the series of fatalities that had affected him all at the same time or the after-effects of his military campaigns and their physically very demanding expeditions? It is difficult to dissociate the two causes; it seems that the first served as a trigger in a body weakened by excessive work. The ultimate testimony of the State was given to him on 3 September 1856: he was promoted to the rank of officer in the order of the Légion d'honneur.

Mr. Bravais (August) 173
No. 1 Annenay Apartment de l'Artich
Le 23 août 1881

[illegible]*H. ruber* var. *ruber*

Endowment

1 st April 1867	3000	Paid to Mrs. Phipps for the 1 st Dec. 11 years 1867
1 st Oct. 1867	5100	and added to the 1 st Dec. 1867

et de l'événement au point de vue de l'histoire de la France, en 1855, en l'absence de l'empereur, avec le
trouvent, en 1855, par le baron de Bismarck, qui a continué à travailler
pour la République de la même manière, avec la prolongation de l'empire de la France
à l'étranger, en 1855 (C. de l'empire en 1855).

Page de registre de l'École Polytechnique

Figure 3. Record of service of Auguste Bravais at the Polytechnic School.

On 21 April, Bravais sat for the last time in his chair at the Academy; on 9 November, he was removed from the Ecole Polytechnique. He was only 44 years old, and his wife was forced to assert his rights to retirement. From his file at the Ministry of War, it is surprising to see that his signature does not appear at the bottom of his records. His doctor said that "his state of insanity no longer allows him to check his conditions of service" (Fig. 3). He still had strength and preserved all the gentleness and the graceful expression of his countenance but his memory was lost without return. He no longer recognized objects or people. Some light came through this cruel night and gave rise to hopes that unfortunately soon vanished. At moments of lucidity, long periods of difficulties followed. In a fit of despair, he burnt all his papers, those studies that required years of experimentation and work. One afternoon when he came back from a walk, he saw his naval officer's uniform on a chair, and cried.

His agony lasted seven years and on 30 March 1863, Auguste Bravais died after a long descent into hell. His grave has disappeared for lack of maintenance and we have forgotten it little by little. Victor-Louis Goybet, his grand-nephew, explained it very well: "Scientists of pure science, such as Auguste Bravais, do not leave in the memory of people of intellectual half-culture the same memories as those who have left tangible results; their memory suffers from this".^[5]

Some Auguste Bravais publications

De la température de l'air à diverses hauteurs au-dessus du sol dans les contrées boréales.

Sur l'influence qu'exerce l'heure de la journée relativement à la mesure barométrique des hauteurs.

Formules pour représenter les variations périodiques des phénomènes météorologiques.

Description d'un nouveau polariscope et recherche sur les doubles réfractions peu énergiques.

Sur les systèmes dans lesquels les vibrations dextrogyres et lévogyres ne s'effectuent pas de la même manière.

Sur un halo observé.

Mémoire sur l'influence qu'exerce la rotation de la terre sur le mouvement d'un pendule à oscillations coniques.

Note sur la vitesse du son.

Note sur l'action qu'exerce un courant circulaire formant la base d'un cône sur une aiguille aimantée placée au sommet de ce cône.

Notice sur le nuage.

Recherche des erreurs de position des points d'un levé sous voiles.

Sur l'observation de la température de l'air.

Note sur le rapport géométrique qui lie le mouvement réel d'une étoile filante à son mouvement apparent.

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[1] Preface by André Guinier for Marie-Hélène Reynaud in *Auguste Bravais, de la Laponie au Mont Blanc*, Annonay, 1991, 237 pp.

[2] Elie de Beaumont, *Eloge historique d'Auguste Bravais*, Paris, 1865, 65 pp.

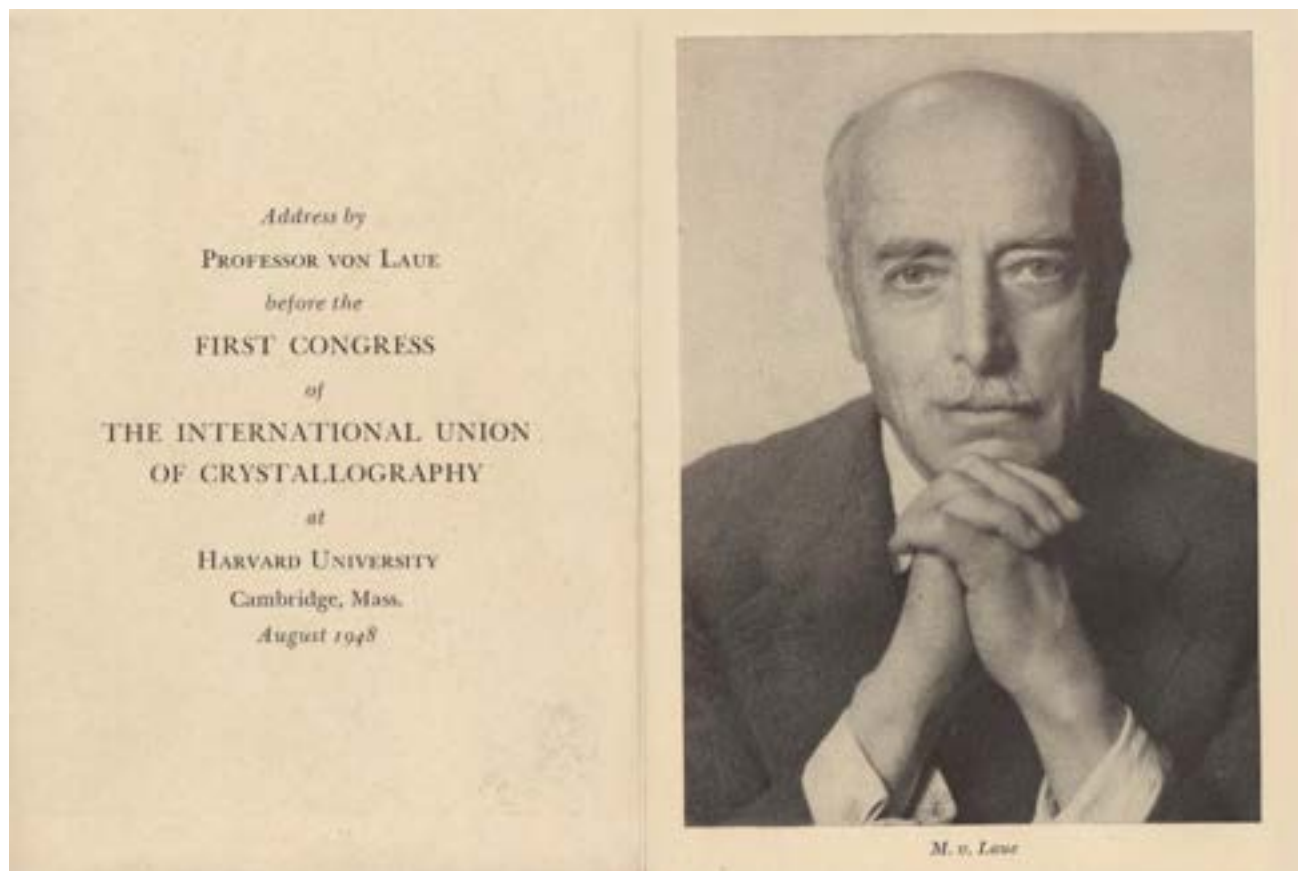
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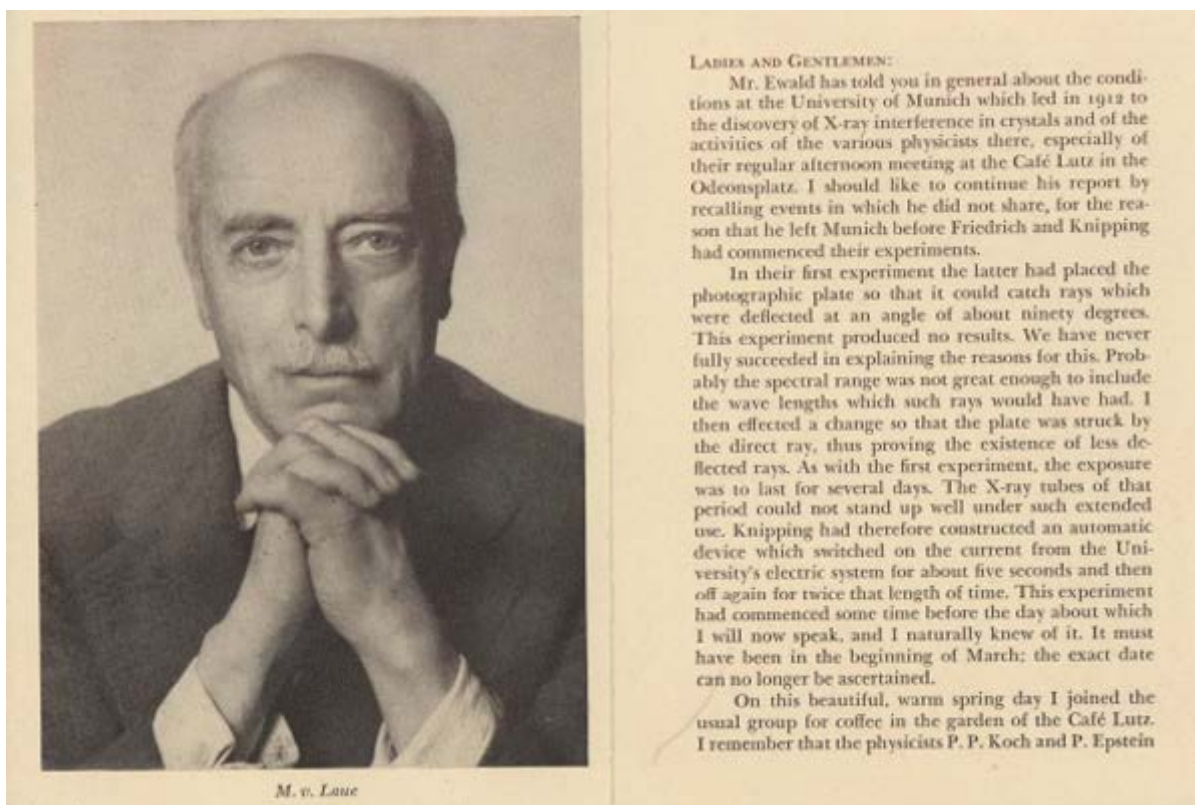
[5] Marie-Hélène Reynaud, *Auguste Bravais, de la Laponie au Mont-Blanc*, Annonay, 1991, 237 pp.

HISTORY OF CRYSTALLOGRAPHY

Address by Professor von Laue before the first IUCr Congress in 1948



Address by
PROFESSOR VON LAUE
before the
FIRST CONGRESS
of
THE INTERNATIONAL UNION
OF CRYSTALLOGRAPHY
at
HARVARD UNIVERSITY
Cambridge, Mass.
August 1948



LADIES AND GENTLEMEN:

Mr. Ewald has told you in general about the conditions at the University of Munich which led in 1912 to the discovery of X-ray interference in crystals and of the activities of the various physicists there, especially of their regular afternoon meeting at the Café Lutz in the Odeonsplatz. I should like to continue his report by recalling events in which he did not share, for the reason that he left Munich before Friedrich and Knipping had commenced their experiments.

In their first experiment the latter had placed the photographic plate so that it could catch rays which were deflected at an angle of about ninety degrees. This experiment produced no results. We have never fully succeeded in explaining the reasons for this. Probably the spectral range was not great enough to include the wave lengths which such rays would have had. I then effected a change so that the plate was struck by the direct ray, thus proving the existence of less deflected rays. As with the first experiment, the exposure was to last for several days. The X-ray tubes of that period could not stand up well under such extended use. Knipping had therefore constructed an automatic device which switched on the current from the University's electric system for about five seconds and then off again for twice that length of time. This experiment had commenced some time before the day about which I will now speak, and I naturally knew of it. It must have been in the beginning of March; the exact date can no longer be ascertained.

were there, also the mathematician Rosenthal, and, I believe, the physicists E. Wagner and W. Lenz. Friedrich and Knipping were missing. But an unusual atmosphere prevailed at the table reserved for the physicists. Instead of conversing as usual, each one silently read a newspaper. I sat down with them, ordered my coffee, and probably took up a newspaper, waiting until a conversation should begin. But none did. One of the company merely made an obscure remark, incomprehensible to me. Shortly thereafter another man made a similarly incomprehensible remark, and so it went, right around the table. I grew more and more mystified. But finally it dawned on me what had happened, and I said, "Well, gentlemen, I assume from your remarks that the interference experiment had a positive result and that each one of you has been told this confidentially. I knew nothing about it until now." And this was indeed what had occurred.

I soon went to the Institute for Theoretical Physics, whose rooms were in the University building and where the experiments were taking place. There I was shown the first interference photograph with copper sulphate, which was later published.

Lost in thought, I then went home. I took no notice of my surroundings. But after some time I found myself standing before the house at number ten Siegfriedstrasse, from which, a year and a half earlier, I had taken my bride. There, on the street, the idea came to me for that theory of space-lattice interference with which you are familiar. It consists essentially of three interference conditions, each of which implies a group of cones. I at once suspected that the circles into which the interference points had grouped themselves on

that photograph must have something to do with these cones. And so I returned to my home at twenty-two Bismarckstrasse, full of hope.

This occurred in the Easter holidays of 1912, and it was still during this vacation that the first diagrams with symmetry were obtained. Sommerfeld was in Munich and naturally knew about the progress of the experiments and theory. But Röntgen was away and did not return until the beginning of the summer semester, early in May. Although the experiments were discussed only in a very small circle, word leaked through to him. He immediately hastened from his institute over to Sommerfeld's which was diagonally opposite, and had Friedrich show him the apparatus and the photographs. He arrived in the highly critical mood which was usual with him on such occasions. But when he saw those symmetrical photographs, he was forced to abandon all his experimental objections. He congratulated Friedrich on his splendid success cordially and sincerely, but added, turning to me, "But those are not interference phenomena. They look different to me."

Despite his doubts, however, Röntgen entered helpfully into the project. I must tell you a rather humorous story about this.

At that time X-ray tubes were still operated in physical laboratories with a Ruhmkorff induction apparatus and with interrupted direct current. We used an electrolytic Wehnelt interrupter which interrupted the current about a thousand times per second and transmitted the vibrations of this frequency into the air but also into the University's electric system. In the evenings as we walked through the wonderful courtyard of the University, which unfortunately lies in

On this beautiful, warm spring day I joined the usual group for coffee in the garden of the Café Lutz. I remember that the physicists P. P. Koch and P. Epstein were there, also the mathematician Rosenthal, and, I believe, the physicists E. Wagner and W. Lenz. Friedrich and Knipping were missing. But an unusual atmosphere prevailed at the table reserved for the physicists. Instead of conversing as usual, each one silently read a newspaper. I sat down with them, ordered my coffee, and probably took up a newspaper, waiting until a conversation should begin. But none did. One of the company merely made an obscure remark, incomprehensible to me. Shortly thereafter another man made a similarly incomprehensible remark, and so it went, right around the table. I grew more and more mystified. But finally it dawned on me what had happened, and I said, "Well, gentlemen, I assume from your remarks that the interference experiment had a positive result and that each one of you has been told this confidentially. I knew nothing about it until now." And this was indeed what had occurred.

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But then the summer semester started in the beginning of May, and with it the lectures on history of art which played a most prominent part in the art-minded city of Munich. Many slides were naturally shown during these lectures, and the projector contained an arc-light, as was usual at that time. That this lamp should have made that same interrupted sound when our experiments were going on, would be clear to physicists. It must be due to some psychological law that this primitive music was contagious to the students. They thought it a great joke to hum along with it. The merriment grew greater and greater until finally the whole lecture was ruined.

The rector of the University naturally ordered a strict investigation into the cause of the disturbance. All of the many committees which are part of a university were set into motion. But in vain. We physicists, who could have explained the whole thing, knew nothing about it.

At the end of the first three weeks of the new semester the matter accidentally came to light. A mechanic, who had also been ordered to look for the source of the disturbance came into the cellar where the Wehnelt interrupter stood, listened, and at once reported it to the higher authorities. Then the waves of general indignation broke over all our heads. All

the various committees came and certainly did not show us the most agreeable side of their natures. They demanded an immediate remedy or else suspension of the experiments. We should gladly have kept the vibrations away from the University current by means of filter coils, if we had only had such coils.

Faced with this need, we turned to Röntgen to ask whether we might draw our current from his institute. Technically this was very simple. We needed only to carry a conducting wire across the university court from the window of one institute to that of the other. And as soon as it was established that the University would thus no longer be disturbed, Röntgen gladly gave his consent.

Just as matters had reached this point, the building committee walked into Sommerfeld's institute. They were the most powerful of all the university committees and apparently the least popular with the professors. They too wanted to let us feel the force of their anger, but we did not give them a chance to speak. Instead we at once told them of the arrangement which we had made with Röntgen. They were nevertheless suspicious. They went to Röntgen themselves to have this confirmed. And they returned a few minutes later in a state of indignation. We had deceived them. Röntgen was absolutely opposed to supplying current from his institute. We must therefore discontinue our experiments at once.

So the four of us sat there, Sommerfeld, Friedrich, Knipping, and I, and actually did not know what we should do next. Luckily our quandry did not last long. The solution came a few minutes later in the person of a mechanic from the Röntgen institute, a fat, affable

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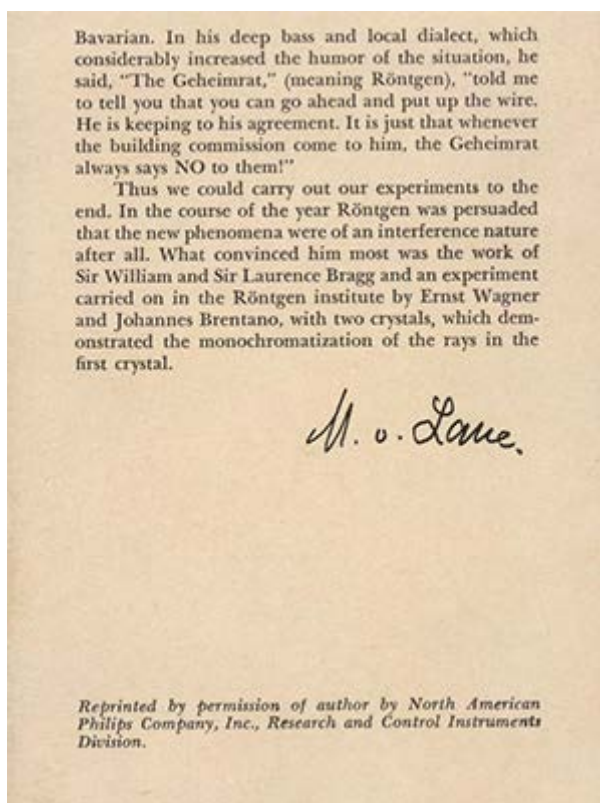
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Thus we could carry out our experiments to the end. In the course of the year Röntgen was persuaded that the new phenomena were of an interference nature after all. What convinced him most was the work of Sir William and Sir Laurence Bragg and an experiment carried on in the Röntgen institute by Ernst Wagner and Johannes Brentano, with two crystals, which demonstrated the monochromatization of the rays in the first crystal.

AWARDS AND PRIZES

IUCr Journal prizes



The IUCr would like to congratulate the following winners of IUCr Journals best student poster prizes.



Ivana Marjanović (second from left) (University of Novi Sad, Serbia), poster "One-Dimensional Silver(I)-5-Sulfosalicylate Ternary Coordination Polymer"; **Predrag Dabić** (right) (University of Belgrade, Serbia), poster "Photoluminescence, Structure and Polymorphism of $K_3ErSi_2O_7$ "; XXV Conference of the Serbian Crystallographic Society (Bajina Bašta, Serbia; 21-23 June 2018). Prizes presented by Anne Spasojevic-de Biré (left) and Tamara Todorović.



Giulia Novelli (second from left) (University of Edinburgh, UK), poster "Carbon molecules in space: a thermal equation of state study of solid hexamethylenetetramine"; **Vittoria Marzaroli** (second from right) (University of Parma, Italy), poster

"Engineering novel porous 3D metallacrown frameworks through the ligand periphery design"; **Breyan Ross** (right) (Max Planck Institute of Biochemistry, Planegg, Germany), poster "DPP8 and DPP9 structure, mechanism and interaction with SUMO1"; ECM31 (Oviedo, Spain; 22-27 August 2018). Prizes presented by IUCr President, Sven Lidin.



Katarzyna Kurpiewska (right) (Jagiellonian University, Kraków, Poland), poster "High pressure protein crystallography (HPPX) lights and shadows", DLS-CCP4 Data Collection and Structure Solution Workshop (Diamond Light Source, UK; 2-9 December 2018). Prize presented by Kay Diederichs, *Acta Cryst. D* Co-editor.

OBITUARY

Aaron Klug (1926-2018)

Sven Hovmöller



Aaron Klug was one of the last giants who were members of the MRC Laboratory for Molecular Biology (LMB) in Cambridge, UK, right from the start. I remember how he showed me “The Hut” in the yard of the Cavendish Laboratory in 1978. He said: “In this building, now used as a bicycle shed, five Nobel Prizes were produced: Watson and Crick for the DNA double helix structure, Max Perutz and John Kendrew for the first protein structures and Fred Sanger for inventing amino acid sequencing. But now, with our huge, modern and well-equipped laboratory there are no Nobel Prizes”. It would take four years until Aaron got the Prize himself, and after that they have come one by one in a steady stream.

Aaron was born in Lithuania in 1926, but his family emigrated to South Africa when he was only two years old. He came to England in 1949 with his wife Liebe Bobrow, a professional dancer, and went to do his PhD at Cambridge University. He wanted to study X-ray crystallography on proteins, but got to work on phase separations in steel. One thing he studied was that of nucleation and growth in a phase change, which later was extended to the self-assembly of tobacco mosaic virus (TMV). He then in 1953 went on to work in J. D. Bernal’s department at Birkbeck College in London. There he met Rosalind Franklin who introduced him to X-ray crystallography and diffraction of helical structures. “From then on my fate was sealed” he recalled in his Nobel speech in 1982.

Rosalind Franklin showed Aaron diffraction patterns from helical structures, including DNA, and he learned to interpret diffraction patterns just by looking at them. This became a great help for several projects, especially when he started to work on electron microscopy. There are two main problems for electron microscopy on biological samples: low contrast and specimen damage. Both can be overcome

by staining the sample with heavy metals (U, Os, I, *etc.*), but at the expense of limiting the resolution. The low contrast is due to the fact that biological samples contain some 50% hydrogen atoms, which are so light that they are hardly detected by X-rays or electrons, and then C, N and O, which are also light elements and of adjacent atomic numbers. It was long unclear if the stain showed the top side of thin samples or perhaps just the bottom half as in a footprint, as would be the case if the stain were sucked in by capillary forces. Klug showed in a brilliant experiment that in fact both sides are seen. The proof was that the diffraction pattern of phage tails must be due to two distinct crystalline patterns one on top of the other, identical but with different orientations. At that time, computers were not yet powerful enough to calculate a Fourier transform of an image, so he had to use a laser beam on the negative electron micrograph.

Klug went on to study both helical viruses (such as TMV) and spherical viruses and showed that the latter were all of icosahedral symmetry. He then showed, with Caspar, that all spherical viruses had to be icosahedral in order for the small protein molecules of the virus shell to cover the much bulkier viral DNA or RNA. A cube has 6 sides of 4-fold symmetry, *i.e.* 24 identical copies of protein, whereas an icosahedron has 12 pentamers, so 60 identical units, and only this is enough to completely cover the DNA or RNA. These are examples of how Aaron Klug frequently combined a deep knowledge of mathematics and physics, with a broad understanding of biology and chemistry, into fundamental breakthroughs in molecular biology. He was also interested in the philosophy of science, as shown by the following example. During attempts to crystallize the coat protein of TMV, they kept getting the uncomfortably large discs of two layers of 17 (!) protein subunits each. They derived a rather elegant scheme for the assembly, but later found out that “Every detail of this scheme is wrong. But the idea is correct!” The idea of course was that the virus assembly never happens haphazardly, but in some highly organized way. Often Nature does things in a smarter way than we humans first think of.

Aaron was, as all crystallographers with some self-respect, also interested in the classical phase problem in X-ray crystallography, *i.e.* the fact that the phases of the diffraction spots are not available in diffraction patterns. He argued that one could look at the interference patterns of adjacent pairs of diffraction spots in the optical transform seen in the laser beam. But then (in 1968) he realised a much better solution: to calculate by computer the Fourier transform of a scanned EM image of the crystal. This directly gave the experimental phases in degrees. He went on (with Erickson in 1970) to show the effects of changing the focus of EM images, where the contrast transfer function (CTF) varied in a way close to that predicted in optics. Already in 1979, with Nigel Unwin, he showed that the crystal structure of a metal oxide could be clearly identified from any of the EM images in a series of images taken at different focus values. This crystallographic image processing has been used in molecular biology, especially on crystalline membrane proteins (Unwin and Henderson 1975), and in inorganic chemistry. Unfortunately, in inorganic chemistry this absolutely fundamental understanding was still denied by many physicists for 40 years, which hampered the development of electron crystallography on inorganic samples. For decades, the crystallographic structure factor phases were directly experimentally available in EM images of proteins and used to determine their structures. In numerous electron microscopy and crystallography conferences this was the situation on one side of the corridor, where biology sessions were held, while the opposite was true on the other side of the corridor. There, the phase information was considered as lost in images as it was in diffraction patterns.

Realising that a single image of a periodically repeating particle, such as for example a spherical or helical virus, contains many different views of the same protein molecules, Klug went on to quantify the Fourier components of such particles. With algorithms and computer programs derived by Tony Crowther and Gérard Bricogne, this allowed 3D reconstructions of both helical and spherical particles. It also allowed Aaron Klug to derive the kind of information needed for 3D structure determination of much bigger objects, including human bodies. This was crucial for whole-body tomography scans in medicine, for which many (including Aaron himself) thought he should have shared the Nobel Prize in Medicine.

After having derived the theoretical basis for electron crystallography, Klug largely continued with X-ray crystallography. He solved a number of very large biological macromolecules such as transfer-RNA, the protein disk of the helical virus TMV and chromatin (with John Finch, Daniella Rhodes and Tim Richmond). During the last decades of his life, he was mainly interested in the structure and function of zinc fingers, common proteins of great biological and medical importance.

As if all of this had not been more than enough for a single person, Aaron Klug also became involved in administration, becoming first the head of the structures division at LMB, then the director of the entire LMB and president of the Royal Society.

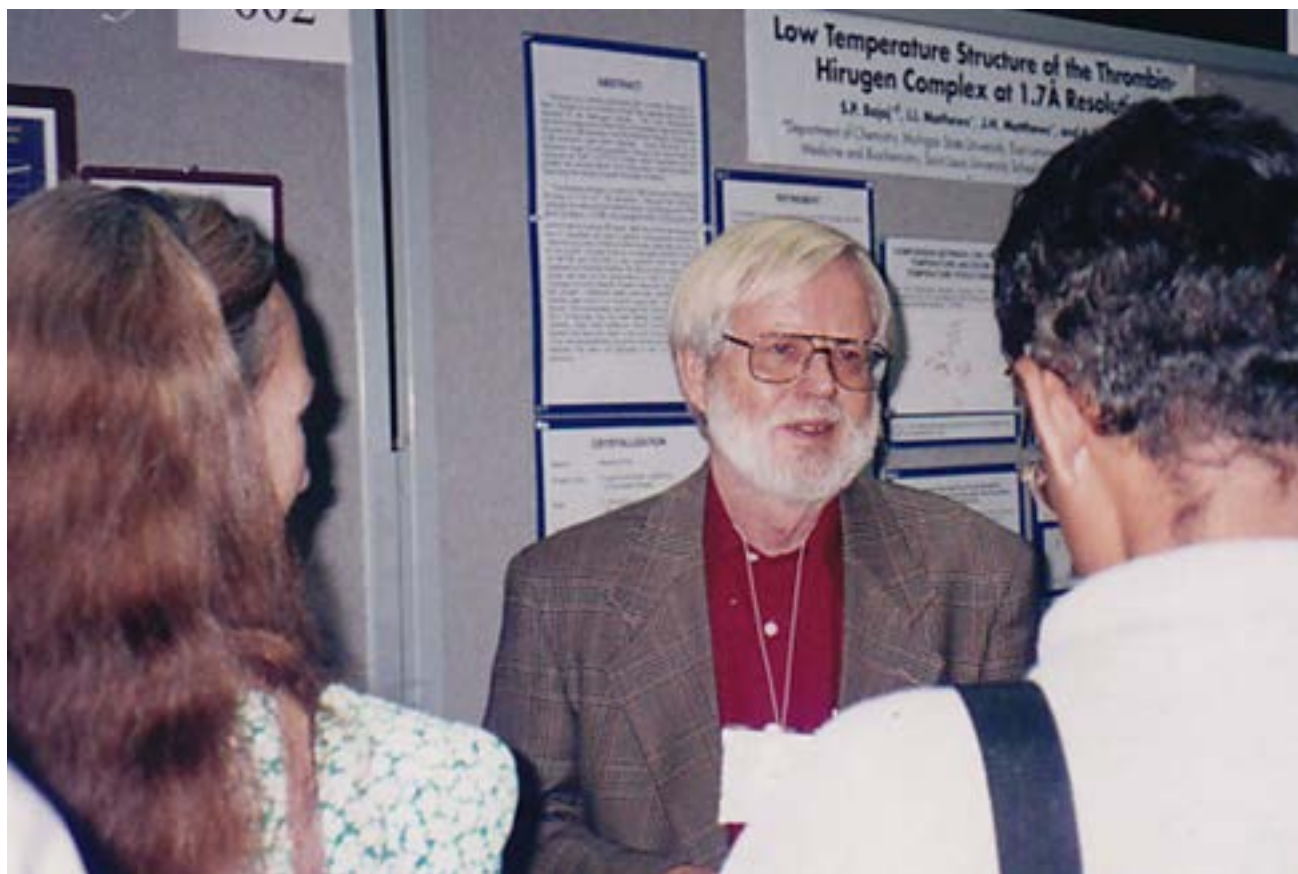
While being very humble as a person, he firmly believed in his theories. A classical example is from an early small meeting for the world's protein crystallographers. While everybody knew the theory of Caspar and Klug that all spherical viruses have icosahedral symmetry, one group presented an exception. Their virus was of cubic symmetry! As confident as Mendeleev was when one element (indium) didn't fit into his Periodic Table and when he frankly declared that the molecular weight must have been wrongly determined, so was Aaron Klug confident that all spherical viruses are icosahedral. So, Aaron interrupted the speaker and said "no that is wrong". When asked how he could know that, he answered "I can't explain it now here, but I will work it out tonight and tell you tomorrow. Please go on." And so he did; next morning he showed that the packing, *i.e.* the space group of the virus crystals, is cubic, but the symmetry of the virus particle is icosahedral. As with Mendeleev, of course he was right.

I was lucky enough to be a Pre doc with Aaron Klug at the LMB for 18 months 1978-1979, the closest I have been (and probably ever will be) to Heaven.

OBITUARY

Håkon Hope (1930-2018)

Martha Teeter with thanks to Marilyn Olmstead, Sean Parkin, Ada Yonath



Håkon Hope died peacefully at home in Davis, CA, USA, on 22 November 2018, surrounded by his family. Born in Førde, Sunnfjord, Norway, on 15 December 1930, Håkon attended the University of Oslo, earning his PhD with Nobel Laureate Odd Hassel as his supervisor. After a postdoctoral fellowship at UCLA on a Fulbright travel grant, Håkon was hired by the Chemistry Department of University of California (UC) at Davis in 1965, becoming full professor in 1973. As an Emeritus Professor of Chemistry at UC Davis since 1993, he remained active in teaching, mentoring students and colleagues, solving crystallographic problems and attending crystallographic meetings, contributing more than 200 publications.

Håkon is most remembered scientifically for his accurate data collection and cryocrystallography of small and particularly of biomolecules. He was a supremely gifted experimentalist, who also understood the physics of data collection better than most. His contributions to cryocrystallography date from his own postdoctoral and graduate student days in Norway, where he developed some of the early cryoinstrumentation. In 1967, he designed and built a cryostat for cooling crystals to about 110 K using a cold $N_2(g)$ stream for the (UC Davis) laboratory Picker diffractometer, according to Marilyn Olmstead, his postdoctoral fellow and Emeritus Professor of Chemistry, UC Davis. His careful specifications for the reduction of turbulence were key to preventing ice formation.

Sean Parkin, Håkon's last graduate student and now Director of the X-ray Facility at University of Kentucky, Lexington, USA, shares: "In terms of small molecules, he was decades ahead of his time. With Ulrich de la Camp, he was the first to demonstrate absolute configuration of light-atom compounds in the late 1960s [*Acta Cryst.* (1972). **A28**, 201-207]. As a follow-on from charge-density work with Fred

Hirshfeld, Ed Stevens (Håkon's graduate student in the early 1970s) and others, he devised experiments to extract accurate hydrogen atom positions from X-ray work [e.g. Hope and Ottersen (1978). *Acta Cryst. B* **34**, 3623-3626]. His work on rapid structure determination [Hope and Nichols (1981). *Acta Cryst. B* **37**, 158-161] presaged the current situation in small-molecule crystallography. His insight in that regard was that the data collection had to give sufficiently good counting statistics, and that scan rate was just one factor involved."

Håkon was the first to apply low temperature combined with a unique mounting technique to protein/ biomolecule crystal data collection. When I met him in 1984, he cleverly devised a way to stabilize pyrophoric small molecules for cryocrystallography using a drop of neutral oil at the end of a fine capillary mounted in a copper pin. With this ingenious method, he could mount the crystal air free, cool it in liquid nitrogen, and transfer it to a nitrogen stream on a diffractometer. He made special tongs with a high thermal mass block to keep the crystal cool from the microscope to the diffractometer.

At the Stanford American Crystallographic Association (ACA) meeting in 1985, we discussed extending his method to protein crystals. We proposed cooling crystals of the small protein I was studying (crambin) to liquid nitrogen temperatures with his method. Later that year, he collected X-ray data to 0.83 Å resolution and 130 K. This cooling greatly reduced thermal vibration, enhanced the intensity of data at higher resolution, permitted stable, full-matrix refinement and clear modeling of more disorder in side chains and solvent that was present only weakly at 300 K.

Another example of Håkon's inventiveness and experimental prowess came to my attention in 1987. I was visiting the Weizmann Institute (Rehovot, Israel) and found that Håkon was also there. He had just created a small glass double-platform support for ribosome crystals grown by Ada Yonath of the Weizmann Institute. With this physical stabilization and application of liquid nitrogen to the crystal, they were able to considerably extend the lifetime of ribosome crystals in the X-ray beam. It was this pivotal event, coupled with Ada's persistence in looking for better crystals and large heavy-atom clusters, that led her and others to the solution of the ribosome structure and Ada's sharing the 2009 Nobel Prize in Chemistry.

Ada summarizes the significance of Håkon's cooling methods: "Håkon's bold attitude led to the development of what became routine in the entire field of biomacromolecular crystallography almost instantaneously, within less than half a year. Thus, not only several ribosome structures could be determined at atomic resolution, over 50,000 new and significant biological structures were elucidated at cryotemperature, many of which were not suitable for the traditional data collection for various reasons."

He continued to develop these cryocrystallography techniques for biomolecules and popularize them. Later he extended them to liquid helium data collection. He worked closely with several synchrotron sites to freely share his experimental procedure and apparatus.

Håkon delighted in teaching crystallography both in class and in informal conversations, at UC Davis Chemistry, at ACA and at IUCr meetings, which he attended since 1968, hardly missing one. He mentored generously, always advocating for his very high standards of data collection and refinement for determination of accurate structures and engaging young and older scientists in the discourse. At UC Davis, he also made "crystallography available to members of the (Chemistry) Department. The possibility of doing crystal structures was exciting for many members of the faculty and the X-ray lab became a significant resource for their research," reports Marilyn Olmstead.

Håkon challenged many to think about their crystallographic data and refinement in order to create the best possible structures. He was able to ensure this attention to detail on an international level as a member of the IUCr Commission on Crystallographic Apparatus (1978-1984) and Co-editor of *Acta Crystallographica* (1984-1993). In 1994, Håkon received the Doctor Honoris Causa from the University of Oslo, Norway. In 2015, Håkon was elected a Fellow of the ACA.

Håkon will be deeply missed by his crystallographic colleagues, both as a friend, colleague and mentor.

OBITUARY

Thomas A. Steitz (1940-2018)

Poul Nissen



Few have exemplified the scale and impact of macromolecular crystallography like Tom Steitz. His lifelong passion was to bring chemical and biophysical mechanisms to life, and it drove him to the frontiers of what crystallography can do, and how to move them.

After his PhD studies with William Lipscomb on carboxypeptidase and postdoctoral studies with David Blow on the structure and mechanism of chymotrypsin, Tom moved first to Berkeley and then to Yale to set up his own research. Early on he presented pioneering studies of large-scale conformational changes in hexokinase that were associated with substrate binding and catalysis. These experiences stayed with him and became a lasting part of his anecdotes and advice. Quickly, Tom's research became devoted to the key principle of life – the central dogma that describes how genetic information in the form of DNA is transcribed into RNA and translated into proteins of function. Understanding how these processes take place and have evolved define our insight into life as we know it, and it was also very complementary to the grand work of his wife Joan Steitz, who had started her pioneering work on RNA through ribosomes and translation. Dedicated to his quest for the mechanisms of the central dogma, Tom's laboratory presented numerous first-in-class structures of protein–DNA and protein–RNA complexes.

As an undergraduate I learnt of his works from Stryer's *Biochemistry*. Later as a PhD student I came much closer to it. I was a student of Jens Nyborg at Aarhus University and worked on the crystal structure of the ternary complex of translation elongation factor EF-Tu, GTP and aminoacylated tRNA. Jens and Tom knew each other from the Blow lab, and we had heard rumours that Tom was also interested in that project after a successful attempt at the related elongation factor G, the ribosomal translocase, together

with Peter Moore. Fortunately, I had the opportunity to meet him at the famous Erice School of Crystallography in 1994. That went well – he was easy to approach for a young scientist like me back then, and when I asked he responded, *e.g.* on their experiences with RNA modelling and refinement, sugar pucker, *anti* and *syn* conformations *etc.* The aminoacyl-tRNA:EF-Tu:GTP project had not really taken off in his laboratory. His honest care and interest for what I had to say and wanted to ask were warming and encouraging, and in science where so many consider it a race for trophies, the openness of his aims, strategies and very preliminary work was unusual and quite an example to follow. As he always put it – it is just not fun if what we are really happy about and want to talk about should remain a secret.

Later that year Peter Moore visited Aarhus and presented the EF-G structure from Yale that he and Tom had determined together with John Czworowski and Jimin Wang (and that Arnthor Aevarsson, Anders Liljas and colleagues had also determined independently in Lund). In 1995 Paul Sigler also came to Aarhus, and he invited me to visit Yale, which I then did the following year after the very first and very exciting meeting of the RNA Society in Madison. To cut a long story short, it was an overwhelming experience to interview all the star groups at Yale, which also included for example Jennifer Doudna, Donald Engelman and Axel Brunger – a superhero community originally nucleated around Fred Richards, and all those laboratories with the very best people.

I had no doubt that the ribosome project with Peter and Tom at Yale was definitely the best choice for a postdoc.

Joining Tom's lab was a transformative experience. When I arrived in 1997, postdoc Nenad Ban, lab technician Betty Freeborn, Peter and Tom had already established a small dedicated ribosome group targeting the *Haloarcula marismortui* 50S subunit that Ada Yonath's research groups in Hamburg, Berlin and at the Weizmann had also worked on for more than ten years, but without a breakthrough on phasing. Nenad however had obtained low-resolution phases and from two independent sources even: (i) a W18 tungsten cluster derivative producing a single major site, which could be determined from Patterson maps and that produced a very low resolution map, and (ii) by molecular replacement using an *H. marismortui* 50S envelope obtained by cryo-EM by Joachim Frank's group in Albany. The W18 site derived from both methods was identical – this was clearly before the days of the 'resolution revolution' in cryo-EM, and the consistency of the two methods was in itself highly rewarding. Very importantly, Nenad, Peter and Tom – with great input also from Jimin Wang, the wizard crystallographer in Tom's group – had just found out before I arrived that the 50S crystals had a very bad tendency for pseudomerohedral twinning. Some of the W18 derivative data sets would only produce Patterson peaks corresponding to a monoclinic form with twinning, whereas others clearly came from an orthorhombic form – $P2_1$ with $C222_1$ twin-symmetry or proper $C222_1$, respectively. That insight was game changing. With the W18 derivatives and compatible native data sets we could sort all data sets and distinguish them as either monoclinic twinned or orthorhombic using scaling statistics, and that was from just a few frames of indexed data during data collection at the synchrotron and using excellent advice in the *DENZO/SCALEPACK* package. After only a month we had identified another two heavy-atom cluster derivatives (a W11 cluster and Ta_6Br_{12}) and found the optimal combinations for MIRAS phasing extending to 9 Å resolution. We could publish the first crystallographic maps of the ribosome showing characteristic features of stalks and the central protuberance. Tom was super excited and came with numerous ideas and suggestions thereafter, including many old tricks from his chymotrypsin and hexokinase work. However, he knew very well how to prioritise ideas, which to go all out for and which to abandon quickly.

Our first step to extend the resolution was to obtain phases and maps from independent 50S crystal forms. One of the monoclinic twinned crystals was apparently only partially twinned – what if we could detwin it? Tom knew of some old Fortran code left in the lab by Adrian Goldman for a twin-fraction determination and a detwinning program that he had developed in the 1980s. We dug it out from old tapes and we also found Adrian's (absolutely brilliant) thesis, where the use of it was described. With help from postdoc Graham Cheetham we rewrote the code for the specific case of pseudomerohedral twinning in $P2_1$, got it compiled and ran it on the partially twinned data set. Amazingly, it worked: a twin

fraction of about 0.35 and the detwinned data set could be solved by the MR procedure. Using higher resolution data sets of the cluster derivative and the *MAMA* multi-crystal averaging program by Gerard Kleywegt and Alwyn Jones from the Uppsala Software Factory, we could extend the maps to 5 Å resolution and localize several structures of large ribosomal subunit proteins and of the ribosomal RNA. This was quite conclusive, we thought, and knowing that Venki Ramakrishnan had reached similar results on the 30S subunit (presented at the 1999 ribosome meeting in Helsinki), the road suddenly seemed to open up towards the finish line, albeit still at some distance. Tom felt it was time for his sabbatical, and he took it in his own lab working with us on the early map interpretations and model building attempts.

Tom insisted that now we gave up on the cluster derivatives and instead turn to ordinary heavy-atom derivatives that we could easily locate by difference Fourier maps – if only we had enough sites we would get a sufficient signal for phasing. Peter Moore further convinced us by calculating transforms of the cluster derivatives to demonstrate that their amplitudes would almost vanish at a broad intermediate resolution range, where the cluster scattering properties disappear due to individual atom scattering interfering destructively. Tom also insisted that we should try the wonderful Os-hexamine compound that Jamie Cate and Jennifer Doudna had used for RNA crystallography. We had a tiny, small sample and indeed it produced 14 sites from a 1 mM soak but we could not get any more of it, and the 14 sites were not quite enough. Instead, we got similar compounds – Ir-hexamine from Jamie and Os-pentammine from a commercial source. It turned out that we should simply soak with as much compound as possible, and using 20–35 mM crystal soaking conditions we identified more than 40 sites and combined SIRAS, MIRAS and SAD phasing that also included a few other derivatives. These procedures were all handled well by expanded versions of *CNS* provided by Axel Brunger and Paul Adams.

At the same time we had developed a procedure to grow thick three-dimensional crystals that reproducibly diffracted to at least 3 Å resolution. With great input from Jeff Hansen we also finally nailed the twinning problem so that all crystals were now reproducibly orthorhombic – we simply needed to keep crystals in 1.7 M NaCl or KCl, not 1.2 M as we had used earlier. A single batch of crystals diffracted even further and we managed to collect a 2.4 Å resolution native data set. Combining phases of 3–4 Å resolution derivative data sets, and performing a very gentle density-modification procedure at 2.4 Å resolution with a solvent sphere radius gradually diminishing from 12 to 2.4 Å (a great tip by Eric de la Fortelle of the *SHARP* group working with Gerard Bricogne), we ended up with electron-density maps of absolutely stunning quality revealing the entire structure of the 50S subunit and basically all details of the RNA and the protein main and side chains. What a moment that was, after years of work – seeing thousands of nucleotides and more than 30 proteins reveal their intimate structure of the 50S subunit and with the peptidyl transferase centre at the middle – the ultimate link between genes and proteins in the central dogma.

Over a few months several of us, now also including PhD students Szilvia Szep, Martin Schmeing and Dan Klein, would trace individual proteins and RNA segments. We were greatly helped by an experimental version of *O* for RNA provided by Morten Kjeldgaard and we could carry out real-space refinement with *TNT*, and finally reciprocal space refinement of the entire 50S subunit with *CNS*. It all just clicked.

It is often said that Tom could have received numerous Nobel Prizes for his work on, for example, tRNA synthetases, RNA and DNA polymerases, and reverse transcriptases, and I couldn't agree more. He really knew how to keep difficult projects going forward, and during my three years as a postdoc on the 50S subunit I never doubted that we were guided in the right direction and always made progress. He would also, in general, be very aware and clear whether a project was 'ripe' or not for structural biology, and he would give strong warnings against simple projects that would not tell us much but would still take time, such as determining structures of individual domains of a protein, where the complex with another macromolecule was the actual goal.

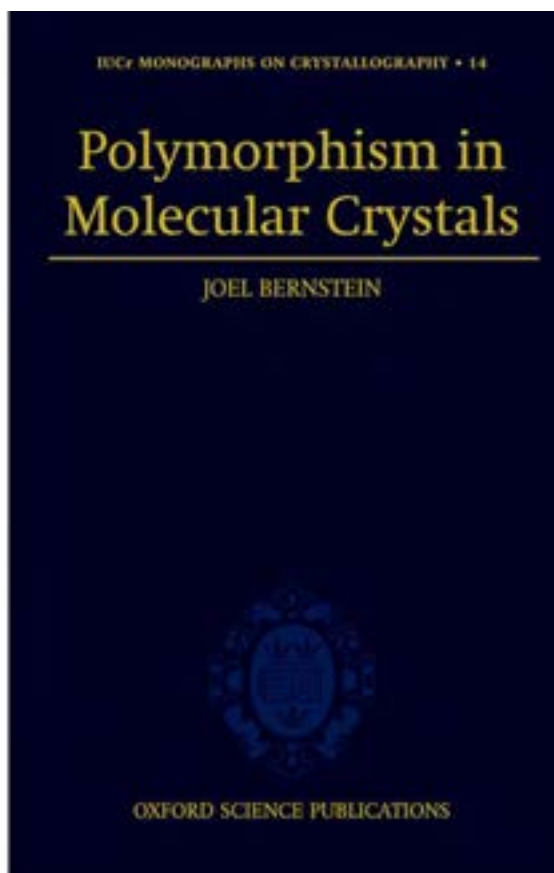
With Tom Steitz's passing we have lost a true hero and superhero of crystallography. In times where we all turn towards cryo-EM we should never forget that crystal structures paved the way and still produce the best and most accurate structures. In hindsight, it is also clear how methods developments in crystallography made it all possible – the developers should be remembered also, and Tom did that.

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OBITUARY

Joel Bernstein (1941-2019)

Ehud KeinanMenahem Kaftory, with recollections from Sonke Adlung (Oxford University Press)



Joel Bernstein at the banquet during the IUCr Congress in Geneva, Switzerland, in 2002, of which he served as Chair of the Organising Committee, and the cover of his famous book.

Joel Bernstein was born on 12 September 1941 in Cleveland, OH, USA, son of Philip and Florence Bernstein. He obtained his BA degree in chemistry from Cornell University (1962) and then after a move to Yale University to study physical chemistry he obtained an MSc in 1964. Continuing at Yale he worked with Basil G. Anex on the solid-state spectroscopy of organic compounds and received his PhD in 1967. Following two-year postdoctoral stints in X-ray crystallography with Ken Trueblood at UCLA and in organic solid-state chemistry with Gerhardt Schmidt at the Weizmann Institute of Science (Israel), he joined the Department of Chemistry of the newly established Ben-Gurion University of the Negev. Later he became the Barry and Carol Kaye Professor of Applied Science at Ben-Gurion University.

Joel's research interests focused on organic solid-state chemistry, chemical crystallography, polymorphism, hydrogen bonding, graph sets, structure–property relations in organic solids, organic conducting materials and pharmaceuticals. He is known for using graph sets to describe hydrogen bonding patterns for comparison and understanding the forces governing structural organizations.

Joel published over 180 research and review articles and book chapters. His well known book *Polymorphism in Molecular Crystals*, published in the IUCr/Oxford University Press (OUP) Book Series and translated into several languages, has become a highly authoritative reference in its field. He published several landmark papers such as *Patterns in Hydrogen Bonding: Functionality and Graph-Set Analysis in Crystals* (Bernstein *et al.*, 1995), *Disappearing Polymorphs* (Dunitz & Bernstein, 1995) and *Graph Set*

Analysis of Hydrogen-Bond Patterns in Organic Crystals (Etter *et al.*, 1990), which combined have more than 9800 citations (Web of Science).

In recent years, he focused on polymorphism of molecular crystals and crystal engineering, using the tools of supramolecular chemistry, and the design and preparation of co-crystals of organic molecules. His group made significant progress in developing a successful strategy for the controlled preparation of co-crystals with a pre-designed structure by recognizing and utilizing specific intermolecular interactions. Their studies involved a statistical analysis using the Cambridge Structural Database, high-level molecular orbital calculations and proof-of-concept experiments on prototypical model compounds. Many subsequent experiments, designed to exploit the principles demonstrated by the proof-of-concept experiment, were successful while others produced unknown crystal forms.

Joel had served as a consultant to many pharmaceutical companies worldwide, including Leo Pharma, Johnson & Johnson, AstraZeneca, Roche, Organon, Sanofi-Aventis, Eli Lilly, Chemagis, Agan Chemicals, Rechter Gideon, Pfizer Pharmaceuticals, Warner-Lambert Pharmaceuticals, TransForm Pharmaceuticals, Millennium Pharmaceuticals, Abbott Laboratories, SmithKline Beecham, Unipharm, GlaxoSmithKline, Teva Pharmaceuticals, 3M Company, Bethlehem Steel Corporation and Plantex Pharmaceuticals. In particular, he served as a testifying witness in litigations on the solid-state chemistry of drugs.

His career was punctuated by visiting professorships at the University of Illinois, Cornell University, University of Minnesota, University of Barcelona (Spain), Cambridge Crystallographic Data Centre (UK), Rand Afrikaans University (South Africa), University of Bologna (Italy), University of Johannesburg (South Africa), Australian National University and Osaka University (Japan). He was a Professor-at-Large at the University of Western Australia, and later became Global Distinguished Professor of Chemistry at New York University Abu Dhabi. In 1999, he was elected a Fellow of the American Association for the Advancement of Science.

Joel was a member of many Editorial or Advisory Boards of scientific journals including the *Israel Journal of Chemistry*, *Structural Chemistry*, *Zeitschrift für Kristallographie*, *Crystal Engineering*, *Crystal Engineering Communications*, *Crystal Growth & Design* and *Journal of Pharmaceutical Sciences*. He was also a member of the IUCr/OUP Book Series Selection Committee. He served the scientific community as President of the Israel Crystallographic Society; as the Israeli representative to the European Crystallographic Committee; and as chair of multiple international meetings, symposia, summer schools and international prize committees. He was an active member of the community of European crystallographers, and a driving force in the formation of the European Crystallographic Association (ECA) and the establishment of the ECA Prize (now Max Perutz Prize).

Joel served Ben-Gurion University on multiple assignments including Director of Undergraduate Studies, Director of Graduate Studies, Chairman of Graduate Studies Committee of the Faculty of Natural Sciences, Vice-Chairman of Chemistry, Steering Committee of the Board of Governors and University Supreme Committee on Appointments and Promotion.

On a personal level, Joel was a true colleague and friend, and his vivid personality and rolling laughter will be remembered by his many friends. He spoke enthusiastically about solid-state chemistry, crystallography and polymorphism, as well as other subjects of science. He was a gifted lecturer who attracted large audiences to packed lecture halls.

Joel married Judy Hurevitz in 1966 (deceased 2001). He passed away on 2 January 2019 and is survived by his two sons from his first marriage, Etan Bernstein and Noam Bernstein, and his wife, Tzipi Eynot.

The Israel Chemical Society, the entire community of Israeli scientists and the world of science mourn the loss of a great scientist.

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Recollections from Sonke Adlung (OUP)

It is a privilege to add a few of my recollections in the aftermath of the entirely unexpected passing of Joel Bernstein. I had the pleasure of meeting Joel first in the mid-1990s, when I started my career as an editor at Oxford University Press. I subsequently worked with him towards publication of his landmark monograph *Polymorphism in Molecular Crystals*. From the outset, I knew Joel to be a tough but pleasant and entertaining negotiator of general ease, first over the phone, then at many meetings. Writing a book like the 1948 classic by C. W. Bunn, *Chemical Crystallography*, was his inspiration, 'a boy's dream', as he later called it. No detail was left without consideration, the page layout, the colour plates, the indexed reference list (unusual, but very helpful), the pricing, the cover in the traditional OUP style, cloth binding and brass blocking. The book was published in May 2002, and immediately became one of the bestsellers at the IUCr Congress in Geneva in the same year, and one of the highlights of the whole of the IUCr/OUP book programme.

Joel showed an amazing commitment to the crystallographic community. Besides his own book and research, and a host of university and wider academic duties, he served as a member of the IUCr/OUP Book Committee, introduced us to new authors, kept us posted about forthcoming awards and meetings, proposed new members to serve on the Committee, and was also closely engaged in issues of sales and marketing. During a trip to South America in 2013, he became the driving force of our sales efforts in Brazil in particular.

It was always a special treat to listen to one of Joel's many interests, starting from science, and including a wide range of related subjects, history, archaeology, law. He was a great storyteller, and there is no doubt that there was at least one other book in him. He knew many renowned scientists and loved to tell about their work but also talk about their backgrounds, their personalities and the connections between them. Joel's stories were always appreciated by his colleagues and also by students all over the world who remained speechless to his wide and endless knowledge. The promise to his wife Tzipi was that his next book would be a collection of these stories. The experience of being involved as an expert witness in a number of patent litigations, and of consulting on issues of polymorphism and crystal forms, inspired him to think about yet another book of the popular science type, a primer for lawyers who are getting into litigations and need to understand at least some of the science involved. While the idea was on and off, in the end it did not materialise.

Keeping *Polymorphism in Molecular Crystals* up to date, however, remained a firm commitment. He drafted first plans for a second edition in 2009, and submitted a formal proposal shortly after the IUCr Congress in Madrid a couple of years later. Despite life becoming 'more complicated' (as Joel put it) and work on the book repeatedly coming to a hold, whenever asked, he made it crystal clear that there was absolutely no inclination to forego or give up on the 2nd edition. Finally, in May 2018, after two years of intense pursuit of the required revisions, we had the pleasure of a celebratory dinner with Joel in Oxford, marking the formal handover of the completed work. It was the charming *modus operandi* he had already chosen some 17 years earlier for the handover of the first edition. For the second, it is tragic that

Joel's best efforts didn't pay dividends for him to see the published book. Extent and price are going to increase, I am afraid to say, but all in line, I hope, with the spirit of our understanding and mutual expectations.

We will miss Joel as an author. We will miss his company, his insights, and the enjoyable discussions at meetings of the crystallographic community. Needless to add, as a publisher, my hope is that his passion for science will live on in the book, and help future generations of readers become as enthusiastic about their studies as he was throughout his life.

IUCR SUPPORTED EVENTS

IUCr supported meetings

These forthcoming meetings are supported by grants from the IUCr Calendar Committee.



**11th Oct 2026 - 16th
Oct 2026**
Indaba10

Skukuza, Kruger National
Park, South Africa



**5th Dec 2026 - 10th Dec
2026**
*African Materials Research
Society (AMRS 2026)*

Nairobi, Kenya

MEETINGS CALENDAR

Meetings calendar

This is a list of meetings of interest to crystallographers occurring within the next twelve months, as recorded in the IUCr Calendar of Events. Please let us know of any that are missing by [completing this form](#) or sending an email to forthcoming.meetings@iucr.org.

	Indaba10 South Africa 11th Oct 2026 - 16th Oct 2026
	Synchrotron Radiation: Science, Knowledge, Innovations, Future (SKIF-2026) Russian Federation 18th Oct 2026 - 23rd Oct 2026
	CCP-EM/Diamond Icknield Workshop United Kingdom 9th Nov 2026 - 13th Nov 2026
	Instruct-ERIC hands-on workshop on Advanced cryo-FIB-SEM methods Germany 9th Nov 2026 - 13th Nov 2026
	Crystal36-AXAA 2026 Meeting Australia 26th Nov 2026 - 2nd Dec 2026
	African Materials Research Society (AMRS 2026) Kenya 5th Dec 2026 - 10th Dec 2026
	Joint Polish-German Crystallographic Meeting 2027 Germany 15th Feb 2027 - 18th Feb 2027

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Director, ICCBS