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LETTER FROM THE PRESIDENT

Best wishes for 2023



LACA V poster-prize award ceremony. Eduardo Gutierrez (second from right) receives his IUCr Journals/structural chemistry prize from IUCr President Hanna Dabkowska (far right) and IUCr Executive Committee member Graciela Díaz de Delgado (third from right). Also pictured (from left): Natalia Alvarez, Session Chair; Andrea Araya, Conference Chair; and José Reyes-Gasga, LACA President.

Hanna Dąbkowska

Here we are approaching the end of 2022. Already. Some of us are getting ready for Christmas (or at least for a short vacation and some family time), others just want to finish this year and move to a new one.

Whereas internet teaching and hybrid meetings will stay with us for good we can now plan for limited travel and for some irreplaceable gatherings in person.

I am just back from the Fifth Meeting of the Latin American Crystallographic Association (LACA), very well organized in a hybrid mode by Andrea Araya in San José in Costa Rica. A lot of progress has been made since the creation of LACA in 2013. Some legal aspects still have to be smoothed out but the energy of the crystallographers there cannot be underestimated. The Fifth LACA School, organized by Andrea Araya and José Reyes-Gasga on the subject of “Polymorphism: Applications in Industry”, was hosted in the Costa Rica National Center for High Technology facilities (hybrid again). It was well attended by students from the LACA region.

In Africa the OpenLab program is slowly coming back after the COVID-induced break. We hope for the active involvement of all the major vendors of crystallographic equipment. Claude Lecomte has organized the first, very successful OpenLab in Mauritania in November 2022; the next one will be coming in May 2023 in Franceville (Gabon). Michele Zema, the IUCr Executive Outreach Officer, has reported that 15 students from Benin, Burkina Faso, Cameroon, Côte d’Ivoire, Ghana, Guinea, Nigeria, Senegal as well as Jamaica and India were selected to participate in the two-week training session on single-crystal diffraction at the X-TechLab in Benin from 21 November to 2 December 2022. Students could bring their own crystals and collect data using the new Bruker AXS D8 Eco diffractometer, which was also used for tutorials and demonstrations. The X-TechLab, funded by the Benin Government and whose implementation was facilitated by IUCr–IUPAP–ICTP *LAAAMP* within the framework of the IUCr-UNESCO OpenLab, is now operational and open for collaborations with researchers from all over Africa. New instruments, including a Panalytical Empyrean powder diffractometer and a microtomograph, will be installed soon and available starting from early next year.

The world is still not a safe place. A brutal war is raging in Ukraina. The scientific community is trying to help displaced Ukrainian researchers. The Polish Academy of Sciences (PAS) and the U.S. National

Academy of Sciences have recently launched a grant program to support Ukrainian research teams. The design of the grant program allows scholars in Ukraine to continue research under the supervision of experienced principal investigators from Ukraine, hosted for up to three years at the PAS. The deadline for grant applications is 16 January 2023.

In Ethiopia we have just had to cancel the IUCr–COSPAR Workshop ”Crystallography for Space Sciences” due to safety concerns. In Iran and other places in the world men and women are fighting for political and social freedom. In Afghanistan women are recently being forbidden to study at the Universities.

As a member of the International Science Council (ISC), the IUCr supports the right to share in and to benefit from advances in science and technology as described in the Universal Declaration of Human Rights and it is very concerned about increasing threats to scientific freedom and other human rights around the world.

At the forthcoming IUCr Congress in Melbourne in August 2023, the General Assembly delegates will vote on formally incorporating our fifth Regional Associate, the African Crystallographic Association (AfCA) – constituted in November 2021. To commemorate this special event, and to mark the 75th anniversary of the first IUCr Congress and the first volume of *Acta Crystallographica*, IUCr Journals are planning to put together a special collection of articles from African researchers, which will be published online to coincide with the Congress.

Please plan to come to Melbourne; it will be an amazing Congress, with many attractions and a very strong program. The abstract submission deadline has been extended to 21 February 2023 so there is still time to present your best results. In recognition of retired crystallographers’ long-term dedication and outstanding contributions to our community, the Congress Organizers have decided to offer them a reduced registration fee. The retiree rate is only available for the Early Bird period, which ends on 31 March 2023. The IUCr President's Fund application deadline is 18 March 2023.

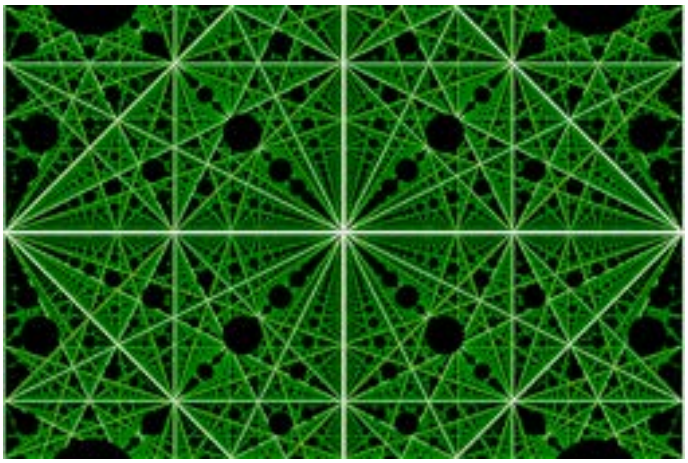
If you have a free minute during the holiday break, please check your entry in the *World Directory of Crystallographers* (WDC). There is a chance that it has not been updated for some time. If you are a Commission Chair, please also check to see if your Members and Consultants are included in the WDC. It all adds up to creating and strengthening this community.

I am also encouraging you all to start (or continue) participating in the IUCr Crystal growing competition for schoolchildren. Other international scientific organizations are copying this very successful program and we are very proud of this fact. Elementary and high-school students need to understand at an early age the beauty of science, and there is a lot of satisfaction from the side of students and coaches when amazing crystals are being presented and highly prized on international forums! See a report from Poland in an earlier issue of the *IUCr Newsletter* here and one from Vietnam in this issue here.

With the end of December approaching fast I want to wish you all a happy and joyful 2023. We intend to make it a successful and important Congress Year. We just hope it will also be healthy and safe.

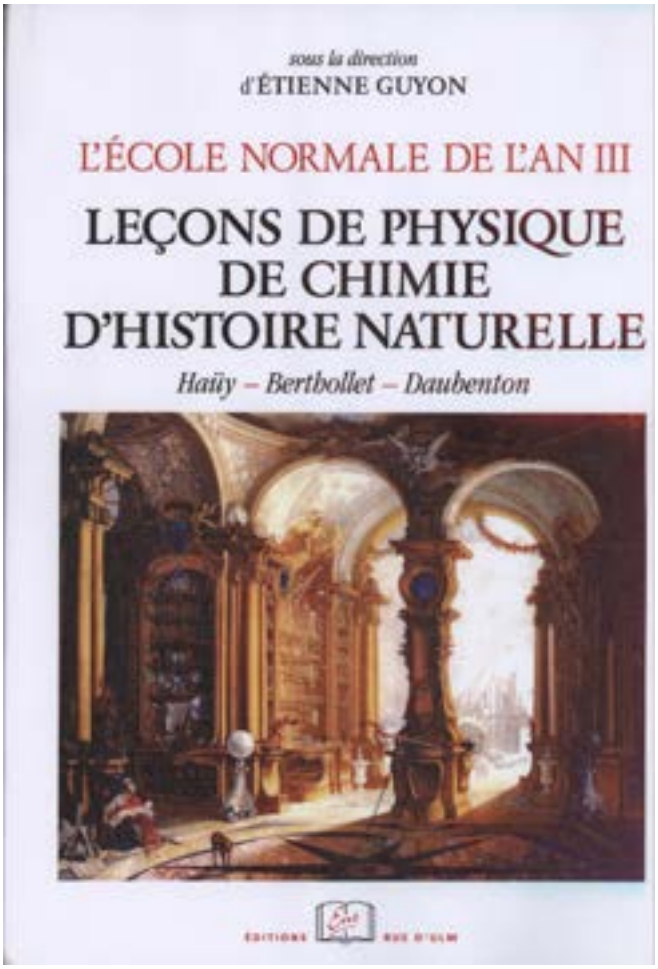
EDITORIAL

Editorial



Mike Glazer

Every quarter, as Editor, I get anxious that we shall not have enough material to publish in the following issue of the *IUCr Newsletter*. But fear not; somehow, the articles keep coming in, often at the last moment, especially recently. So, in this issue of the *IUCr Newsletter*, we have much interesting material. I have always encouraged articles on the history of our science, as I believe that it is important for scientists to be aware of how our forefathers struggled to come up with the ideas that today we take for granted.



For example, Jean-Claude Boulliard, Delphine Cabaret and Paola Giura have written an important and detailed account of the life and work of the French cleric René-Just Haüy, sometimes regarded as the

father of crystallography. Based on an observation of a broken crystal of Iceland spar (calcite), he inferred that crystalline matter consisted of repeating units (he did not know what they consisted of), which he called "*molécules intégrantes*." Although he was not the first to think in such terms – Robert Hooke and Johannes Kepler, for example, also suggested something similar – but it was Haüy who put this on a more scientific basis, for example, through his law of rational indices. We forget, however, just how controversial, and even dangerous, such ideas were in the time and place that he lived (France in the 1790s). Materialism at that point came to be indissociably associated with atheism and atheism with political enemies of the French government. As an example of how Haüy had to be careful, there was an interesting series of lessons published in the archives of the École Normale [1] at the time between someone simply called the "Professeur" and a pupil on the question of heterogeneity or otherwise of solid matter. It is evident that the "Professeur" is Haüy of course!

Readers may recall that some time ago, we published several articles in the *Newsletter* about the work of Juan Manuel García-Ruiz ("Juanma") (see an example here) and his study of crystals found associated with the remains of ancient hominids. In this issue, there is an article by Wulf Depmeier celebrating the well-deserved award of the DGK Liebau Prize to Juanma earlier this year. This is followed by an article from Juanma himself, describing some fascinating experiments with chimpanzees where they were introduced to crystals. Most thought-provoking is the way that, given a crystal of quartz, they soon began to take a particular interest in the apparent hexagonal symmetry as seen by looking down the long axis of the crystal. So there seems to be something special about symmetry that causes a response in the chimpanzee's brain, supporting Juanma's original suggestion that the discovery of crystals may have played an essential role in the original development of thought processes in humans and an awareness of their surroundings.

Another topical article is a contribution from Istvan Hargittai, this time on the observation of the so-called star polyhedra, a motif that seems to appear in many places. Again, it is the symmetry that attracts attention.

And yet again, the importance of understanding symmetry for crystallographers is raised by Carol Brock, who points out that the IUCr has now made freely available the symmetry diagrams for the 17 plane groups (also known as the wallpaper groups). Carol also reminds us of Escher's wonderful drawings. Escher's work had been initially spotted by the crystallographer Caroline MacGillavry, who subsequently brought Escher's work to our attention. I expect that all crystallography teachers have used such drawings to illustrate symmetry principles to students, especially regarding the concept of periodicity in crystals. I would make a point here, though, that the plane groups are two-dimensional symmetry groups, whereas there are no really two-dimensional crystals: atoms are three-dimensional, aren't they? However, it is perfectly possible to have three-dimensional materials, such as graphene, whose periodicity is only two-dimensional (best described by one of the 80 sub-periodic layer groups). In assessing crystal symmetry, it is important to distinguish between crystal structure on the one hand and the concept of periodicity (usually described by the lattice) on the other.

Again, on the historical theme, Brian Toby has written in memory of Ted Prince, Tony Santoro and Judy Skalick, who are no longer with us. They were three important figures who worked at NIST (National Institute of Standards and Technology, USA) for many years and were well known to many of us. I did not know Judy very much, but I remember several discussions with Ted and Tony. Ted was a formidable mathematician whom I found to be most impressive. Tony had strong opinions, which he expressed freely. My discussions with Tony were always enjoyable and lively: a great character.

Talking about history, 2023 marks the 75th anniversary of the IUCr, founded just after the terrible period of World War II. Jenny Martin has announced that crystallographers around the world will be invited to participate in a refresh of the IUCr's vision/purpose and values through an online survey in 2023 with the results to be announced during the International Crystallography Congress in Melbourne later that year. By the way, you can find out details of the Congress here.

As usual, we have some obituaries. Sadly, this time all of them were personal friends. Václav Janovec was a colleague working in the scientific area relative to my own research, namely the crystallography of ferroelectrics, and someone with whom I used to discuss symmetry and domain effects in crystals. Ian Munro was the person I first met when I began carrying out early experiments using the NINA synchrotron in Daresbury (UK) and was an enabler for us to carry out experiments, often under challenging conditions. Basia Oleksyn was a friend whom I used to meet during my visits to Kraków, Poland, in the 1980s.

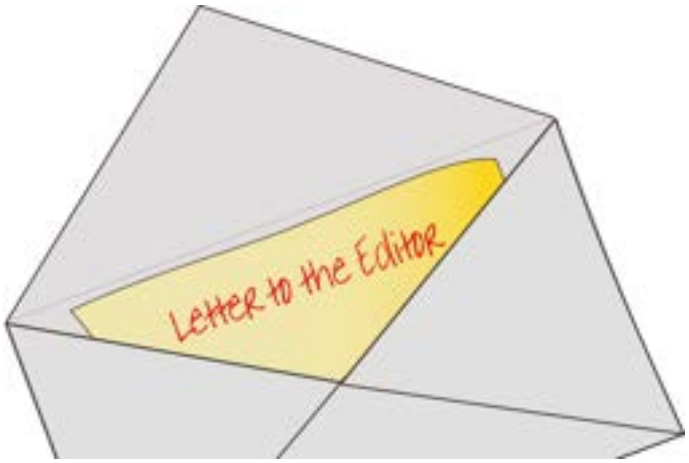
Finally, on a more cheerful note, I am pleased to be able to congratulate Richard Welberry for his award of the Bragg Medal for his work on diffuse scattering, received during the recent meeting of the Society of Crystallographers in Australia and New Zealand (SCANZ) held in Bendigo.

Note

[1] I am grateful to Caroline Warman of Jesus College Oxford for drawing my attention to this document.

LETTER TO THE EDITOR

An open letter to the IUCr leadership regarding the current protests in Iran



Shanti Deemyad

12 December 2022

Iranian scientists have been an integral part of the global scientific communities and continuously contributed to the advancement of science and technology. I graduated from Sharif University of Technology in 1998 with a degree in Physics and moved to the west to continue my education. Today, more than half of my life has been spent far away from Iran and is dedicated to scientific research and education. However, I never felt far from the Iranian academic community, as the scientific community around the world is inherently connected. The past three months have been exceedingly troubling times for the Iranian scientific community and students. Today, I'm writing this letter to ask the IUCr leadership, a community that I've been connected to for many years, to voice their support for Iranian academics and researchers in these anxious times.

Iranian women are leading a cultural renaissance with massive support from the university students with the rallying cry "Woman, Life, Freedom". University campuses have been at the center of the waves of protest sweeping through Iran, and the academic community of Iran has suffered enormous damage. Hundreds of students have been arrested on campus and sent to prison, University administrations in Iran have been complicit in the abduction of student protesters on campus and have additionally expelled a large number of students for participation in on-campus protests. As such, the academic career of many scientists, who are amongst the brightest minds of Iran, is in disarray and their lives are in danger. University campuses have a universal standing as places for fostering the free exchange of ideas, including peaceful protests. As scientists, there is a tie that binds us to these students and requires us to protect their right to free speech on campus. While the context of this letter is the ongoing struggle for political and social freedoms in Iran, my request is only about the catastrophic consequences of government crackdown in academia. As do all professional societies, the IUCr has also taken positions where political strife and violence has threatened scientists. My hope is that this effort shows our solidarity with and helps avert further harm to the academic community in Iran. I would like to encourage the IUCr to reiterate the following shared values in an open letter and

Clearly condemn the attack and arrest of students and professors in Iranian Universities.

Reiterate its commitment to free speech on University campuses worldwide.

Condemn violence on university campuses.

Ask the Iranian Universities to reinstate students and scholars who have been dismissed or suspended due to participation in peaceful protests.

State its support for free and open internet access for all University students and faculty in Iran.

Demand the release of student and faculty members arrested due to protest from Iranian prisons.

Thank you for your consideration,

Respectfully



Shanti Deemyad

Relevant news links

The New York Times: 'Geniuses' Versus the Guns (6 October 2022)

Nature: 'I could not keep silent' (12 October 2022)

Physics Today: STEM scholars worldwide express solidarity with Iranian protesters (19 October 2022)

Oslo based Iran Human Rights Asks Universities Worldwide to Condemn the Islamic Republic's Encroachment of University Campuses (30 October 2022)

The Guardian: Dozens arrested as Iranian security forces attack university campuses (4 November 2022)

ISNA (Iranian government news agency, use Google Translate): Disciplinary actions against protesters at Sharif University, including the suspensions of 10 students in one day (19 November 2022)

Universityworldnews: Students barred from campuses as state steps up crackdown (22 November 2022)

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FEATURE ARTICLE

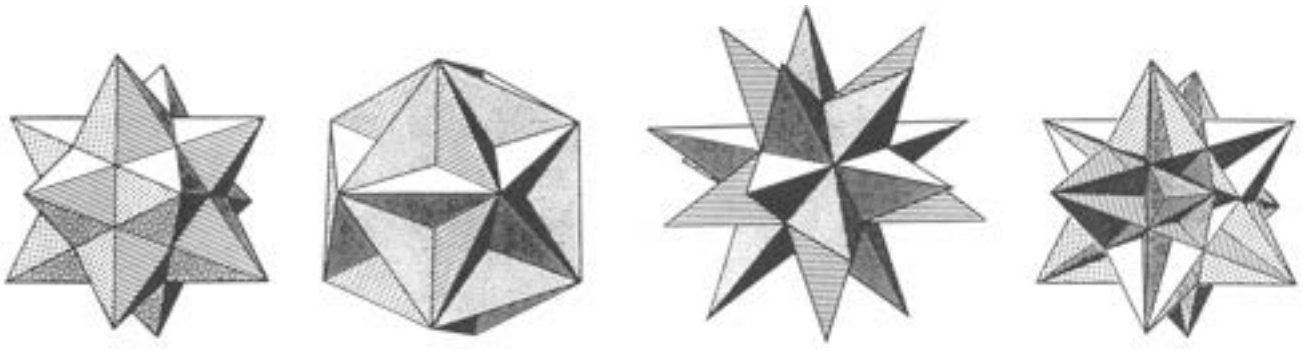
Star polyhedra



Detail of the interior of the shopping mall at One Columbus Circle, Manhattan (photograph by the author).

Istvan Hargittai

Let’s start with some definitions [1]. There are five regular polyhedra: the tetrahedron, cube (hexahedron), octahedron, dodecahedron and icosahedron. They are also called Platonic solids because they were an important component of Plato’s natural philosophy. The faces of the regular polyhedra are regular polygons: regular triangles, regular pentagons or squares. A regular polyhedron has regular and equal faces, and their vertices are surrounded alike. When we speak about the five regular polyhedra, a qualifier should be added: they are *convex* regular polyhedra. A polyhedron is convex if every dihedral angle is smaller than 180°. The dihedral angle is the angle formed by two polygons joined along a common edge. If the convex restriction is lifted, the number of regular polyhedra rises from five to nine. The additional ones are the four regular star polyhedra, depicted here after Cundy & Rollett [2].



The four regular star polyhedra from Cundy & Rollett [2], from left to right: small stellated dodecahedron, great dodecahedron, great stellated dodecahedron and great icosahedron.

My interest in the star polyhedra dates back to an accidental “discovery” in the early 1990s. At that time, it was still possible to climb out onto some small balconies at the top of St Peter’s Basilica, Vatican City (such adventures have been blocked since because of safety precautions — I learned about this during a subsequent visit). A captivating view appeared from one of those small balconies: it was a bird’s eye view of the Sacristy of the Basilica. At a closer look, a beautiful star polyhedron could be seen, just beneath the cross. This experience initiated some studies and inquiries [3].

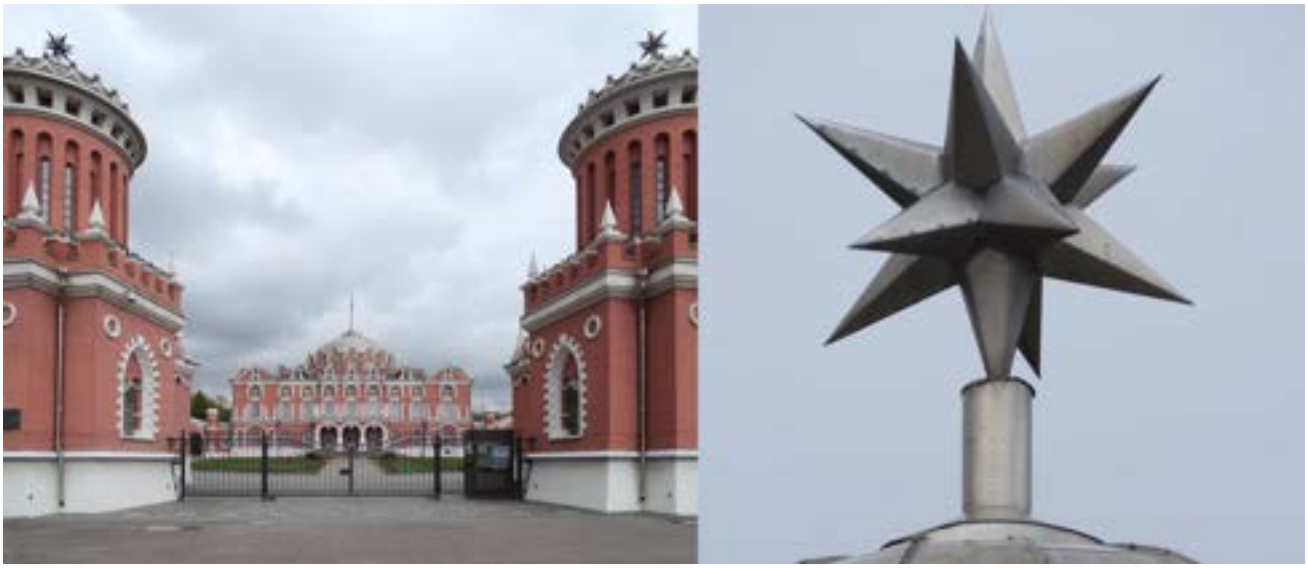
The Sacristy was built by the architect Carlo Marchionni in the years 1776–1784. The beautiful star polyhedron at its top is a great stellated dodecahedron, also called Kepler’s great stellated dodecahedron. However, it is not perfect, as two of its 20 triangular pyramids are missing in order to accommodate the vertical stand of the cross above the polyhedron.



Left: the Sacristy of St Peter’s Basilica in Vatican City, as viewed from one of the small balconies at the top of the Basilica. Right: the star polyhedron at the top of the Sacristy (photographs by the author).

On a subsequent visit, I contacted some Vatican officials to inquire about the significance of the star polyhedron at the top of the Sacristy, but nobody seemed to know about its origin or significance. As I visited the interior of the Sacristy, I noticed several small ornate stands on the altar, holding similar star polyhedra.

Once I had noticed the top decoration of the Sacristy, I started noticing star polyhedra elsewhere, and they appeared to be quite common with frequent decorations at the tops of church towers and other prominent places [3]. Often, the star polyhedra decorating public places are not exactly regular, but slight deviations do not disturb the viewing pleasure. There is a gradual transition between genuine star polyhedra and just a bunch of spikes radiating from the center. An example of a not quite regular star polyhedron is presented here from the Petrovsky Palace in Moscow [4].



Left: the central section of Petrovsky Palace at 40 Leningradsky Avenue, Moscow, with two towers at its entrance with a star polyhedron on top of each. Right: a close up of one of the star polyhedra (photographs by the author).

The Petrovsky Palace was designed by Matvei F. Kazakov and built in the years 1776–1782, so it was a contemporary of the Sacristy in Vatican City. The Palace was built by the order of Catherine II, also known as Catherine the Great. Its purpose was to serve as a resting place for the Tsar or Tsarina when traveling from St Petersburg to Moscow. At the time, it was well outside Moscow, at a considerable distance from the destination of the sovereign's trip; today it is well within the Moscow city limits. Travelers arrived at the Moscow Kremlin fresh and rested after this stopover. In the Soviet era, the Palace housed the Zhukovsky Air Force Academy. The kosmonauts (the Russian word for astronauts) Yury Gagarin and Valentina Tereshkova and the airplane designers Sergei Ilyushin and Aleksandr Yakovlev studied here, amongst many others. Eventually, the Air Force Academy moved out, the Palace was renovated, and it has served close to its original purpose: functioning as a hotel for traveling dignitaries [5].

The star polyhedra of the Petrovsky Palace do not correspond to any of the regular star polyhedra, but correspond to one of the 59 stellated icosahedra [The 59 Icosahedra – once opened, this site presents a rotating model (animation) of the stellated icosahedron No. 18], as suggested by Nikolai Dolbilin of the Moscow Steklov Institute of Mathematics [6]. On Magnus Wenninger's so-called Wenninger's List, this polyhedron stands under No. 34 (https://en.wikipedia.org/wiki/Great_triambic_icosahedron).

I conclude this note with a challenge to the reader to find the closest identification among star polyhedra for the decoration depicted above from the building at One Columbus Circle, Manhattan, New York; at the time it was the Time-Warner Building.

References

[1] Hargittai, M. & Hargittai, I. (2009). *Symmetry through the Eyes of a Chemist*, 3rd ed., pp. 76–90. Springer.

[2] Cundy, H. M. & Rollett, A. P. (1961). *Mathematical Models*. Oxford: Clarendon Press.

[3] Hargittai, I. (1996). *Math. Intell.* **18**, 52–54.

[4] Hargittai, B. (2019). Editor. *Culture and Art of Scientific Discoveries: A Selection of István Hargittai's Writings*, p. 25. Springer Nature.

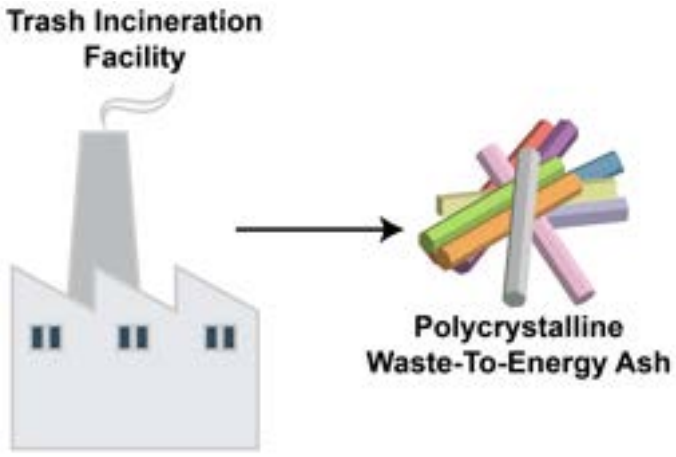
[5] Hargittai, I. & Hargittai, M. (2019). *Science in Moscow: Memorials of a Research Empire*, p. 148. Singapore: World Scientific.

[6] Dolbilin, N. (2021). Private communication.

Istvan Hargittai is at Budapest University of Technology and Economics, Hungary.

FEATURE ARTICLE

Crystals in trash



Vikram Kumar, Nishant Garg

The 2015 American Crystallographic Association Transactions Symposium on *Crystallography for Sustainability* highlighted the impact of crystallography-based research on sustainability (Helliwell, 2015*b*). Specifically, the fundamental crystallography-related research on health, structure-based drug design and energy, and investigation into crystal structures for hydrogen storage, has directly addressed the United Nations Millennium Development Goals on combating diseases and ensuring environmental sustainability (Helliwell, 2015*a*). Through this article, we intend to disseminate how powder diffraction with in-house laboratory and synchrotron X-ray sources is contributing to waste management and valorization – an application of crystallography that is key to finding alternative feedstocks for energy-intensive industries and enhancing environmental sustainability.

Traditionally waste management encompasses three practices: recycling, incineration for energy recovery and landfilling. Amongst these three practices, recycling is the most preferred, followed by incineration for energy recovery and landfilling. In contrast to recycling, landfilled materials are lost forever and hinder progress toward a sustainable materials system (Olivetti & Cullen, 2018). As an alternative, waste incineration in controlled facilities allows energy recovery and has the potential to contribute toward the sustainable materials system (Walser *et al.*, 2012). This is because the product of the waste incineration process is the waste-to-energy ash – a material that can become part of the sustainable materials cycle. Specifically, waste-to-energy ash could substitute traditional feedstocks in environmentally intensive industries, such as cement and metals (Kumar & Garg, 2022; Cheisson & Schelter, 2019). Despite these possibilities of becoming a part of the sustainable materials cycle, at present, the waste-to-energy ashes are mostly landfilled because of two factors. First, there can be tremendous variability in the ash composition. The variability comes from the differences in waste composition and the fluctuations in operating parameters, such as temperature and O_2 content, at an incineration facility (Kumar & Garg, 2021). Second, the ashes can be a repository of heavy metals, which may render them hazardous. The hazardous nature of ash depends on the heavy-metal speciation, which needs to be better understood for waste-to-energy ashes. Because of these uncertain factors, the waste-to-energy ash is not a reliable feedstock for any industry, so it is landfilled.

In our current research, we seek to uncover the compositional variability and heavy-metal speciation in waste-to-energy ashes by studying a diverse set of ashes collected from spatially distinct waste-to-energy facilities in the United States. In the United States, ~10 million tons of waste-to-energy ashes are landfilled annually. Therefore, by understanding the diversity in composition, we aim to integrate these ashes into the sustainable materials cycle. However, understanding the mineralogy of materials as complex as these ashes is challenging. This is because, in the scientific literature, ~150 distinct mineralogical phases have been reported to constitute waste-to-energy ashes (Piantone *et al.*,

2004). The scientific literature primarily relies on in-house laboratory powder diffraction experiments to identify and quantify the mineralogy of waste-to-energy ashes. However, there are multiple technical limitations to the in-house laboratory powder diffraction measurements for complex systems such as waste-to-energy ash. These limitations include (a) differences in the mass absorption coefficient of phases present in the waste-to-energy ashes, (b) limited penetration depth of X-rays, (c) preferred orientation effects for platelet and needle-like particles, (d) uncertainty in identifying phases because of peak overlaps, and (e) the anisotropic diffraction peak broadening (De la Torre *et al*., 2001). These limitations increase the uncertainty in identifying the mineralogical constituents of the waste-to-energy ashes and question whether the reported ~150 distinct mineralogical phases are actually present. In our research, we are addressing these limitations by probing the mineralogy of waste-to-energy ashes with penetrating synchrotron X-rays.

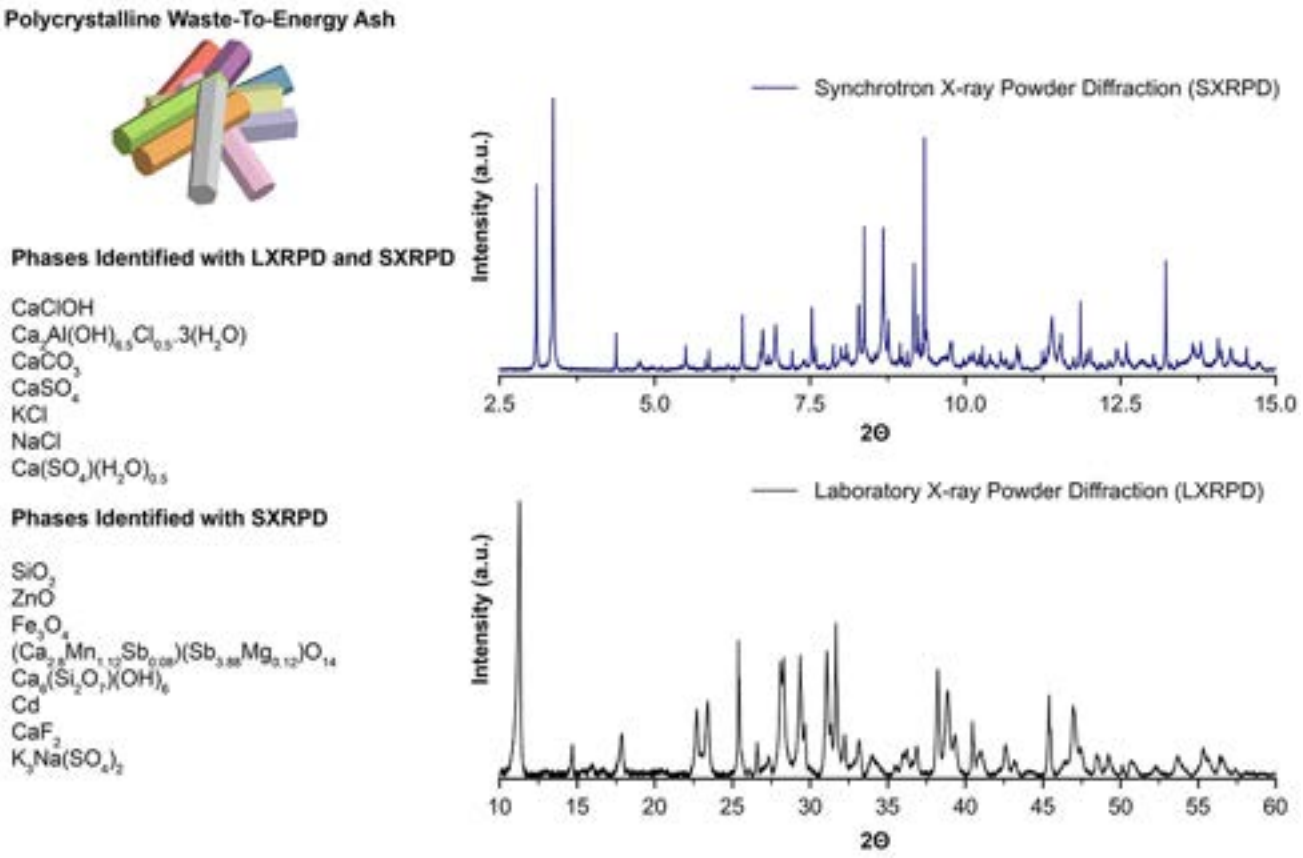


Figure 1. Example laboratory (LXRPD) and synchrotron (SXRPD) X-ray powder diffraction patterns for a polycrystalline waste-to-energy ash. The laboratory diffraction pattern was collected with Cu *K*α radiation (λ = 1.5418 Å), whereas the synchrotron pattern was collected at 0.45891 Å. The peak widths for SXRPD are smaller when compared with the LXRPD, which enables the identification of additional phases. With SXRPD, we can identify minor constituents and heavy metals speciation, understanding which is essential for employing waste-to-energy ash as an alternative feedstock for energy-intensive industries, such as cement and metal.

Synchrotron X-ray-based investigations on waste-to-energy ashes have been performed in the past (Yu *et al*., 2009; Hsiao *et al*., 2001). Most of these investigations probed the mineralogy of waste-to-energy ashes with X-ray absorption near edge structural (XANES) and extended X-ray absorption fine structural spectroscopy (EXAFS). While XANES and EXAFS are excellent characterization methods, their utility for probing the mineralogy of multielement specimens, such as the waste-to-energy ash, is restricted by their element-specific nature and the lack of standard databases containing XANES and EXAFS spectral patterns of pure minerals (Castorina *et al*., 2019). However, these restrictions do not apply to the synchrotron X-ray powder diffraction experiments as the diffraction pattern contains the mineralogical information of multiple elements, and there are excellent databases, such as ICSD, ICDD and COD. So, we employed synchrotron powder diffraction experiments to investigate the mineralogy of waste-to-energy ashes. Example diffraction patterns for a waste-to-energy ash collected in the lab and at the synchrotron are illustrated in Fig. 1. We note that the laboratory-based X-ray powder diffraction

experiments indicate the presence of CaClOH (calcium chloride hydroxide), $Ca_2Al(OH)_{6.5}Cl_{0.5}.3(H_2O)$ (hydrocalumite), $CaCO_3$ (calcite), $CaSO_4$ (anhydrite), KCl (sylvite) and $Ca(SO_4)(H_2O)_{0.5}$ (bassanite) (Fig. 1). By relying on laboratory-based powder diffraction experiments, we cannot identify the presence of minor mineralogical constituents and the speciation of heavy metals. However, with synchrotron powder diffraction measurements, we can identify the minor constituents as well as the heavy-metal speciation. The minor constituents in the ash are SiO_2 (quartz), $Ca_6(Si_2O_7)(OH)_6$ (jaffeite), CaF_2 (fluorite) and $K_3Na(SO_4)_2$ (apithalite) (Fig. 1). Most importantly, with synchrotron powder diffraction experiments, we identify the speciation of heavy metals – Zn as ZnO (zincite), Fe as Fe_3O_4 (magnetite), Mn and Sb as $(Ca_{2.8}Mn_{1.12}Sb_{0.08})(Sb_{3.88}Mg_{0.12})O_{14}$ (ingersonite) and cadmium as Cd (Fig. 1). These results demonstrate how critical synchrotron-based experiments are in understanding the chemistry of complex systems such as the waste-to-energy ash.

Environmental sustainability is intricately tied to the sustainable materials cycle. To facilitate the development of a sustainable materials cycle, alternative feedstocks such as waste-to-energy ash should serve as feedstocks for energy-intensive industries, such as cement and metal. However, our poor understanding of their complex chemistry severely limits their utilization as an alternative feedstock. Our ongoing research addresses these limitations by employing synchrotron powder diffraction experiments to shed light on mineralogy and heavy-metal speciation of waste-to-energy ash. By understanding their complex chemistry, we are optimistic that the waste-to-energy ash will likely become a feedstock for industry, not a landfill material.

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IUCR ACTIVITIES

The 75th anniversary of the IUCr – refresh of vision and values



Jenny Martin

Happy Birthday to the IUCr, which marks its 75th year in 2023! To celebrate this momentous occasion, crystallographers around the world are invited to participate in a refresh of the IUCr's vision/purpose and values.

Why?

The world has changed dramatically over the last 75 years and continues to change at a rapidly increasing pace. We need to be ready to change with it.

Now is the time to acknowledge our past, celebrate our achievements and plan for our future. We want your input on what the IUCr should aspire to be, and where the IUCr should focus its attention.

How? When? Where? And What?

An online survey will be conducted in early 2023. Look out for your invitation to take part.

The outcomes of the online survey will feed into an in-person workshop scheduled for 22 August 2023 at the IUCr Congress in Melbourne. The workshop will develop a draft vision/purpose statement and draft IUCr core values.

The draft vision/purpose statement and draft core values will be presented as recommendations for endorsement at the General Assembly in Melbourne.

The draft recommendations will be made available for comment by the IUCr community for a short period after the Congress and then a final recommendation will be endorsed by the Executive Committee.

The IUCr's refreshed vision, purpose and values will underpin the IUCr's future strategy/mission, planning, policies, priorities and milestones.

Watch your inbox for news of the survey, and if you are joining us for the Melbourne Congress, don't forget to express your interest in the workshop on Tuesday 22 August (1pm – 4pm). We look forward to gathering your thoughts and opinions on the IUCr.

Professor Jenny Martin AC FAA is a Member of the IUCr Executive Committee.

Note from the IUCr

An invitation to complete the survey will be sent to everyone in the *World Directory of Crystallographers* (WDC). If you are not registered in the WDC or believe your details to be out of date, please register here or update your entry here.

Some of the WDC web pages have recently been updated to have a more modern look and feel. Additional functionality has also been added, such as the ability for registrants to edit individual sections of their personal details (see example below).



FEATURE ARTICLE

Symmetry diagrams for the 17 plane groups now freely available



Carolyn Pratt Brock

It is very good news that the IUCr has decided to make the tables of the 17 plane groups (also known as the wallpaper groups) freely available. Seven of the 17 are shown in the *Teaching Edition* of *International Tables for Crystallography* (Aroyo, 2021) but the full set has been available only in Volume A of *International Tables* (Aroyo, 2016). The plane groups are very often used for teaching periodic symmetry because it is much easier to understand relationships in two dimensions than in three. Having the tables available at no cost is an important contribution to the educational mission of the IUCr.

To access the information for the plane groups visit the homepage of Volume A, select *plane group* from the drop-down menu in the *Go to* box, and choose the specific plane group from the drop-down menu in the *No.* box.

Although the identities of the 17 plane groups have been known for over a century (Federov, 1891; Pólya, 1924), they first appeared in *International Tables* in 1952 (Volume I of the 'Red Series'). Even much later several sets of competing symbols were in use (Schattschneider, 1978). A particular problem was confusion about the labels for *p*3*m*1 and *p*31*m* (Fig. 1).

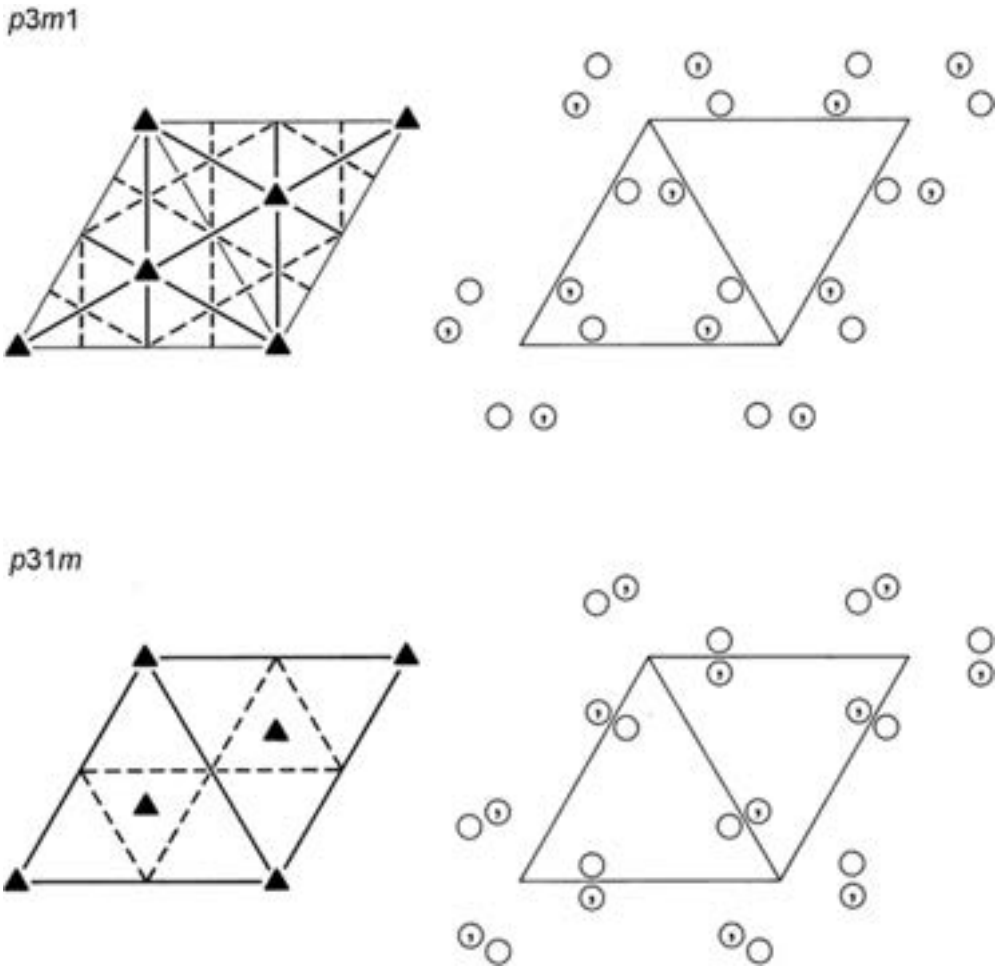


Figure 1. Diagrams of the plane groups *p*3*m*1 and *p*31*m* as they appeared in the 1952 Volume I of *International Tables*. Triangles indicate threefold rotation points, thicker solid lines indicate mirror lines and dashed lines indicate glide lines. Circles and circles enclosing a comma are enantiomeric.

In teaching symmetry, the tables of plane groups are often used in conjunction with C. H. MacGillavry's (1965) book *Symmetry Aspects of M. C. Escher's Periodic Drawings*, in which there are 41 plates of examples. A third edition of the book was published by the IUCr in 2017 (Fig. 2).



Figure 2. Cover of the third edition of the MacGillavry book.

The history of the MacGillavry book is interesting; much of what follows is taken from Doris Schattschneider's definitive book (1990) about Escher's periodic drawings. Both Escher and MacGillavry were Dutch.

Escher knew about crystallographers well before crystallographers knew about Escher. During a visit to his parents in 1937 he showed some of his drawings to his half-brother Berend, a Professor of Geology at the University of Leiden. Berend then sent Escher a list of ten papers (authors F. Haag, G. Pólya, P. Niggli, F. Laves and H. Heesch) published in *Zeitschrift für Kristallographie* between 1911 and 1933, along with a note suggesting that at least the drawings might be of interest. Escher studied several of the papers very carefully. He transcribed the 1924 article by Pólya, including all its illustrations, into a copybook.

Crystallographers first learned of Escher's drawings in 1952, when MacGillavry, a Professor of Chemical Crystallography at the University of Amsterdam, saw an exhibit of Escher's work at the important Museum Boijmans in Rotterdam (now the Museum Boijmans Van Beuningen). MacGillavry returned to the exhibit a few days later, accompanied by all the students and staff of the crystallography laboratory. The first appearance of an Escher drawing in a crystallographic publication is thought to have been in 1955, when Professor Pieter Terpstra of the University of Groningen used the drawing of a horse and rider as the frontispiece of his book *Introduction to the Space Groups* (Fig. 3). In 1959 Professor J. D. H. Donnay from Johns Hopkins University and Dr Gabrielle Donnay from the Carnegie Institution for Science visited Escher's studio and asked him to lecture at the 1960 IUCr Congress in Cambridge, England. A few months later MacGillavry visited the studio and encouraged him to accept the invitation. Escher then wrote to his son:

"*the nicest thing to have happened to me recently was a visit yesterday afternoon … from a lady, Professor MacGillavry, who … came with her sister-in-law, who was also somehow interested in divisions of the plane, and the two of them had their eyes glued to my prints from half past two till after half past*

five. What a pair of smart ladies! It's such a relief to have visitors at last who don't stare at my creatures uncomprehendingly, but who can chuckle with amusement at anything worth chuckling at."

(quotation taken from p. 103 of Schattschneider, 1990).

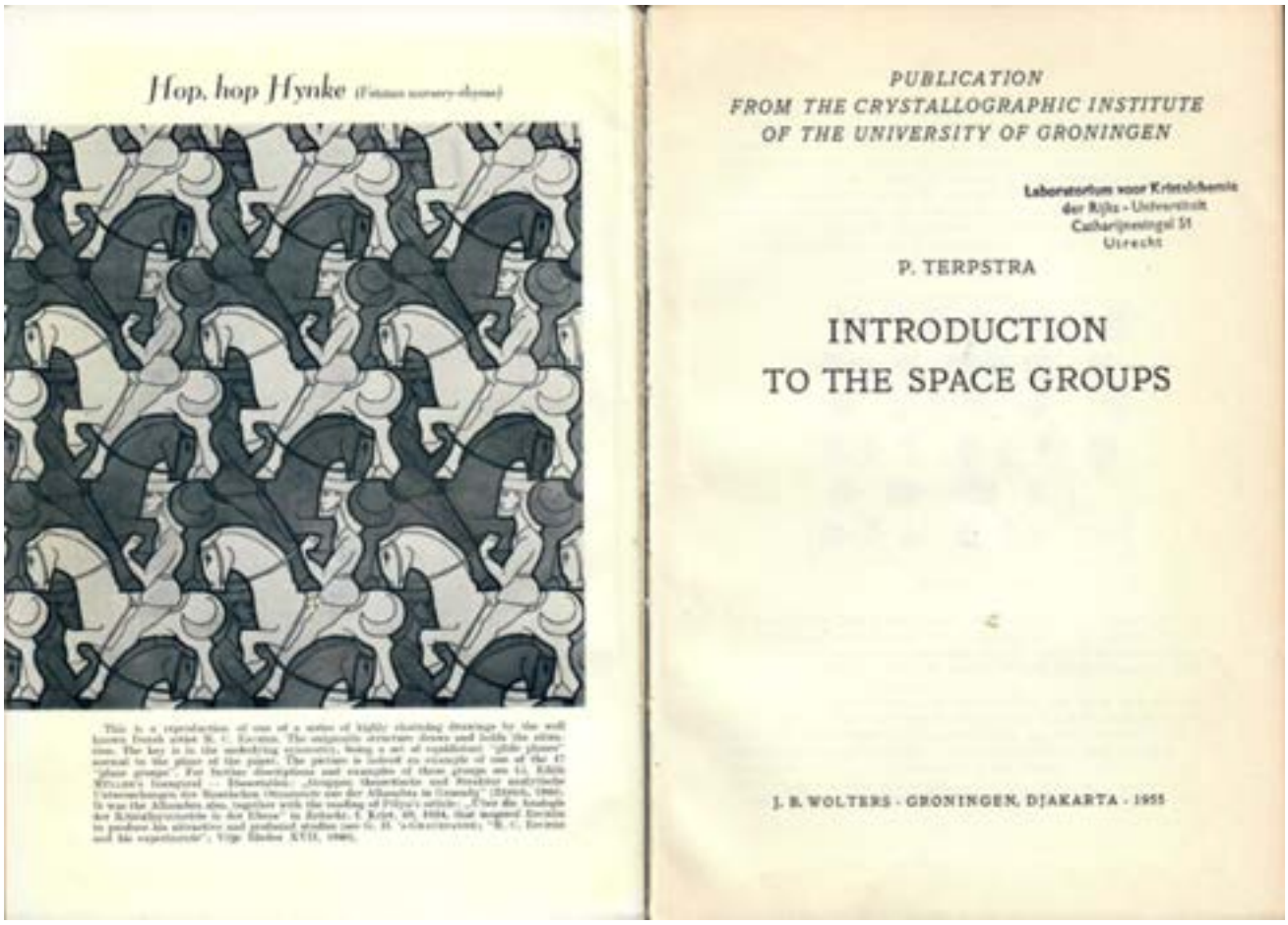


Figure 3. Frontispiece and title page of Terpstra's 1955 book. The text above the drawing is part of a Frisian children's song; the figure caption gives some information about Escher.

The talk at the 1960 Congress was a great success. Both the large main hall and an overflow room linked by closed-circuit television were filled, and Escher's talk was received very enthusiastically. An accompanying exhibit of Escher's work had been arranged, and many crystallographers bought prints. Some years later, when Escher's work had become widely popular, some of those owners found their home-insurance premiums had suddenly increased.

Escher's report of his experience at the 1960 Congress is part of the website of the museum *Escher in Het Paleis*, which is located in The Hague. At the end of the webpage there is a picture showing Escher and MacGillavry standing together. In the background are several bricklaying patterns, in which the Amsterdam school was interested and used for teaching.

After the 1960 Congress the IUCr commissioned MacGillavry to work with Escher on a book illustrating the plane groups. The book appeared in 1965. Included are 13 drawings that have classical symmetry, 22 that have black/white symmetry (*i.e.* antisymmetry) and six that have polychromatic symmetry. At MacGillavry's request, Escher created two new drawings for the book and improved five others; five more drawings in the book were created after Escher participated in the 1960 Congress. Escher graciously granted the IUCr permission 'to permit reproduction of any of the drawings included in the book when such reproduction is requested for teaching or scientific purposes' (Fig. 4).



M. C. ESCHER
VAN HEEMSKERKLAAN 2B
BAARN (Holland)
Telef. 02426

Baarn, 15-XII-1966

Dear Dr Boom,

With reference to the recent talk which I had with Dr Smits on the telephone, I am writing to confirm that I have given permission to the International Union of Crystallography to have an unlimited number of reprints published of the book "Symmetry Aspects of M.C. Escher's Periodic Drawings", and that I forego the right on any royalties on the income from the sale of copies of any such reprint editions. I would also like to confirm that I would like to leave it to the judgement of the responsible Officers of the Union to permit reproduction of any of the drawings included in the book when such reproduction is requested for teaching or scientific purposes.

Yours sincerely,

M.C. Escher

Figure 4. M. C. Escher’s letter of 15 December 1966 to the IUCr about how his drawings in the MacGillavry book may be used.

At the 1975 IUCr Congress in Amsterdam a new set of three prints of Escher’s periodic drawings (Plate 13 of the 1965 book and two others) were sold. During the Opening Ceremony, MacGillavry gave the Congress Discourse, which was titled *Order and Beauty*. I was very happy to be able to meet her during one of the poster sessions and to tell her that it was her book that had led me to the field of crystallography.

Notes on C. H. MacGillavry’s name

MacGillavry was a Professor and the Head of the Crystallographic Laboratory at the University of Amsterdam. In the 1993 obituary by Aafje Looijenga-Vos that was published in the *Proceedings of the Royal Netherlands Academy of Arts and Sciences* (KNAW), the name is given as Carolina Henriëtte Mac Gillavry. That version is probably authoritative although the version used professionally was C. H. MacGillavry. Vos, two decades younger than MacGillavry and also Dutch, was a crystallographer, a professor at the University of Groningen and very active in the IUCr.

MacGillavry’s first given name can be found as Carolina, Caroline and Carolien; all three versions occur in IUCr publications. The first spelling is perhaps the most correct but many people who knew her professionally used the second. The third spelling is Dutch.

The second given name, if written, usually appears without the diacritical mark.

The family name, Mac Gillavry, is written as MacGillavry in all but a few of her scientific publications, but her father (Donald Mac Gillavry, a brain surgeon) seems to have always included the space. A web search shows that the separating space is still in common use.

In the family she was called Lien. Her doctoral students called her Mac.

There was indeed a Scottish ancestor: William Mac Gillavry, 1751 (Elgin, Scotland)–1810 (the Netherlands). He was Carolina's great-great grandfather. A MacGillavry clan website says that William fought in 1794 in the Highland Regiment under Major General Dundas with the allied troops against the French revolutionary army. After being wounded he was taken to the town of Zwolle, where he recovered, supported himself as a teacher of English, married and founded the Dutch branch of the Mac Gillavry clan.

All the drawings in the MacGillavry book that have classical symmetry are built from at least two different units (*e.g.* a bird and a fish) so that the boundaries between them can be seen easily. In the drawings built from a single unit, adjacent units are distinguished by color. If there are two colors then the symmetries of the drawing can be analyzed in three ways, *i.e.* by considering the two colors as different, the same or opposites (Fig. 5).

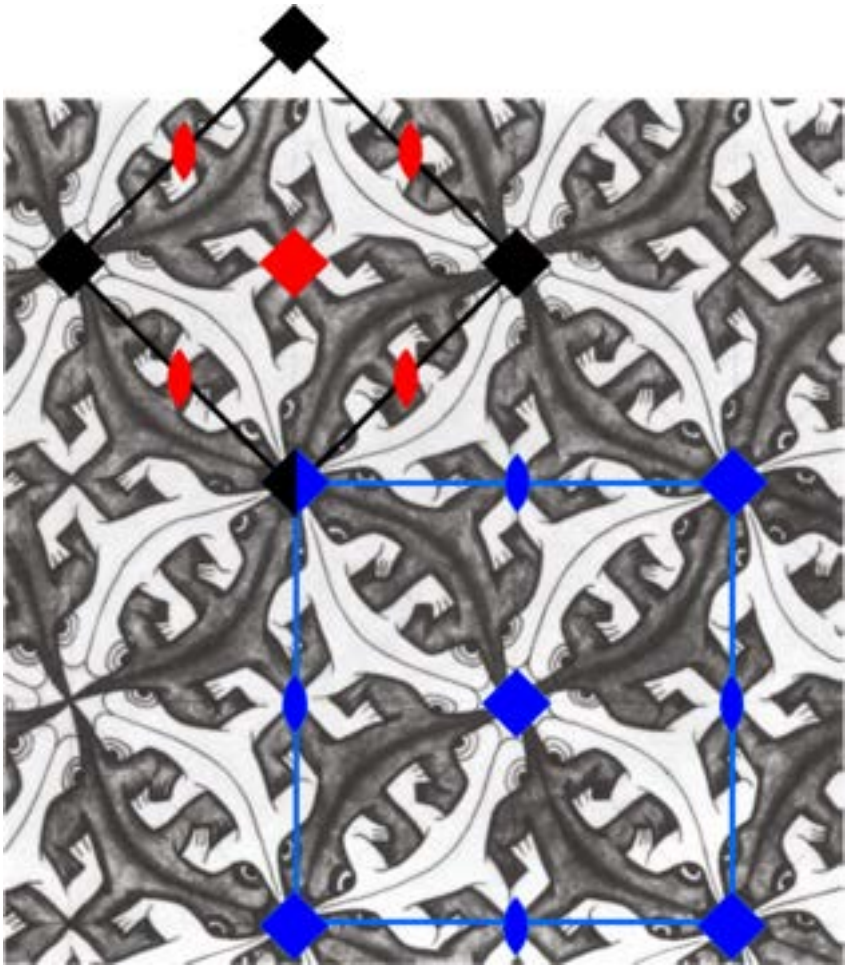


Figure 5. Plate 25 of MacGillavry's book marked to show the symmetry of the conventional unit cell (darker lizards not equivalent to lighter lizards; group *p*4) and the antisymmetry (or magnetic) unit cell (symbol p'_c4, $p'4$ or p_p4; group 10.4.52 in Litvin's 2013 compilation). For the smaller magnetic cell, the classical symmetry elements are black and the antisymmetry elements are red.

If the two colors are considered antisymmetric, *i.e.* are related by an operation of antisymmetry that changes the colors (*e.g.* black to white) or the direction of the magnetic moment (parallel or anti-parallel to a given direction), there are 46 possible plane groups. The combination of the antisymmetry operation with the ordinary plane-group operations results in the compound antisymmetry operations, *i.e.* a successive performance of ordinary plane-group operation and the operation of antisymmetry, *cf.* Figs. 5 and 7. Allowing combined antisymmetry operations makes it possible to derive the 80 antisymmetry plane groups, which include the 46 black-and-white or magnetic plane groups, the 17 'white' plane groups (*i.e.* no antisymmetry operations) and the 17 'grey' plane groups. The grey groups contain an additional anti-symmetry version of every symmetry operation and so superimpose differently colored

(*e.g.* black and white) units.

Diagrams of these groups are available in Danny Litvin's extensive (>12,000 pages) compendium of magnetic space groups that was published by the IUCr in 2013 as an open-access e-book (Fig. 6) and that built on the work of Shubnikov, Belov *et al.* (1964). The tables for the plane groups can be found by searching *Part 2. Tables of Magnetic Groups* (98 MB) for *Index of Two-Dimensional Magnetic Space Groups* (p. 2279 in the current edition). The tables for the 80 groups fill the following 161 pages.

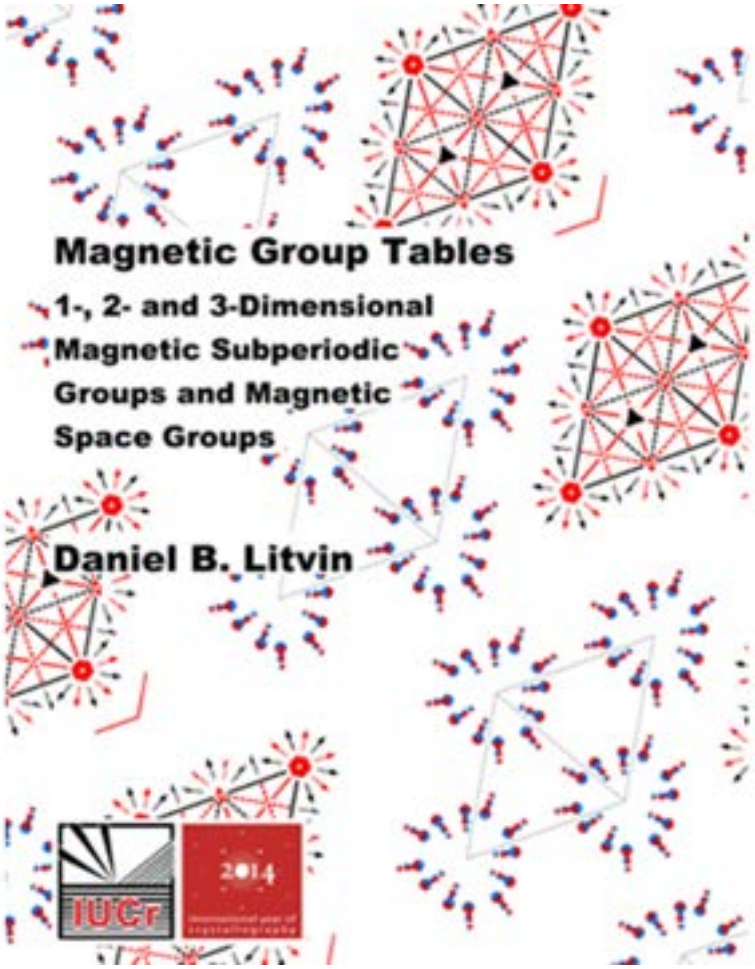


Figure 6. Cover of the Litvin e-book.

The diagrams for the group of an Escher drawing with antisymmetry are shown in Fig. 7. The classical symmetry elements are black whereas the antisymmetry elements are red. The arrows in the group diagram represent the magnetic moments. Classical rotations affect magnetic moments and position vectors in the same way but classical inversion has no effect on the magnetic moment. A mirror line that changes x,y to x,y then changes the magnetic moment from u,v to u,v.

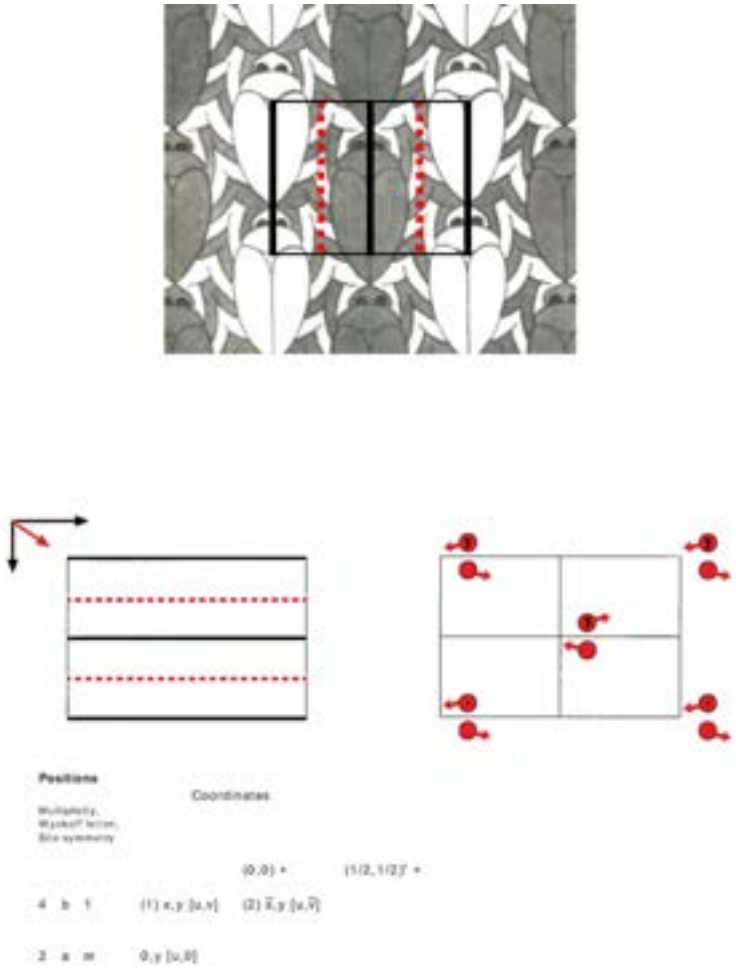


Figure 7. Part of Plate 19 of the MacGillavry book along with the diagram for its antisymmetry group (c_p1m1, no. 5.4.22 in Litvin's 2013 compilation; in other systems the symbols are p'_cm, p'_c1m and c_pm). The generated lattice vectors, given in the upper-left corner of the symmetry-element diagram, are color coded; the red is coupled with the antisymmetry operation whereas the black are not.

The symbols for the magnetic groups have not yet been standardized but progress is being made in that direction (Campbell *et al.*, 2022). The last page of the third edition of MacGillavry's book provides the symbols for the antisymmetry groups for Plates 14–35 in five different systems; Litvin's symbol is accompanied by his group number.

Escher had no formal training in higher mathematics but did correspond with several prominent mathematicians (*e.g.* Pólya, Coxeter, Penrose) and published two books [*e.g. Grafiek en tekeningen* in 1959; see pp. 337*ff* in Schattschneider (1990) for a complete list of writings by and about Escher]. He also explored polychromatic symmetry, a topic that mathematicians have not yet finished analyzing (see Senechal, 1988). Schattschneider's (1990) book contains extensive reproductions of pages from Escher's notebooks as her stated goal was to answer the question: *How did he do it?* Studying her book provides insight into Escher's creative process.

Other sets of drawings with 2D periodicity were inspired by Escher's work, two of which have strong connections to crystallography. On the occasion of the 1981 IUCr Congress in Ottawa, François Brisse (1981) created a set of 17 drawings based on Canadian themes. In Arthur L. Loeb's book *Color and Symmetry* (1971) there are 86 geometrical 2D patterns that illustrate color groups. Loeb, a senior lecturer at Harvard in the Visual and Environmental Studies Department, earned a PhD in chemical physics at that university after having left Holland as a teenager at the beginning of WWII. Later he came to know Escher well.

The efforts of all of these people have provided a wealth of material for teaching periodic symmetry, solving intriguing puzzles and pondering the more complicated problems of polychromatic symmetry. Having the IUCr's plane group diagrams freely available is an important step towards making this

material easier to understand. The complete information about plane groups does not seem to be available anywhere else.

Acknowledgements

I am very grateful to Doris Schattschneider, who made many comments on the first draft of this article. Danny Litvin, Mois Aroyo, Ton Spek and Marjorie Senechal were also very helpful. This also seems a good place to thank Henk Schenk and Peter Strickland for putting together the third edition of the MacGillavry book, which was not a small project.

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IUCR CONGRESS

IUCr2023 abstract submission deadline extended



We want to thank and acknowledge all of you who have submitted abstracts to the 26th Congress and General Assembly of the International Union of Crystallography Congress 2023. The enthusiastic response from our global community has met all expectations. We are excited that our goal to create a content-rich programme is coming to fruition.

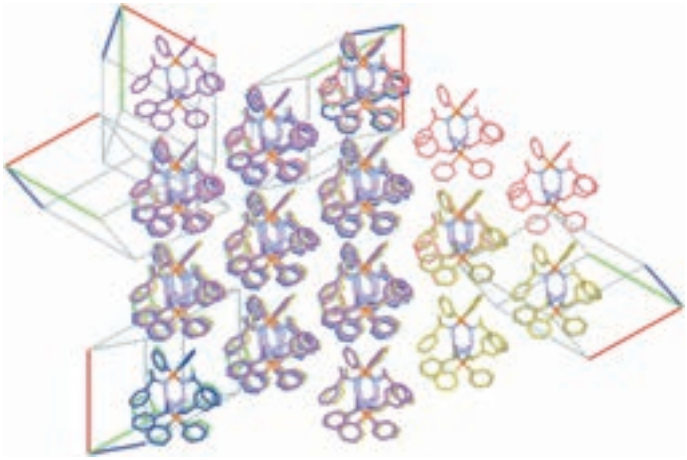
In light of the multiple requests, we have listened. We have re-opened the Call for Abstracts to allow additional time for those who need it. The submission portal will now remain open until 21 February 2023.

Please note also that Early Bird Registration ends on 31 March 2023. All deadlines and dates can be found on our website.

From the IUCr2023 team in Australia, we wish you, wherever you are in the world, a safe and happy holiday season.

COMMENTARY

Learning from approximate periodic symmetry in organic P1 structures



Victor G. Young

The article by Brock (2022) is the result of an ambitious 3+ year long project to study the occurrences of approximate symmetries in the space group *P*1. Brock selected the November 2019 version of the Cambridge Structural Database (CSD; Groom *et al.*, 2016), where 2592 reports of organic crystal structures (based on Z, Z' and an R value ≤ 0.05) were found. Using a number of criteria this set was distilled down to 1407 $Z = Z' > 1$ and 1049 $Z = Z' = 1$. In the former group, molecules (including cations and anions) within asymmetric units were evaluated for possible approximate symmetries: 2, 21, 3, 31, translations, inversions or glides. Entries in the latter group were retained if some possible approximate symmetry was detected within the molecule(s). A subset of crystal structures was removed from both sets if the symmetry indicated these would be better described in a higher-symmetry space group. Brock's conclusion is that approximate symmetry is pervasive in *P*1 crystal structures.

There are a number of notable findings that are worth considering. About five-sixths of the $Z = Z' > 1$ group and three-quarters of the $Z = Z' = 1$ display evidence of some approximate symmetry. Enantiopure materials mimic inversion symmetry about one-third of the time. Approximate rotational symmetry is found about two-fifths of the time. Perhaps more of a surprise, for achiral and racemic materials, approximate glide or mirror symmetry is found more often than approximate inversion symmetry. Wherever possible Brock points out if the approximate symmetry leads to a better description as a two-dimensional structure with a corresponding layer group designation. For these $p2_111$ and $c211$ are the most common with $p112$ as a distant third.

In the *Results* section, the lead observation is that overlooked crystallographic symmetry is common for crystal structures composed of achiral or racemic materials, but is uncommon for enantiopure materials. About 8% of the achiral or racemic structures are better described in a different unit cell or higher-symmetry space group. This is precisely the same conclusion as found by Richard Marsh in the past generation (Marsh, 2009). The statistics presented on recent publications versus previous decades is not encouraging with the overall trend remaining about the same.

Many readers perhaps perused this article when it first appeared, but did not dive into the deposited materials Brock used to determine the results and conclusions. There is a wealth of information within these six files including additional commentary on all crystal structures considered, illustrations of selected structures by approximate symmetry, illustrations of the aforementioned selected structures, a spreadsheet of the *P*1 $Z > 1$ structures, a spreadsheet of the *P*1 $Z = 1$ structures and a spreadsheet showing cell transformations and calculations of layer offsets. There is an enormous amount of data presented in the files to be gleaned. For example, I found one memorable crystal structure of mine (CSD refcode QUPBIN; Ha & Young, 2009) in the listing, where I learned it had a layer group designation of *pba*2.

It will be interesting to see if this article will inspire better software tools to assist the experimental crystallographer with some additional information when there is approximate symmetry within the crystal structure. When I started my career some 30 years ago it seemed rare in my experience to have any crystal structure with more than one molecule in the asymmetric unit. That observation has changed considerably in recent years. Just this spring and summer I had a period where most of the crystal structures completed in my laboratory had two or more molecules per asymmetric unit, or $Z' > 1$, with several being $Z' = 8$. This phenomenon appears to be due in part to the complexity of the molecules our chemists and scientists are designing, as well as the relative ease our modern instrumentation has to collect diffraction data on small, weakly diffracting specimens with relatively large unit cells. In any event, Brock's article provides useful tools we crystallographers can use to describe crystal structures with pseudosymmetry.

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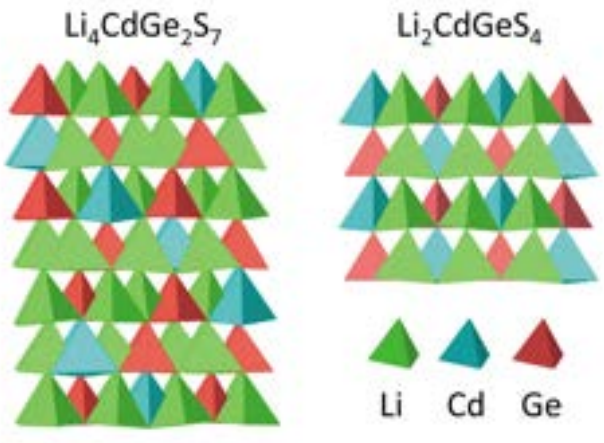
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COMMENTARY

The centre cannot hold



Arthur Mar

An enduring paradigm in solid-state chemistry is that the structures of many ionic solids can be built up by placing cations within the interstitial sites of a stacked arrangement of close-packed anions. Filling half the tetrahedral sites results in structures containing corner-shared tetrahedra as found in diamond: a zincblende (or sphalerite) family based on cubic closest packing and a wurtzite family based on hexagonal closest packing (Parthé, 1965). The names, taken from the polymorphs of ZnS, draw attention to the fact that most of these compounds are sulfides or selenides. When several types of metal cations are introduced, the possibilities for how they can be distributed become immense, depending on the occurrence of order or disorder. Determining the correct site distribution is essential for understanding the relation of structure to physical properties. These compounds are typically semiconducting and have attracted enormous attention over the years as attractive candidates for materials applications. Among these 'diamondlike semiconductors,' $Cu(In,Ga)S_2$ is already well established in thin-film solar cell technology (Ramanujam & Singh, 2017) and Cu_2ZnSnS_4 is a promising lead-free alternative to halide perovskite solar cells (Wallace *et al.*, 2017). New classes of thermoelectric materials based on similar compounds are being investigated (Miller *et al.*, 2018). In a related application that takes advantage of the ability to control band gaps, nonlinear optical (NLO) materials based on these diamond-like semiconductors can convert coherent light to other desired wavelengths, as in the operation of a laser (Liang *et al.*, 2017). Existing NLO materials made of oxides that function in the UV–visible region are well developed, but NLO materials made of sulfides or selenides would have smaller band gaps, making them suitable for the IR region. An IR NLO laser could then be used for medical treatment or nighttime illumination. As an essential criterion for a compound to exhibit NLO behaviour, its structure should be noncentrosymmetric.

As part of their longstanding investigations of diamond-like semiconductors as IR NLO materials, Craig *et al*. (2022) report the synthesis of the quaternary sulfide $Li_4CdGe_2S_7$, which is remarkable in several respects. First, it demonstrates the compositional richness that has yet to be fully realized among diamond-like semiconductors. Most quaternary representatives have the composition I_2–II–IV–VI_4 (as in the popular kesterites Cu_2ZnSnS_4 mentioned above), whereas those with the composition I_4–II–IV_2–VI_7 are rare and further examples surely remain to be discovered. Second, the authors provide convincing evidence for an ordered distribution of Li, Cd and Ge atoms within tetrahedral sites, which is not necessarily an easy task. The resulting structure is a lower symmetry, noncentrosymmetric derivative of the rarer family of diamond-like semiconductors based on hexagonal stacking. Although Pauling's rules for ionic solids are recognized to have limitations (George *et al.*, 2020), they were applied to give a satisfying rationalization of the structural features, including support for the site distribution of cations. Crystallographers sometimes engage in what may appear to be esoteric debates (to outsiders) about whether a structure is centrosymmetric or not (Marsh, 1986). In the end, does it really matter? Within

other contexts, such as chiral magnetism and superconductivity, this question is essential (Cheong & Xu, 2022; Smidman *et al.*, 2017); for optical materials, it is no exception. This leads to the third point. When microcrystalline samples of $Li_4CdGe_2S_7$ are exposed to near IR light, a strong second harmonic generation (SHG) response is observed, giving a change in colour in the visible region, detectable by the naked eye. This observation clinches the assertion of a noncentrosymmetric structure. For practical use, NLO materials have to satisfy several other stringent conditions, including phase matchability, high wavelength transparency, high laser-induced damage threshold and ease of crystal growth. $Li_4CdGe_2S_7$ shows promising characteristics, with an SHG response competitive with existing benchmark materials such as $AgGaS_2$ but with a much improved laser-induced damage threshold. Although many strategies have been proposed to 'design' materials having noncentrosymmetric structures, including computational and informatics approaches (Balachandran *et al.*, 2017; Song *et al*., 2020), there is no substitute for experimental verification. Careful crystallographic analysis remains a useful guide for choosing the correct space group, but it is even better if the conclusions are supported by measurements of physical properties, such as the observation of NLO behaviour.

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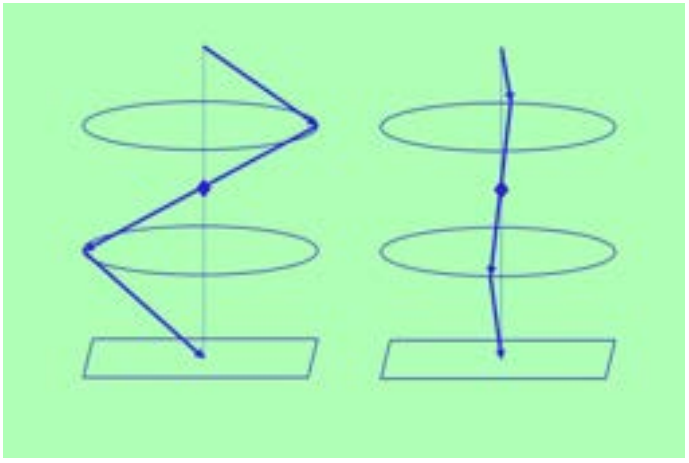
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COMMENTARY

Towards a new level of quantitative treatment of 3D electron diffraction data – in-pattern optical distortions



Tatiana E. Gorelik

The availability of aberration correctors for transmission electron microscopes leads to a significant improvement of the achievable resolution (Batson *et al.*, 2002); for beam-stable materials, sub-ångstrom resolved images can routinely be obtained using modern TEMs. Lens aberrations are inherent properties of electromagnetic elements (Haider *et al.*, 1998). Consequently, their effect is also present in electron diffraction patterns, which are formed at the back focal plane of the objective lens. In addition to the properties of the objective lens, electron diffraction patterns are affected by the characteristics of the diffraction/projector lens system and by the deviation of the electron beam from the optical axis of the microscope, whether intended (precession electron diffraction) or unintended (owing to misalignment).

Electron crystallography based on the analysis of 3D electron diffraction data is a rapidly developing field, demonstrating remarkable achievements in structure analysis of nano- and microcrystals of diverse nature – from minerals to proteins (Gemmi *et al.*, 2019; Gruene & Mugnaioli, 2021). Different instrumental approaches including dedicated electron diffractometers (Heidler *et al.*, 2019) are available. The data reduction is performed using either dedicated programs for electron diffraction (Kolb *et al.*, 2011; Gemmi & Oleynikov, 2013; Palatinus *et al.*, 2019; Wan *et al.*, 2013) or X-ray software [*e.g. XDS* (Kabsch, 2010), *DIALS* (Winter *et al.*, 2022), *MOSFLM* (Battye *et al.*, 2011)]. The structure solution is typically performed with X-ray programs [*SHELXT* (Sheldrick, 2015), *SIR* (Burla *et al.*, 2015), *Superflip* (Palatinus & Chapuis, 2007), *Phaser* (McCoy *et al.*, 2007)]. The success of dynamical refinement, reliably delivering hydrogen-atom positions (Palatinus *et al.*, 2017) and the absolute configuration (Brázda *et al.*, 2019), clearly demonstrated the potential and necessity of *dedicated approaches* for the quantitative treatment of effects specific to electron scattering.

Aberrations of electron optical systems bring a distortion field in 2D electron diffraction patterns. These distortions unavoidably propagate into the 3D ED data and deform the complete reciprocal space. The presence of the distortions usually does not hamper the indexing, but may introduce inaccuracy of the lattice parameters, and can lead to improper integration of intensities due to displacement of reflection predictions when mapped back onto 2D frames.

In this issue of **IUCrJ**, Brázda *et al.* (2022) present a comprehensive analysis of different types of distortions present in electron diffraction patterns, their propagation into the reconstructed reciprocal space, and elaborated methods for their detection and correction. These methods are already implemented in the new version of *PETS2* – widely used dedicated software for 3D ED data reduction

(Palatinus *et al.*, 2019).

In a general form, the positional shift of a point due to a distortion can be separated into its radial Δr and tangential Δt components [Brázda *et al.*, 2022; equations (6) and (7)]. The axial symmetry of the optical system sets selection rules on the orders of the circular harmonic and polynomial terms, so that $n + m$ should be odd (Smith, 2007; Linck, 2022). For different distortion types, the formulae for radial and tangential distortion components can then be deduced (Table 1), containing different power dependence on r. Magnification, rotation and elliptical distortions [Fig. 1(*b*)] contain linear dependence on r, parabolic [Fig. 1(*c*)] is quadratic with r, and barrel [Fig. 1(*d*)], pincushion [Fig. 1(*e*)] and spiral [Fig. 1(*f*)] have cubic dependence on r. The angular part of the distortions, which depends on the azimuth π, is zero-order for magnification, rotation, spiral and barrel–pincushion distortions (they do not depend on φ), first-order for parabolic distortion (the period is 2π), and second-order for elliptical distortion (the period is π).

Table 1
Different types of distortions observed in 2D electron diffraction patterns – formulae for the radial and tangential displacements

ρ_{01}, τ_{01}, φ_{r2}, ρ_{23}, φ_{r1}, ρ_{12}, ρ_{03}, τ_{03} are scalar coefficients.

Distortion types	Radial and tangential distortion components
Magnification/scaling factor	$\Delta r = \rho_{01} r$, $\Delta t = 0$
In-plane pattern rotation	$\Delta r = 0$, $\Delta t = \tau_{01} r$
Elliptical	$\Delta r = \cos\left[2\left(\varphi - \varphi_{r2}\right)\right] \rho_{23} r$, $\Delta t = \cos\left[2\left(\varphi - \varphi_{r2} + \frac{\pi}{4}\right)\right] \rho_{23} r$
Parabolic	$\Delta r = \cos\left[\left(\varphi - \varphi_{r1}\right)\right] \rho_{12} r^2$, $\Delta t = \cos\left[\left(\varphi - \varphi_{r1} + \frac{\pi}{2}\right)\right] \frac{\rho_{12}}{3} r^2$
Barrel–pincushion	$\Delta r = \rho_{03} r^3$, $\Delta t = 0$
Spiral	$\Delta r = 0$, $\Delta t = \tau_{03} r^3$

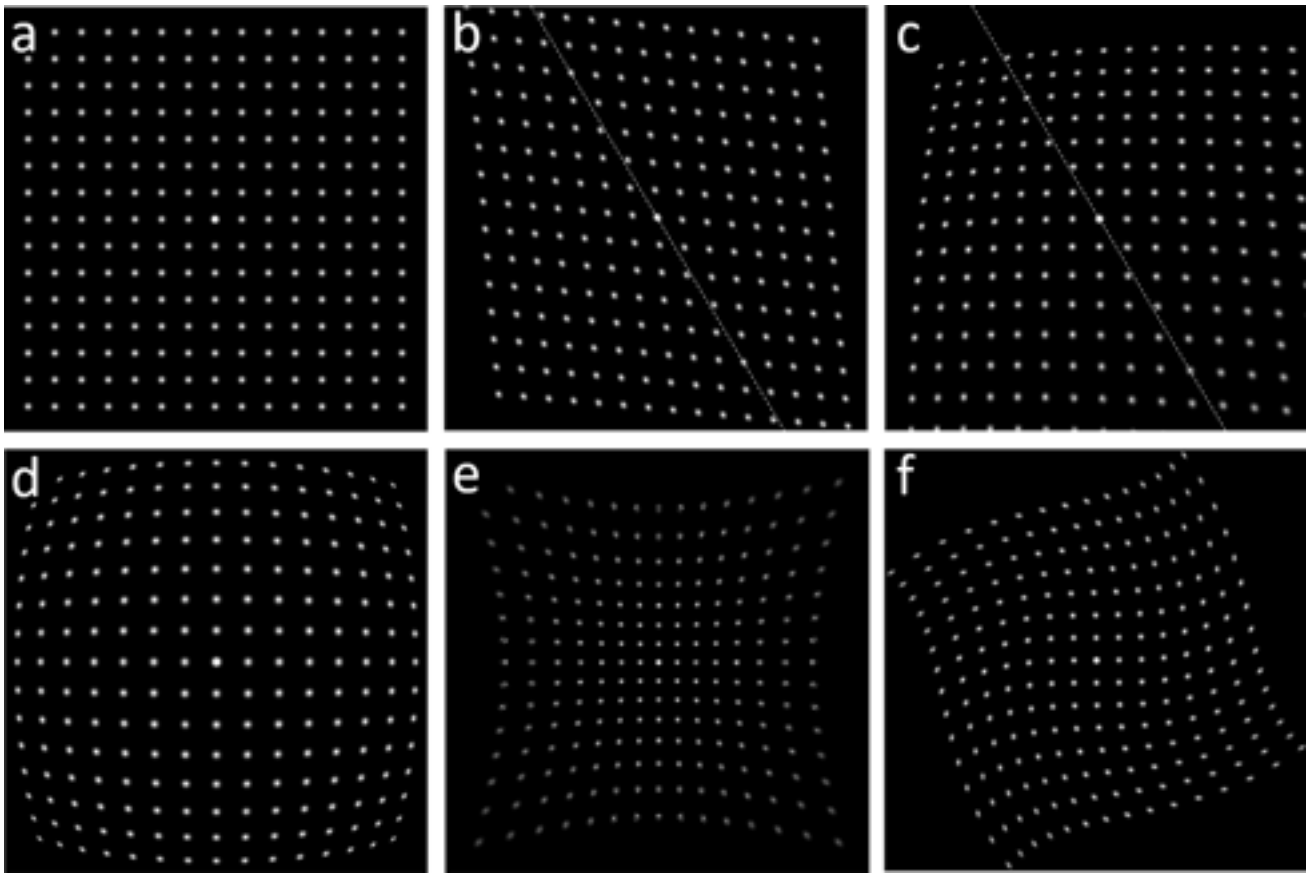


Figure 1. Different types of distortion in electron diffraction patterns: (*a*) original undistorted image, (*b*) elliptical distortion with the distortion axis inclined 30 away from the vertical axis, (*c*) parabolic (coma) distortion, (*d*) barrel with a negative ρ_{03} parameter, (*e*) pincushion with a positive ρ_{03}, (*f*) spiral distortion.

An important point of the study of Brázda *et al.* (2022) is the elaboration of the relationship between different types of distortions and the possibility to correct for them for a given dataset without any

additional information. The *magnification distortion* is equivalent to the scaling factor and is fully correlated with the lengths of the unit-cell vectors. This makes it impossible to decouple from the lengths of the unit-cell vectors, and correct for, without any additional knowledge. The *rotation distortion* correlates completely with the tilt axis position in the frames, which also makes it difficult to separate, yet it does not affect the values of the unit-cell vectors, solely resulting in the rotation of the orientation matrix.

The *elliptical distortion* represents a complex case: the component along the tilt axis (and orthogonal to it) is equivalent to stretching or contracting of the complete reciprocal space along the tilt axis, and therefore distorts the lattice perfectly linearly, resulting in the change of the unit-cell parameters (*i.e.* it is fully correlated with the unit-cell metric). The component away from the tilt axis does lead to the distortion (twisting) of the lattice, which can be corrected for. For a full correction of elliptical distortion, additional knowledge on the crystal class or an additional dataset from a differently oriented crystal is necessary (under the assumption that the elliptical distortion is the same for the two datasets). Distortions with quadratic and cubic dependence on *r* described by Brázda *et al.* (2022) lead to specific deformations of the reciprocal lattice, and can be refined simultaneously with the unit-cell parameters.

Accounting for the specified distortions in electron diffraction data has a number of implications. Apart from the obviously more accurate unit-cell parameters, enabling the crystal system determination, and improving the integration of intensities, the final structure models provide a more accurate bond geometry, and finally, better accuracy of the unit-cell parameters improving the findability of the structures within the databases.

In the first publication of the series, Brázda et al. (2022) consider the effect of distortion within 2D frames. The next step is the correction for misalignment of individual frames. It has been demonstrated that the in-frame distortion correction combined with the frame orientation allowed for better visibility of hydrogens in cobalt aluminophosphate (Brázda & Palatinus, 2022) compared with uncorrected data extraction reported in 2017 (Palatinus *et al.*, 2017), and significantly improved (Krysiak, 2022) data reduction and structure analysis of hydrous layer silicate RUB-6 (Krysiak *et al.*, 2020). We therefore look forward to seeing a significant step forward in the accuracy of electron diffraction structure analysis in general, driven by the implementation of more accurate models of electron diffraction data geometry.

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COMMENTARY

Making ripples in the comparison of calculated and experimental maps for real-space refinement and assessment by analytic modelling of local resolution

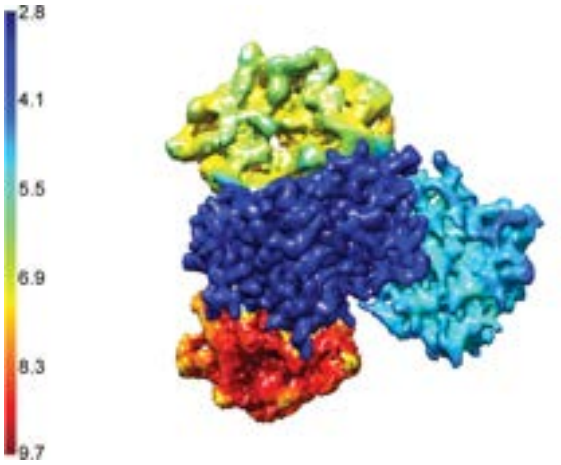


Figure 1. Large differences in local resolution are typically observed in cryoEM maps and the work of Urzhumtsev and Lunin allows the refinement of the local resolution of the map as an atomic parameter. In the figure, resolution variations are represented as identified by *DeepRes* from the simulated map of the 39 kDa human cartilage glycoprotein tetramer filtered at 3, 5, 7 and 9 Å. Reproduced from Ramírez-Aportela *et al.* (2019).

Isabel Usón

Our experimental knowledge of structure in atomic detail is derived from the electron density or electrostatic potential map interpreted as an atomic model. Conversely, we calculate the theoretical map from our model and comparison of both sources is used to refine (Urzhumtsev & Lunin, 2019) and improve this knowledge or assess its correctness. In this issue of **IUCrJ**, Urzhumtsev & Lunin (2022) revisit first principles underlying imperfections in the experimental maps in order to propose a map calculation with variables to account for atomic displacement and local resolution linked to each atom. The new maps reflect the observed inhomogenous resolution with superior accuracy and their expression is nearer to physical reality, along with the useful feature of simplifying the necessary calculation of derivatives with respect to all parameters.

The last decade has seen an expansion of powerful experimental structural techniques, the ‘resolution revolution’ in cryoEM (Kühlbrandt, 2014), micro-electron diffraction (Clabbers *et al.*, 2022) or serial crystallography from tiny crystals (Standfuss & Spence, 2017), that are gaining importance in expanding the basis for macromolecular structural knowledge. These methods provide information down to the atomic level but frequently, resolution varies to a large degree across different areas of the map, leading to the observation of very different local limits as illustrated in Fig. 1. The effect, prominent in maps where the main distortions are caused by harmonic disorder of the structure and limited resolution, may also be relevant in X-ray or neutron crystallography and is presented in a general way. Addressing differences in local resolution is recognized as essential to avoid misleading and over-interpretation of cryoEM reconstructions (Vilas *et al.*, 2020). The work of Urzhumtsev and Lunin illustrates the shortcomings and limitations of accounting for this phenomenon through a combination of atomic displacement parameters and global resolution cut-off. While the atomic positional disorder blurs atomic densities, the resolution cut-off, alongside this, generates Fourier ripples, which significantly contribute to

the map far from the atomic centre. Both types of distortion can be described by the same mathematical operation of a convolution but require different functions. Instead, the authors suggest a method to calculate model maps at every point, extending the concept of a local resolution down from a region to the characterization of each individual atom. This value will naturally be adjusted on the fly in the course of refinement.

In the absence of an analytic expression of the convolution between the Gaussian function accounting for displacement and the interference function limiting resolution, the latter has been recast into a shell decomposition allowing the calculation, in a closed analytical form, of the atomic model map distorted by restricted resolution and positional disorder.

The particular implementation and large-scale refinement tests on real data remain to be explored for each envisaged application, and it is anticipated that such development will soon follow. Nevertheless, the present work provides proof of principle of the superior effect of accounting for Fourier ripples with synthetic data calculated for a protein model and establishes the computational advantages.

The availability of accurate predicted models for protein components of macromolecular complexes (Jumper *et al.*, 2021; Baek *et al.*, 2021) opens new opportunities while demanding advancements in the treatment of errors in experimental determinations. Enhancing the quantitative comparison of calculated and experimental maps will be decisive in extricating unbiased experimental information beyond prior knowledge and the authors – along with the contribution in this paper – raise a number of questions remaining to be addressed. These include the inverse problem of calculating their parameters from the experimental map, the extension of the model to anisotropic displacement parameterization or subatomic resolution scenarios in charge-density studies or the current limitations in the absence of complete data and the need for optimally accounting for atomic scattering where unaccounted environmental effects or dynamic effects occur (Gruza *et al.*, 2020; Samperisi *et al.*, 2022). None of these considerations detracts from the interest of their proposed map calculation and application in refinement but rather adds to the debate.

This development will enable real-space refinement in a more appropriate way and thus be welcomed by the community once implementations tailored to each envisaged application are available in refinement software. In the meantime, this theoretical proposal stirring discussion on how to best connect model and experiment for a critical and accurate assessment is timely, and is a development that will make ripples in the structural sciences.

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Note: The first follow-up paper on practical applications has recently been published in *Acta Cryst. D*.

CRYSTALLOGRAPHY IN AFRICA

Recent outreach activities of AfCA in Banjul (Gambia) and Boké (Guinea Conakry)

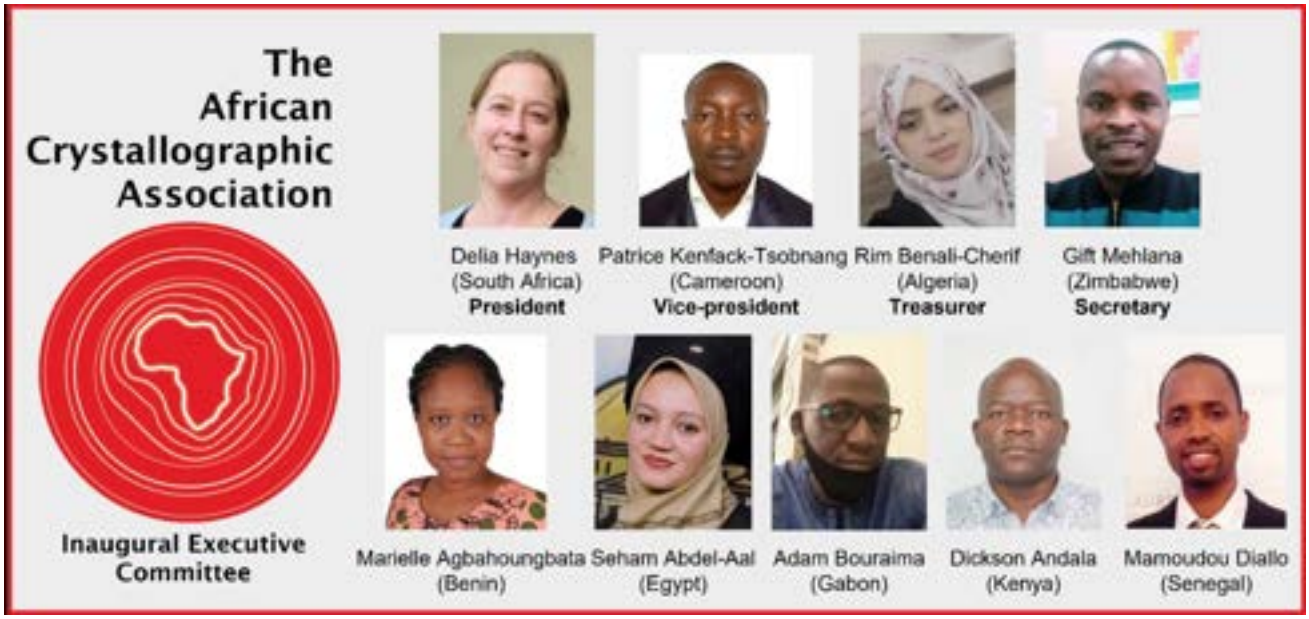


Participants in the first seminar on crystallography in The Gambia.

Mamoudou Diallo

AfCA's milestones in the dissemination of crystallography in Africa

About 15 million people died in the first two years of the COVID-19 pandemic, according to figures from the World Health Organization (WHO) (Adam, 2022). This pandemic threat has not only triggered an urgent public health declaration of international concern but has also put the global economy at risk. Science, of course, holds the key to countering this pandemic, but our inability to "see" the agent responsible is generating fear and, in some individuals, disbelief, while limiting the strategies that can be applied. Crystallography, of course, plays a unique role in helping to resolve this crisis as it can determine the structures of molecules at the atomic scale and sometimes at breathtaking speed. Recognizing the opportunity to communicate to the broader African scientific community the research opportunities offered by crystallography, as well as the value of crystallographic information, the African Crystallographic Association (AfCA) has begun organizing educational events on crystallography to promote this science on the continent. The objective of this initiative is to bring crystallography education and training to some African countries where this fundamental discipline is still lacking. During the last five months, two crystallographic seminars were organized in two different African countries, namely the Gambia and the Republic of Guinea.



First Seminar on Crystallography in the University of the Gambia (Banjul)

The first Seminar on Crystallography in the Gambia was organized in collaboration with the University of the Gambia-Science Students Association (UTG-SSA) on 1 June 2022 at the AUF digital Lab on the Brikama Campus. This first ever seminar on crystallography was intended to bring education and training of structural sciences to the participants, particularly those in Chemistry and Biology lacking ready access to crystallography courses at their institution. The impressions given at the end by the President of the UTG-SSA and the Information and Communication Ministry say it all ... .

The seminar was centered on the application of crystallography in the natural science courses, namely Chemistry, Biology, Physics and Mathematics. It was attended by 35 students from the various departments of the Division of Physical and Natural Sciences to listen and learn from the lecturers about this interesting discipline of science. Delia Haynes, the current president of AfCA, opened online the seminar with a brief presentation of the Association, and Marielle Agbahoungbata, one of the AfCA regional representatives, said a few words online regarding the advancement of the discipline in the region. Mamoudou Diallo, present on site, conducted the rest of the seminar. In the morning it was mostly about structural biology. Mamoudou gave a lecture entitled “The Role of Crystallography in the Fight against Covid-19”.



The participants listening to the lecture on the role of crystallography in the fight against Covid-19 given by Mamoudou Diallo.

After the coffee break, another – much more pedagogical – lecture followed on the theoretical understanding of the geometry of crystals. During this second lecture, key concepts of crystallography like symmetry, crystal structure, unit cell and crystal systems were introduced to the participants. In the afternoon, a two-hour workshop on the use of the *Mercury* software for visualizing molecular crystal structures was held. The crystal structure of benzene was used as an example. Students were shown not only how the atoms in benzene are arranged in patterns with six carbon atoms at the vertices of a regular hexagon and one hydrogen atom attached to each carbon atom but also the packing of this molecule was discussed and the structure–properties of this compound were studied. Through this workshop, they were able to see how the use of molecular visualization tools like *Mercury* to inspect X-ray crystal structures is essential towards understanding the properties and the applications of materials.

Also from a pedagogical standpoint, Mamoudou gave examples of how crystallography can be used to find protein structures and drugs. The students were then able to relate the information acquired to topics they studied in some biology courses. It was a total of 6 hours of crystallography lectures. A day of really hard work for both the students and the tutors but it was worth it!

It is hoped that more seminars like this will be organized. Students and young academics interested in crystallography will then have the opportunity to participate in these great scientific exchanges, which will promote the growth of the community working around crystallography.

Reaction of some participants from the first Seminar on crystallography in the Gambia

Words of the President of the UTG-SSA:

“Every society around the globe encounters problems such as increasing local and global pandemics. With application of science and technology and applying the knowledge of crystallography we will go a long way to improve the treatment of challenging and reoccurring diseases. The science students of the UTG, especially those in the natural sciences had no experience and exposure in the era of the science of crystallography. Therefore, the UTG-SSA under the leadership of President Ousman A.M Touray deemed it necessary to organize such interactive and educative seminar that may act as a catalyst to inspire young scientists of the Gambia. Such inspiration will enable the students and young academics to take up the mantle through research to figure out societal problems as a tool to providing solutions to those problems. The 17th executive council of the UTG-SSA is looking forward to welcome again Dr. Mamoudou Diallo and the entire members of the African Crystallographic Association for a visit to the University of the Gambia. The association will also want to seize this opportunity to commend Dr. Mamoudou Diallo for his invaluable contributions for the success of this event”.

Words of the Information and Communication Ministry (UTG-SSA):

"*Thanksgiving Message to the Participants. When knowledge becomes a raw material wisdom serves as the only ingredient to make the composition a real substance with unquenchable sweetness. The 17th Executive Council of the UTG-SSA is pretty jubilant to express appreciation to all the participants including all the lecturers for using their precious time to witness one of the biggest and most educating seminars ever. It was a seminar characterized with new scientific vocabularies and ideas that aroused the attention of the students with unquantifiable enthusiasm. While knowledge is like a baobab tree and which no man can ever claim ownership, the 17th executive council wishes to acknowledge that the knowledge learned today was one of its kind and will surely conduct similar activity on different areas in the world of academics. The participants indeed gained knowledge at free cost, while the welfare ministry didn’t rest on their oars, serving participants with food to boost their interest in the seminar and enable them to focus more. Indeed, it was a great magnum opus*".

AfCA seminar at the Institut Supérieur des Mines et de la Géologie in Boké (Guinea Conakry)

As for the second seminar in the Republic of Guinea, it was held at the Institut Supérieur des Mines et Géologie de Boké on 9 August 2022. This Higher Institute of Mining and Geology is one of the Guinean higher education institutions located in the region of Boké in the northwest of Guinea. Created in 1962 as the Faculty of Geo-Mining within the Polytechnic Institute of Conakry, it was established as an Institute in 1991, with the main mission of training students in the various professions of geosciences and the environment. On this occasion, AfCA was invited by the General Director of the Institute to organize the seminar on crystallography. The AfCA Vice President Patrice Kenfack Tsobnang, participating online, opened the seminar with an introduction to AfCA's vision, objectives and actions. He then turned the floor over to Mamoudou Diallo for a thorough presentation. Unlike the seminar in The Gambia, in Guinea the participants (especially the master students and the teaching staff of the institute) had experience in geometric crystallography. The seminar was therefore much more engaging in terms of exchanges, discussions and question-and-answer sessions. This question-and-answer session lasted about an hour before the coffee break.



Mamoudou Diallo talking about the science crystallography at the higher institute of Mining and Geology of Boké.

After the break, the discussion focused on some of the academic issues they are facing, especially the revitalization of crystallography teaching at the institute, which is almost at a standstill. This is because most of the experts are now retired and there are no new teachers in this field. In addition, they expressed the need to equip their institute with a new powder diffractometer to facilitate their research and teaching activities. The ambition expressed by the participants at the end of the seminar was that they are ready to join forces with other national institution members to create the Guinean Crystallographic Association, which will allow them – with the acquisition of the new equipment – to make the institute a pole of development of crystallography in the sub region.



Participants of the seminar on crystallography held in the Republic of Guinea with Patrice Kenfack Tsobnang participating remotely.

Reference

Adam, D. (2022). "15 million people have died in the pandemic, WHO says", *Nature*, **605**, 206–206.

OUTREACH

From a local to a national Vietnamese Crystal Growing Competition



Ngan Bich Nguyen, Luc Van Meervelt

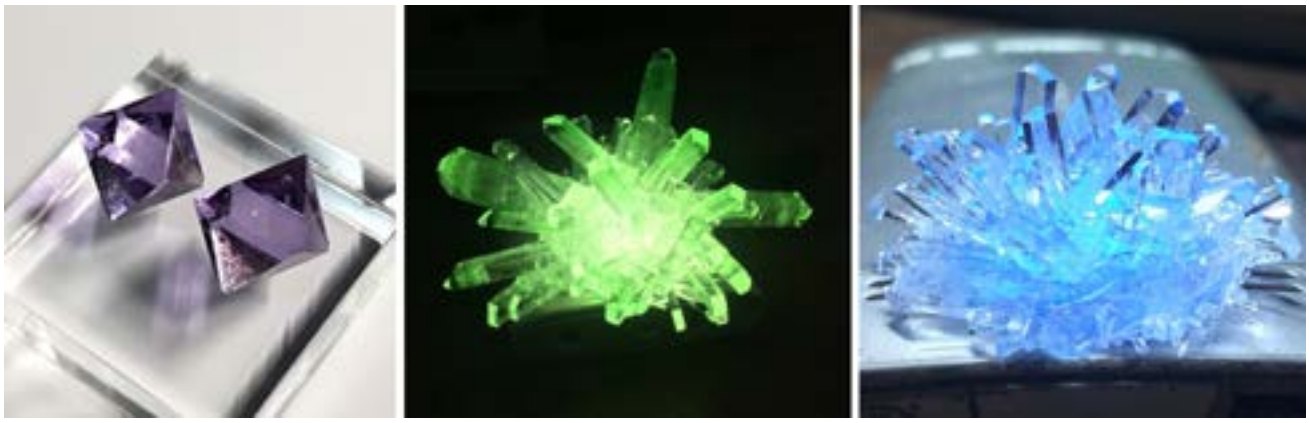
The Vietnamese Crystal Growing Competition (V-CGC) was initiated in 2014 as part of a collaboration between the chemistry departments of KU Leuven and Hanoi National University of Education and funded by VLIR-UOS (Belgium). Initially, the competition concentrated on the region of Hanoi, but in 2019 the initiative was extended all over Vietnam as one of the work packages of the MOMA project “Research-based curriculum development in molecular and materials sciences Vietnam” funded by the Erasmus+ program of EACEA.

Many schools participated in the IUCr Crystal growing competition launched in 2014 as part of the celebrations for the International Year of Crystallography. From 2016 to 2019, Vietnamese teams won several silver medals and a gold medal in 2018. During the COVID-19 pandemic, while the international competition was temporarily halted, the Vietnamese competition was successfully organized locally. The V-CGC is open to all school children from 11 years up to and including undergraduate students, divided into two groups of under and over 15 years. There are two categories: growing a single crystal and a video clip competition. The same guidelines as for the IUCr competition are used for the judging of the entries.



Laureates, their teachers and the organizers at the grand ceremony of the Vietnamese Crystal Growing Competition in the period 2019–2022.

During the difficult period of the pandemic, we have learned and achieved a lot. Vietnam is a rapidly developing country but has many schools in remote areas where learning conditions are minimal. The opportunity for their school children to conduct scientific experiments is relatively rare. Fortunately, thanks to the crystal growing competition, they can start with very simple everyday tools (such as a cup, a spoon, a piece of cardboard, a wire *etc*.) and a very popular substance in the local market, namely alum. After a short introduction to crystals and crystallization, the children can get started quickly with the help of their teacher. The interesting thing about the crystallization of alum is that it is easy to obtain a small single crystal, but it is more difficult to obtain a larger single crystal. Therefore, these experiments are suitable for both the novice and the experienced experimenter. The children work together at school (or online), familiarizing them with soft skills such as group work, problem-solving and communication skills. In addition, research skills and self-learning are further developed. For the latest round in 2022, the V-CGC welcomed 120 entries (for both categories together) from 110 participating groups coming from 38 schools. On 15 September 2022, a prize awarding ceremony was held in Quy Nhon, where the laureates (and their teachers) of the 2019–2022 editions were honored. Some crystals made by Nguyen Duc Thang, one of the laureates of the V-CGC 2021–2022, are shown below.



From left to right: crystals of chromium potassium sulfate (chrome alum), potassium dihydrogen phosphate with green food dye and potassium dihydrogen phosphate with copper sulfate (5–10% m/m).

More information is available here.

OUTREACH

Glasses and minerals in the spotlight at Sorbonne University



Making a diamond-type crystal model with jelly beans.

Cécile Duflot, Arie van der Lee

Eight years have passed since in 2014 crystallographers world-wide celebrated the International Year of Crystallography at numerous events. It was an excellent opportunity to explain the benefits of crystallography to a wider public from young to old. Since then small-scale public events have continued to take place, especially crystal growth competitions for school kids. In the UK the Big Bang Fair takes place annually, often with events related to crystallography whereas the French equivalent to this Fair is the ‘Fête de la Science’ or Science Festival, which is held every October with science events all over the country for schoolkids during working days and for all interested people during the weekends.

The year 2022 marked the commemoration of the bicentenary of René-Just Haüy’s death. Haüy was one of the most famous French mineralogists and one of the fathers of modern crystallography, thanks especially to his four-volume *Traité de Minéralogie*, which was published in 1801. This commemoration was the reason for the International Mineralogical Association to declare 2022 as the International Year of Mineralogy. In parallel, the UN General Council approved in 2021 a joint application by the International Commission on Glass (ICG), the Community of Glass Associations (CGA) and ICOM-Glass that 2022 was to be declared as the United Nations International Year of Glass.

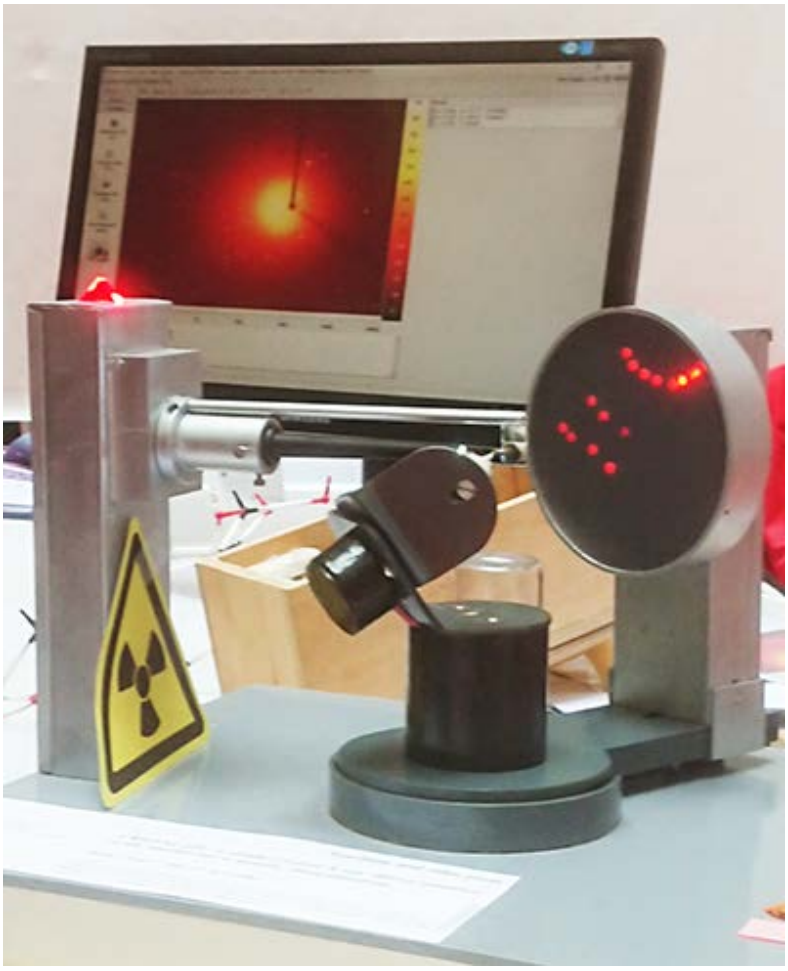
In France, glass scientists, mineralogists and crystallographers decided to join their efforts to demonstrate the contributions of their science to society's welfare at the occasion of the 2022 edition of the French Science Festival at Sorbonne University under the title: Glasses and Minerals in the spotlight. The Pierre and Marie Curie campus of Sorbonne University was chosen for this thematic event, because of the historical context since the creation by imperial decision of the mineralogy chair at the Sorbonne in 1809.

Ten different themes were defined for this event: making mirrors from crystals; minerals and the living; making or ‘blowing’ glass; making geometric atomic models from jelly beans; light and crystals; making ice with pressure; growing salty and sweet crystals; the multiple facets of glasses; how to make stained glass panels; and how to look inside minerals and crystals with X-rays. In addition, special visits were organized to the magnificent Minerals Collection – 13,000 samples of which 1500 are displayed – which is also located at the Pierre and Marie Curie campus.



Design poster. © IMPMC - Cécile Duflot.

The Glasses and Minerals event attracted 533 school kids from elementary to high school on Friday 14 October 2022. The Pierre and Marie campus recorded 11600 visitors over the three days from Friday to Sunday 16 October for this event and the other events taking place on the same campus.



The single-crystal X-ray diffractometer scale model CRISTAL-ITE used at the Science Festival at Sorbonne University [Giorgi & Berchadsky (2022). *J. Appl. Cryst.* **55**, 149–153]. © Arie van der Lee.

The ‘small talk’ with the visitors and the school kids was as usual delightful and very interesting. What do you say to an eight-year-old boy who asks you to look inside the crystal he just polished at another stand with the rotating single-crystal diffractometer model that you have shown him just before? I have cheated you, boy: it is just a model of a real diffractometer …. Maybe we can do the experiment with real X-rays later …. It was also the occasion to explain the fundamental differences between a glass and a crystal or mineral. Whereas crystalline matter is very precisely defined by the IUCr, a mineral material is not. A possible answer could be that a mineral is always natural and very often crystalline, but it can also be glassy. And for sure a crystal has an ordered atomic arrangement, but a glass has not. Much conversation covered of course all the applications that crystalline and mineralogical materials have in society and their role in everyday life.



Overview of the Glasses and Minerals event in the Atrium of the Pierre and Marie Curie campus. © IMPMC - Cécile Duflot.

These experiences of scientific dissemination and outreach to the wider public remain extremely valuable for both the scientists organizing them and also for the visitors who come to the events and maybe never realized the importance that mineralogy, crystallography and glass science have in their daily life. Fellow mineralogists, crystallographers and glass scientists, do not give up your efforts to present your work to non-scientists!

AWARDS AND PRIZES

The ECA General Interest Group on Education (GIG-03) Poster Prizes at ECM33

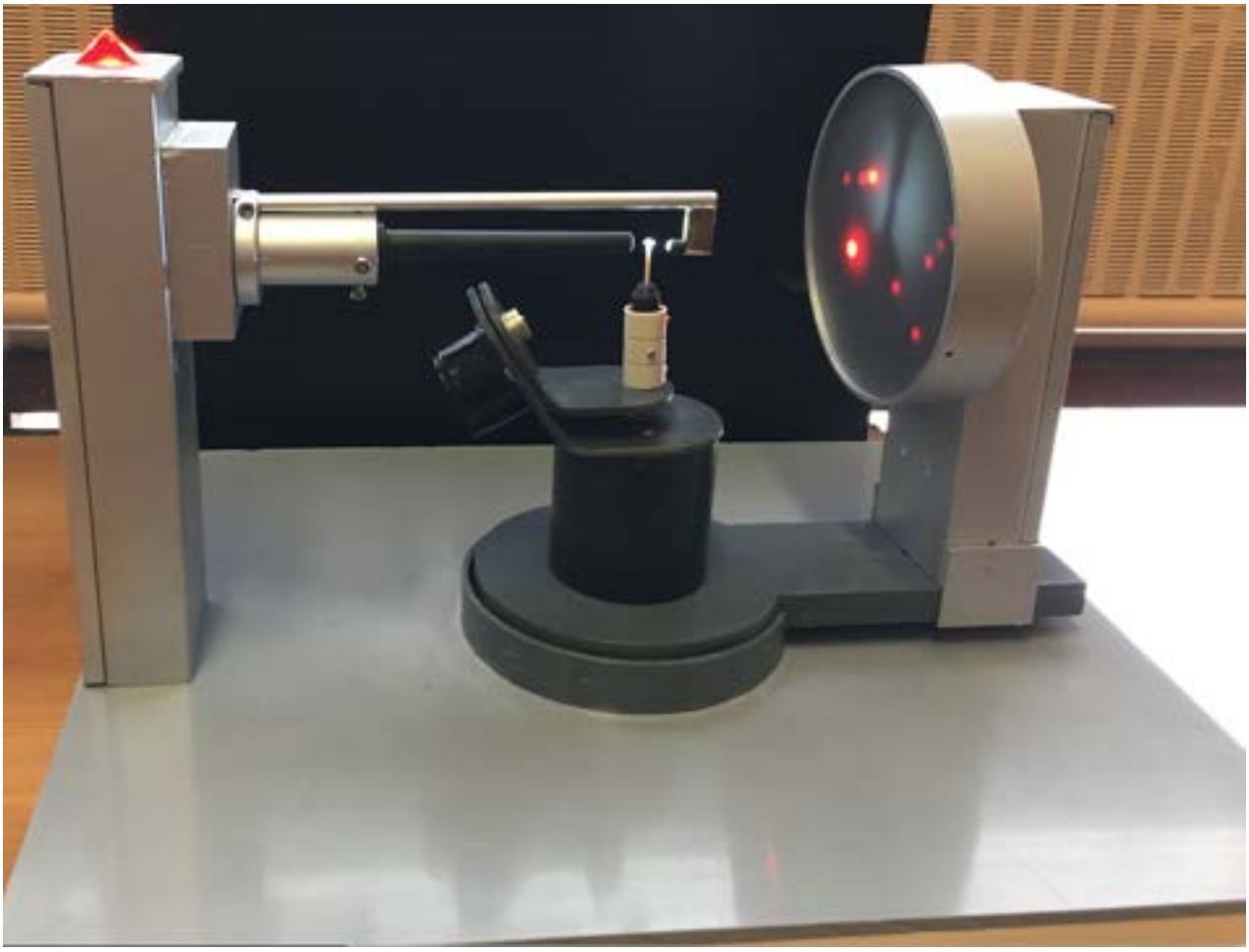


Presentation to Erhard Irmer (Germany) by John R. Helliwell (UK) of the ECA General Interest Group (GIG-03) Education in Crystallography Poster Prize at ECM33 (Versailles, France; August 2022).

John R. Helliwell

The ECA's GIG-03 on Education in Crystallography had two poster prizes. Firstly, Oxford University Press (OUP) donated a teaching book from the IUCr OUP Book Series as one of the GIG-03 poster prizes. For this Prize, the winning poster was by Erhard Irmer from Göttingen, Germany, whose poster was entitled "Expanding horizons - the use of crystallographic structures in high-school chemistry classes". His poster described both diffraction and interference of waves from two slits as well as crystal structures from the Cambridge Structural Database teaching subset. Erhard described his exploration of "what teachers dare to describe for their students in their chemistry classes" as "often teachers or students have little knowledge of crystallographic techniques". In consultation with Sonke Adlung of OUP, who was staffing the Exhibition Stand, the book *Symmetry in Crystallography: Understanding the International Tables* by Paolo Radaelli (see https://academic.oup.com/book/2799) was selected as the Prize. As an explanation for the choice of this book, we mention that the IUCr 2023 "Bragg Your Patterns" project for schoolchildren was highlighted in the ECM33 GIG-03 Microsymposium in the talk of Helen Maynard-Casely (Australia) and the approach of Paolo Radaelli's book of "first examining simple patterns as found in architecture and art" provided a connection. To hope for a connection in the schools of our *International Tables* is maybe too much; we will see what Erhard Irmer makes of it in due course.

The second poster prize was sponsored by the American Chemical Society's journal *Crystal Growth and Design*. The selected winner for this Prize was by M. Giorgi and Y. Berchadsky of Aix Marseille University, France, and entitled "CRISTAL-ITE: a single crystal X-ray diffractometer scale model for scientific dissemination". This poster very nicely linked to the education of new researchers.



The single-crystal X-ray diffractometer scale model of M. Giorgi and Y. Berchadsky of Aix Marseille University, France; reproduced with their permission.

The poster prize judges were Teresa Duarte (Portugal), Annalisa Guerri (Italy; Chair), John R. Helliwell (UK) and Marta Morana (Italy).

SPECIAL REPORT

One hundred years of Anton Paar: from a machine shop founded in 1922 to a global corporation a century later



Company founder, Anton Paar.

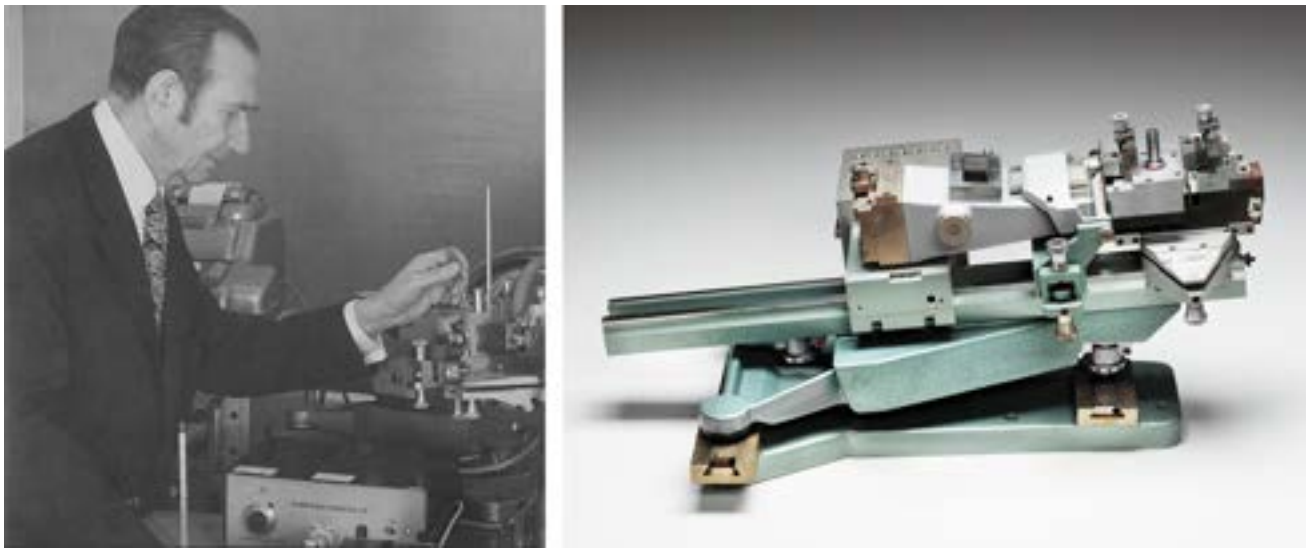
In 1922, Anton Paar established a machine shop on Heinrichstraße in Graz, Austria, starting off with just a hand drill, a foot-operated lathe and four machine vices. His clients were mainly local butchers and bakers. Ten years later, his daughter, Margareta Platzer, began to increasingly take over the business and introduced precision technologies and precision mechanics to the workshop. A year earlier, she had become the first female master machinist in Styria and began setting up the workshop's first contacts with universities in the Graz area.



Anton Paar's daughter Margareta Platzer at work. His other daughter, Hermine, did the company's accounting for a number of years.

During Margareta Platzer's era, the company started manufacturing parts for scientific devices. The first one? The famous Kratky small-angle X-ray camera, designed by Professor Otto Kratky in the 1950s, yet modern SAXS systems are still produced by the company today. The production of the Kratky camera marked the start of Anton Paar's entry into the world of measurement technology on the one hand and into X-ray structure analysis on the other. In the following decades, many new technologies and product areas were added including temperature chambers for X-ray diffraction in the 1960s, X-ray optics through the purchase of AXO DRESDEN GmbH in 2019, and an automated multipurpose powder X-ray

diffractometer in 2021.



Otto Kratky with his small-angle X-ray camera, the predecessor of the company's well known SAXS systems.

In 1954/1955, the workshop relocated to a new factory in Graz-Strassgang. The company now has more than 3700 employees and in June 2022, over 2000 of them gathered at the company headquarters to celebrate the centenary. A week of special events and activities – from hands-on workshops and product training to sightseeing tours and food trucks – was capped off with a banquet dinner at the magnificent Graz convention center.



One hundredth anniversary group picture at the Anton Paar headquarters in Graz, Austria (June 2022).

As part of the company’s celebrations, it is donating a measuring instrument to each of five universities in Colombia in 2022 to support the country’s education sector and strengthen cooperation between Anton Paar and the scientific community. Anton Paar is already involved in an education charity project in India, which has so far supported over 2,500 children through school renovations and the provision of

basic supplies – with further assistance planned in the future.

The non-profit Santner Private Foundation has owned the company since 2003. The foundation has two purposes: the promotion of non-profit science and research, and the prevention of drug addiction and the support of projects to combat addiction.

To find out more about the company's centenary, please click here.

SPECIAL REPORT

News from the Cambridge Structural Database



3D searching.

3D search crystal structures online

3D searching is now possible online using WebCSD. This allows you to search the Cambridge Structural Database (CSD) with constraints on specific parameters: angle, centroid, plane, vector or point on line (dummy points in *ConQuest*). This feature is now available to all users with a full CSD licence, including academic licences. You do not need to perform an installation or update, the change will be visible next time you log in.

Learn how to set up a 3D search in this tutorial blog.

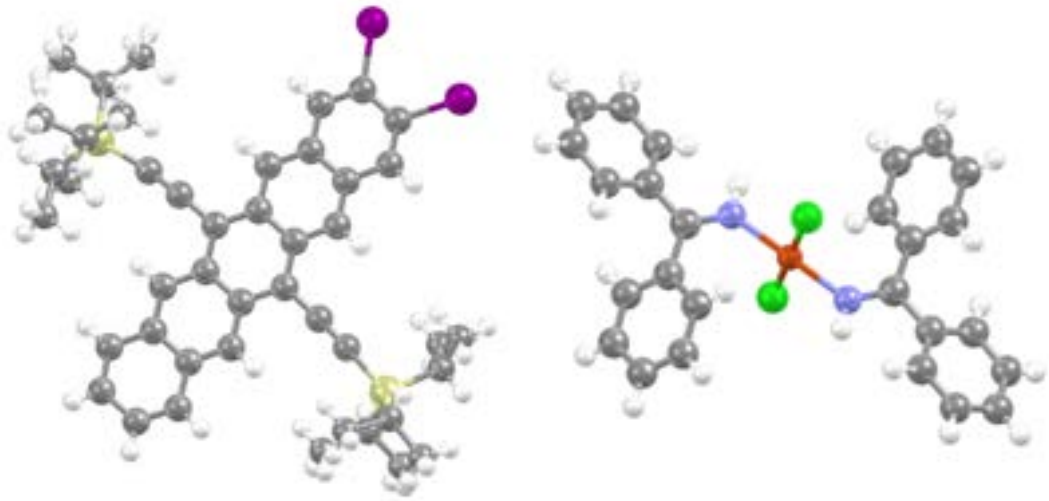
The CSD has hit 1.2 million structures

We are delighted to report that with your help, the CSD has now hit 1.2 million structures! The November 2022 data update contains over 8000 unique structures. Alongside this data release, we are also making enhancements to our CSD software portfolio to help you get the most out of this wealth of data. Learn more about our data and software releases and how to stay up to date here.

Conclusions of the 7th Crystal Structure Prediction Blind Test

In the 7th Crystal Structure Prediction (CSP) Blind Test that ran from October 2020 to September 2022, seven structures of 2D systems that had been experimentally analysed but not published (‘blind’) were released to participants along with some experimental conditions.

The seven 2D structures included Cu- and Si-containing systems that pushed the boundaries of CSP beyond the pharmaceutical sector to areas such as electronics and photonics. Other structures included one of the most challenging systems in CSP Blind Test history – a large, highly polymorphic, pharmaceutical drug candidate – along with agrochemicals and a food flavouring.



Target systems included an optoelectronic system containing silicon (left) and a metal-organic system containing copper (right).

More experimental data was released over the course of the test to simulate real world conditions.

Participants included groups from both industry and academia, and all compounds successfully had their experimentally observed crystal structures predicted by at least one group from landscapes of 1K+ potential structures.

In one challenge, a PXRD pattern for an observed crystal structure was provided alongside the 2D chemical structure. This emulated a common situation where a single crystal structure is unable to be obtained, but a poor-quality powder pattern is. This showcased an application of CSP to industrially relevant molecules.

CSP is an ever-evolving discipline and the 7th Blind Test identified future challenges including disorder prediction that had previously been disregarded owing to its complexity but is now more industrially relevant to solve as bigger molecules with more flexible groups are being seen in drug development; more challenges that reflect industrial reality; and continued broadening beyond pharmaceuticals to solid-state devices.

“Thanks to collaborative initiatives like the CCDC blind test, the complex field of CSP is advancing rapidly, taking advantage of machine learning techniques and the availability of ever-more powerful computing resource,” says Dr Jürgen Harter, CEO, CCDC. “I look forward to future Blind Tests addressing challenges such as structure ranking, overprediction and disorder.”

A scientific paper with full results is being prepared and will be submitted for publication in 2023. Preliminary detailed results, including how many groups correctly predicted each target, the lowest rankings, CPU time used and details of methodologies are available by emailing hello@ccdc.cam.ac.uk.

CCDC training, events, webinars and conferences

CCDC is planning more webinars and Virtual Workshops for 2023 so do check our events page for more details on dates and topics. If you would like to suggest topics for our sessions in 2023 you can email us at hello@ccdc.cam.ac.uk. If you can’t wait until 2023 we also have five free online courses where you learn about structural chemistry and the CSD. Find out more here. We will also be sponsoring and presenting at the PCCr3 crystallography meeting in Nairobi, Kenya, in January 2023. If you’re attending please say hello to the CCDC team!

MEETING REPORT (IUCR SUPPORTED)

Electron Crystallography School 2022



Tatiana Gorelik, Philippe Boullay

From 29 August to 1 September 2022, this year's Electron Crystallography School took place in Caen, France, continuing the tradition of electron crystallographic schools in Europe. It was hosted by ENSI Caen, France, and organized by Philippe Boullay (CrisMat, Caen) together with Stéphanie Kodjikian (Institut Néel, Grenoble), Tatiana Gorelik (HZI Braunschweig) and Mauro Gemmi (IIT, Pisa). Further details can be found on the website.

The school comprised a very rich programme, extending over four days of lectures and tutorials in diverse contemporary fields of electron crystallography. The lectures mirrored this broad scope, ranging from teaching basic crystallographic concepts, towards specifics of electron diffraction as dynamical and inelastic scattering. More practical issues were discussed in tutorials on electron diffraction data reduction and structure determination software. Particularly warmly received was the poster session with numerous contributions from the participants. A number of industrial sponsors made use of the sponsor session and presented new solutions for electron crystallography.

Academic contributions to the school came from 12 renowned scientists acting as lecturers from different European Universities, namely Philippe Boullay, Joke Hadermann, Christophe Lepoittevin, Ute Kolb, Mauro Gemmi, Hongyi Xu, Pascal Roussel, Lukas Palatinus, Jan Pieter Abrahams, Stéphanie Kodjikian, Dominique Housset and Tatiana Gorelik.

The school received strong interest, with 41 attending participants from France, Czech Republic, Italy, Belgium, Sweden, Germany, The Netherlands, Singapore, Spain, Portugal, Poland, Israel, Austria, Australia and the UK. This high attendance was helped by its setup, being organized as a satellite to the European Crystallographic Meeting ECM33 in Versailles, France. We were particularly happy to greet newcomers from established X-ray crystallographic laboratories, willing to expand their research to the electron crystallography field, either having recently purchased a TEM, or having established a tight cooperation with an electron crystallography laboratory.

We proudly highlight the strong role of female scientists, where the school managed to reach a 2:1 male:female balance for the lecturers. From the attendee perspective, the gender balance even reached an approximately 1:1 male:female balance, which may point to a stronger role of female scientists also as lecturers in the future. Budgetary support was provided by several institutions, comprising several industrial and academic sponsors. The IUCr travelling grants for students and young researchers were awarded at the social dinner. The six recipients (shown below), from EU and non-EU countries, included Barbara Gruza (Poland), Ekaterina Vinokurova (Germany), Hans Gildenast (Germany), Jacob Whittaker (the Netherlands), Walter Wong (Singapore) and Yan Li (Australia).



Winners of the IUCr travelling grant award (top). Barbara Gruza (bottom left). Yan Li (bottom right)

Yan Li (The University of Queensland, Australia)

It's been a fantastic experience to attend the ECS workshop in the final year of my PhD. Thank you for offering me the IUCr travel grant, which significantly benefitted my trip from Australia to Europe. The ECS workshop provides a great platform to improve my knowledge about characterization techniques such as 3D ED. I believe this school will help to enhance my research work and provides the possibility to find new collaborations. It is an excellent opportunity for me to learn the theoretical and practical aspects of micro-ED/ 3D-ED techniques. The knowledge I will obtain from this workshop will significantly help my current project to develop further. Last but not least, I want to thank all the community.

Barbara Gruza (University of Warsaw, Poland)

I am very thankful to the IUCr for the opportunity to participate in this school. I gained a good foundation in the subject of electron diffraction on crystalline materials. I will certainly benefit from both the discussed theoretical aspects and the computer training. Furthermore, I learned about topics that I wasn't even aware of. Conversations with scientists from the field undoubtedly broadened my horizons and helped me in setting my scientific career path.

Lastly, regarding the organization of the school and the electron crystallography landscape in Europe in general, we would like to mention the supportive role of the EU funded project NANED, having established the network of leading electron crystallographic laboratories in Europe, and special interest group SIG4 of electron crystallography of the European Crystallographic Association, who are involved in diverse activities in the field of electron crystallography.


Tatiana Gorelik
Philippe Boullay

MEETING REPORT (IUCR SUPPORTED)

25th International Conference on the Chemistry of the Organic Solid State (ICCOSS XXV)



Panče Naumov, Durga Prasad Karothu, Luca Catalano

The 25th edition of the International Conference on the Chemistry of the Organic Solid State (ICCOSS XXV) marks an important milestone in the ICCOSS series of conferences, which for nearly half a century has been gathering the organic solid-state research community. We are thrilled to have hosted this event in one of the most distinct cultural, spiritual and historic cities of Europe, the city of Ohrid in Macedonia. Marking half a century of this conference series, the theme of this conference was "*(Re)building bridges in the solid-state research community*", as a highlight of our determination to bring the community together in a post-pandemic world. The conference took place in a venue on the shores of Ohrid Lake, a double UNESCO World heritage site, and the oldest lake in Europe. The lake is also one of the three oldest on Earth and, having existed continuously for approximately 1.4 million years, it is a living museum of endemic life forms. The picturesque town of Ohrid, one of the oldest human settlements in Europe, is a religious and cultural center of Eastern Europe, and nearly 1100 years ago the Ohrid Literary School was founded here, which is considered to be the first Slavic university.



Alan Eaby, one of the recipients of the ICCOSS Award for young researchers. He was also awarded the Joel Bernstein Memorial Poster Award. Prizes presented by Luca Catalano.

The conference included four plenary speakers coming from four continents. It was opened by a plenary lecture from Craig Eckhardt (University of Nebraska-Lincoln) who led the audience through the past half a century of evolution of solid-state research. This was followed by an insightful talk by Aurora Cruz-Cabeza (University of Manchester) who provided an overview of the challenges of molecular flexibility for solid-state and crystallization. The conference was wrapped up by plenary lectures from Masako Kato (Kwansei Gakuin University), on soft crystals, and Len Barbour (Stellenbosch University), who elaborated on the future of solid-state chemistry and presented quotes from leading young researchers in the field.



Tomislav Stolar. One of the IUCr Journals Poster Prize winners. Prize presented by Luca Catalano.

This 25th conference continued the tradition of this series by being diverse and inclusive. There were 116 registered participants coming from 23 countries, with most participants coming from the UK and USA, followed by the UAE, Germany, Israel and other countries, with a favorable female-to-male ratio and age distribution. Eighty-two speakers presented their research in the oral sessions, with a very close number of male and female speakers in the final speakers' list. The conference participants included a good number of both junior and established speakers from South-Eastern Europe, providing an opportunity to present their work in times of financial and mobility constraints. The oral sessions were preceded by introductory notes from the chairs and co-chairs, which was found to be an effective approach in bringing up to speed participants who are not familiar with a specific session topic. The new role of a session co-chair ensured balanced participation of junior researchers. In addition to talks that focused exclusively on organic molecular materials, the presentations also included reports on crystallization, structure or properties of inorganic or metal-containing materials. The conference was preceded by a workshop on neutron and X-ray methods for structural analysis of organic materials, organized by Tomče Runcevski (Southern Methodist University) and Robert Dinnebier (Max Planck Institute for Solid State Research).



Weronika Kras. One of the IUCr Journals Poster Prize winners. Prize presented by Luca Catalano.

The recipients of the ICCOSS Award for young researchers, sponsored by the IUCr, were Alan Eaby (Stellenbosch University), Alyssa Thornton (Georgetown University) and Jasna Alić (Ruđer Bošković Institute). The recipients of the four IUCr Journals Poster Prizes were Shodai Hasabe (Waseda University), Weronika Kras (University of Manchester), Tomislav Stolar (Ruđer Bošković Institute) and Kristine Krukle-Berzina (Latvian Institute of Organic Synthesis). The recipients of the four RSC Chemical Science Poster Prizes were Yuki Hagiwara (Waseda University), Alyssa Thornton (Georgetown University), Cameron Wilson (University of Edinburgh) and Hema Kuntrapakam (Weizmann Institute of Science). For the first time, this event also included awards for women researchers, sponsored by the ICCOSS, with Rishika Rai (IISER Thiruvananthapuram), Zeinab Saeed (Khalifa University) and Samantha Le Roux (Stellenbosch University) as the winners. The Joel Bernstein Memorial Poster Award was awarded to Alan Eaby (Stellenbosch University).



Shodai Hasabe. One of the IUCr Journals Poster Prize winners. Prize presented by Luca Catalano.

MEETING REPORT

Workshop report: Structural resolution by single crystal and powder X-ray diffraction + Remote control of a single-crystal diffractometer



Rim Benali-Cherif

A workshop on Structural resolution by single crystal and powder X-ray diffraction + Remote control of a single crystal diffractometer took place at Abbes Lagrour-Khenchela University (Algeria), on 6 and 7 November 2022, thanks to the unfailing support of the university Rector and the support of Faculty of Science and Technology staff, and especially to the immeasurable efforts of the local organizing committee.

In a studious and relaxed atmosphere, more than 140 participants present at Khenchela (we recorded 221 pre-registrations) enjoyed two days of a workshop dense in conferences and workshops, and intense in scientific and technical exchanges. These crystallographic days *par excellence* were a great success, and brought together students, doctoral students, researchers and industrialists from around 30 universities and research establishments. The mornings were devoted to courses and conferences and the afternoons to workshops, led by professors who are among the best crystallographic specialists in Algeria.



Participant-to-participant and speaker-to-participant interactions were numerous during the workshops and theoretical sessions, allowing discussion of recent advances in the field of single-crystal and powder XRD. The accessibility and availability of the trainers was a major asset of this workshop.



Workshops (single crystal and powder).

The workshop was embellished by a very nice exhibition of used equipment and museum pieces for X-ray diffraction from the research unit of Chimie de l'Environnement et Moléculaire Structurale (CHEMS), moderated by Professor Merazig Hocine. This museum allowed participants to see, ask questions and understand the functioning of these strategic devices.



Diffraction Museum Exhibition.

The 'Remote lab' project, an idea for a remote laboratory launched by Professor Claude Lecomte on 31 August 2022, was presented during this meeting. During this workshop and for the first time in Algeria, a remote measurement was carried out on a single-crystal diffractometer of the Laboratory of Cristallographie, Résonance Magnétique et Modélisations (CRM^2), piloted remotely from Abbes Laghrour Khenchela University by Dr El-Eulmi Bendeif.



Remote lab.

Presentation of AfCA

During this meeting, Dr Rim Benali-Cherif, president of the workshop, presented and highlighted the actions and roles played by the African Crystallographic Association (AfCA) in the promotion of crystallography on the African continent, due to the quality of the educational interventions and the support. These were able to capture the audience, thus allowing the effective transfer of knowledge.



Acknowledgements

We thank the Universities of Khenchela, Jijel, Constantine 1, Bouira and Lorraiane (France), and SINAL Algeria and la direction générale des oeuvres universitaires for their support.


UNIVERSITE ABBES LAGHROUR DE KHENCHELA
Organise
La première édition de workshop International sur
06 et 7 novembre 2022

AWARDS AND PRIZES

Liebau Prize awarded to Juan Manuel García-Ruiz



Wulf Depmeier

On the occasion of its annual conference in Munich, Germany (14–17 March 2022), the German Society for Crystallography (DGK) presented the *Waltrude und Friedrich Liebau Prize* for the Promotion of Interdisciplinarity in Crystallography for the year 2022 to Juan Manuel García-Ruiz, CSIC Professor at the University of Granada, Spain. Because of the COVID pandemic, the annual conference had to be held virtually, so the certificate could not, as usual, be handed over by the chairman of the DGK. As the award winner spent the first half of 2022 as a Senior Fellow at the Institute for Advanced Studies (Hanse-Wissenschaftskolleg, Bremen–Oldenburg), located in Delmenhorst, his host in nearby Bremen and co-author of important publications, Professor W. Bach (University of Bremen), agreed to hand over the certificate.



Professor García-Ruiz (left) with Professor Bach.

The decision of the prize committee to select the awardee was justified on the certificate with the following words translated into English:

"...for his fundamentally innovative considerations of the biological origin of microfossil structures as well as for his future-oriented examinations of chemical activity of self-organized mineral aggregates, which contribute to a new understanding of the importance of inorganic mineral building units for the development of natural biorelevant molecules under geochemical conditions and thus essential building blocks to establish a plausible prebiotic chemistry."

In this context, the recently quoted advertisement for a W3 professorship at the Faculty of Geosciences of the Ludwig Maximilians Universität, Munich, is interesting, as it reflects the high topicality of the award, as the job description quoted in part explains:

"The Faculty of Geosciences of the Ludwig Maximilians Universität München invites applications for a Full Professorship (W3) of Mineral Earth and Life Interaction commencing on 01.04.2024. The Mineral Earth and Life Interaction professorship is intended to further strengthen the Faculty of Geosciences in the field of Earth and Environmental Sciences. Applicants are expected to have innovative and internationally visible research activities focused on the interaction of the mineral world and living organisms, as well as the ability to interface with the environmental sciences. Relevant research areas should cover the multi-scale structural relationships of biomaterials that contribute to a deeper understanding of the interaction of inorganic and biological processes. Research activities might include the formation of biomineral composites as well as processes that dissolve, convert and transform minerals. The focus should be predominantly on mineral components. It is desired that applicants employ state-of-the-art structural research methods, such as electron, photon, neutron or scanning microprobe techniques, atomic diffraction, nanoscale imaging and/or microchemical techniques."

In addition to the certificate and the appropriate words of praise, the Liebau Prize comes with a considerable amount of prize money. The prize sponsors, Professor Friedrich Liebau from the University of Kiel, who died in 2011, and his wife Waltrude, provided the foundation with share capital and stipulated in the statutes that the prize money is to be raised from interest income or from donations or private donations. As is well known, interest rates have developed negatively over the past decade, so that there was a real danger that further award ceremonies would no longer be possible without access to capital, which was denied. Following a call from the Board of Directors, the members of the DGK unanimously agreed to a voluntary increase in the annual membership fees in order to raise the prize money. Incidentally, the same applies to the DGK's Max von Laue Prize for young scientists, which is subject to similar conditions.

A more detailed appreciation of the awardee and his merits is included (in German) in Vol. 52 of the *DGK-Mitteilungen* and is available for download. The present short note confines itself to a few general remarks, and preferably those of topical relevance. Professor García-Ruiz is called Juanma by his friends. As I hope to count myself among them, I will occasionally use this name.

First, I would like to mention Juanma's diverse activities to spread his profound knowledge about almost every aspect of crystallization to almost everyone. He not only shares his experience with his students and colleagues but also with school children of all ages, where he knows how to arouse interest and enthusiasm for crystals and their beauty. For the first category, there are the well known International Crystallization Schools of Granada, which are annually alternately inorganic or biologically oriented. For the second category, there are crystallization competitions for school children, whose sheer number of participants (approximately 14,000 annually in Spain alone) are self-explanatory. He also scores points with the lay public, where he has caused a stir in various media, for example, with his reports on the giant Naica crystals (*El Misterio de los Cristales Gigantes: Edición comentada del guión de la pelicula Triana*, Science and Technology 2015).

Juanma is very interested in promoting and cultivating connections between crystallography and related scientific communities. For example, in 2016 he led the first COSPAR–IUCr workshop on *Crystallography for Space Sciences – an International School and Capacity Building Workshop* held in Puebla, Mexico (BUAP) as well as in the nearby charming village of Tonantzintla, San Andrés Cholula, on the premises of the Instituto Nacional de Astrofísica, Óptica y Electrónica (INAOE). Hanna Dabkowska, current President of IUCr, attended the event as a representative of the union; see Hanna's account in the 2016 *IUCr Newsletter* (old series). Incidentally, I was also present. This was a welcome opportunity for me to look back on my first visit to Mexico (1981, after the 12th IUCr Congress in Ottawa, Canada) when I spent a pleasant few days in and around INAOE.

The COSPAR–IUCr workshop was organized under the auspices of the IUCr and IAU (International Astronomical Union), both members of the International Science Council (ISC). COSPAR is the abbreviation for the Committee on Space Research. Like other committees, it was established to assist the ISC and its 200+ member organizations in pursuing their respective scientific goals, should the specific competencies and skills of the committee be required. Therefore, the *raison d'être* of COSPAR is clearly interdisciplinary, and the purpose of the workshop was to familiarize young international students with some aspects of space exploration and its relation to crystallography. Participants received first-hand information from leading international specialists from various fields of space exploration. Among the numerous contributions, a special one deserves mention. This was the NASA Mars mission *Mars Science Laboratory* (start 2011) and its rover *Curiosity*. Participants with a keen interest in crystallographic methods were particularly attracted to *CheMin*, a portable and remote-controlled X-ray powder diffractometer tasked with studying Martian rocks on site. The *CheMin* project leader explained how the instrument works, and how the relevant data were transmitted over a distance of around 70 million kilometers to our planet for further study. A demonstration project was planned for the workshop, in which a replica of *CheMin* would be installed on the nearby Popocatépetl volcano. Sampling and diffraction would be carried out on site, and the data would then be transmitted to the INAOE for data analysis by the participants. Unfortunately, that plan fell victim to an unexpected event when the volcano

entered a severe eruption phase. It could have been worse, as the eruption produced an intense ash rain so that the sampling could be carried out practically on the doorstep of the INAOE and the functionality of *CheMin* could be convincingly demonstrated.

One of the main themes of the workshop was the search for the origin of life on Earth and elsewhere. Professor García-Ruiz is one of the main players in this field of research, as evidenced by numerous publications. He is particularly intrigued by the possibility that inorganic materials may have played a major role and that both large-scale geological processes and widespread but small-scale physicochemical and catalytically controlled chemical reactions operate in confined volumes. Juanma was also involved in several aspects of planning for the *ExoMars* (Exobiology on Mars) mission. Organized under the leadership of the European Space Agency (ESA), this highly interdisciplinary project aims to search for traces, or perhaps even remnants (but likely extinct) of primitive life on Mars. It was hoped that this approach would provide clues as to whether primitive life forms might also have existed on the young Earth or whether they originated on the hitherto lifeless planet. The educated guess of geoscientists justifies this approach that Earth and Mars evolved more or less in parallel for the first ~500 million years after their formation, before Earth's geodynamics set in, resulting in convection currents in the mantle and plate tectonics. Continuous formation and decay of the Earth's crust would have destroyed all evidence of possible life. Mars is essentially unaffected by such dynamics, and possible remnants of early life would have stood the test of time there.

Juanma was elected IDS (Interdisciplinary Scientist) of the *ExoMars* project. This was because one of his main scientific interests was the investigation of self-organization phenomena in biological and geological structures, with possible implications for the origin of life. To appreciate the importance of crystallography for the planned investigations, the *ExoMars* rover was christened *Rosalind Franklin*. This was a tribute to the great scientist Rosalind Franklin (1920–1958) for her important work in connection with the elucidation of the structure of DNA. The launch window for *ExoMar*s was planned for the period between August and October 2022. This plan fell victim to a side effect of the February 2022 Russian invasion of Ukraine. ESA, the leading science agency of the *ExoMars* project, decided to end the hitherto pleasant and successful cooperation with the Russian State Space Corporation Roscosmos. It is currently unclear when, or if, there will even be a future for *ExoMars* and the *Rosalind Franklin*.

To better characterize Juanma as a scientist, it makes sense to mention his activities in the Spanish program *Explora*, where he devised the concept and chaired the Scientific Advisory Board. Scientifically demanding projects that are risky in terms of achieving their goals are funded. Such projects often focus on the (blurred) boundaries between established scientific disciplines. Even if some projects will (honorably) fail, others can be successful and change established thinking and action. It might even be that this disrupts old ideas in favour of radically new emergent thinking. The *Experiment!* program of the Volkswagen Foundation and the *Reinhart–Koselleck* program of the German Research Foundation (DFG) seem to follow a similar approach.

Presumably, as a result of the approach described, Juanma seems to be deeply convinced that the border between the realm of crystals and that of living matter is not well defined and sharp, but blurred; there could be a gradual transition between both sides. In this context, it is appropriate to mention the research topic of Juanma during his stay at the Institute of Advanced Studies Bremen, Oldenburg, namely Biomorphs in Science and Art.

Following his belief, Juanma seems, supported by some evidence, to have developed an idea that crystals hold a certain special place in the totality of natural things, and that the contemplation of crystals might have provided a direction for the development of the early human mind. This would then have led to early forms of a sense of symmetry, beauty and later art, and possibly associated with various forms of transcendence. He has published the following interesting article on this, *2001: the Crystal Monolith*, which is characterized by the following remarkable combination of keywords: crystals; crystallography; abstract thinking; paleoneurobiology; *Kubrick, 2001: a Space Odyssey*. The article provoked a comment from J. R. Helliwell: *Wrestling with questions at the edge of science methods* in the *IUCr Newsletter* in

2018 as well as an editorial comment by A. M. Glazer, where both recommended reading the article and reflecting on the ideas expressed there. (The author of these lines also later felt encouraged to write another comment entitled *Some humble side-notes on quartz, handedness and possible evolution of the human mind* in the *IUCr Newsletter* in 2019).

At the IUCr25 Congress in Prague (2021), Juanma gave a well received keynote lecture, building on his earlier works and which was supplemented by new ideas and historical evidence combined with experimental observations. The title also reflected his research topic at the Institute for Advanced Studies and was *The crystal and the rose: on the influence of crystals and crystallography on art and mind*. A summary can be found in *Acta Cryst. A*. He also reported the remarkable observation that not only infants, but also monkeys, have a clear tendency to prefer regularly shaped, or maybe even symmetrical, patterns over less regular or unsymmetrical ones. Juanma is planning corresponding systematic behavioral experiments on monkeys.

In a 2021 post for the *IUCr Newsletter* entitled *Ancient crystal collectors*, Juanma commented on a recent finding from palaeo-archaeologists. These findings seem to support his ideas about the possible relationship between crystal shape and consciousness-raising in hominins as our early ancestors. Juanma offers some arguments for an explanation of the find. I agree with most of them but tend to have a slightly dissenting opinion in a particular case. In his essay, he shows a photo of 30 or so calcite crystals that were excavated at a site in southern Africa and were obviously collected by hominins around 100,000 years ago and preserved by them for unknown purposes. All crystals in the photo are rhombohedrally shaped and their surfaces are more or less corroded by weathering. While well formed as-grown rhombohedral crystals of calcite are well known from other places in southern Africa. The occurrence of calcite in the close-by vicinity of the digging is reported to be restricted to massive crystal aggregates within a dolomitic limestone deposit. Therefore, the rhombohedral shapes were most probably formed by cleavage, either by accidental impact from the environment or caused intentionally by appropriate handling. The scientists involved in the excavation, and Professor García-Ruiz alike, seem to prefer the latter possibility and in addition, they are convinced that any usage of these crystals as primitive tools can be ruled out, given their poor mechanical properties (low hardness, cleavage). I agree with that. In addition, Juanma challenges the idea that optical properties might have drawn the hominins' particular attention to the calcite crystals shown. Thereby, he focusses on birefringence, or double reflection, as a characteristic property of calcite, and he suggests that the poor quality of the finds prevented this effect from being observed. I agree, and one may add the likely underdeveloped technical skills of the hominins and the obstacles to finding suitable means for observing double reflection.

Instead of the latter rather tricky property, I would like to suggest another, more easily observed optical property, namely the reflection of light from flat surfaces. Mineralogists often use the different reflectivities, or luster, of minerals as a simple means for distinguishing between different mineral species. The perfect cleavage of calcite results not only in extremely flat surfaces but also in a particular luster on the rhombohedral cleavage planes. Because this is associated with iridescence, the luster is then labeled as pearl-like. The occurrence of iridescence requires crystals of the highest quality and freshly prepared cleavage planes. The effect lasts for only some time, after which the luster becomes less brilliant and loses the iridescence: the luster is then labeled glass-like. Nevertheless, such a cleavage plane is still highly reflective of sunlight. Because of the relatively low resistance of calcite to corrosion by water and particularly carbon dioxide, the flatness of the crystal faces, and hence the reflectivity, are likely to wane over the course of millenia, unless the crystals are protected from moisture.

As a particularly outstanding property, the reflected rays from a flat surface can be observed over a great distance – tens of meters or more – provided that the reflecting plane and the observer are properly oriented. In a figurative sense, one might then say that a kind of information channel has been opened between the crystal and the observer. Even a not-too-heavily corroded crystal surface can still be recognized by its luster. I suspect that this optical effect might have partially contributed to the attraction of calcite to hominins living in this part of Africa. One may speculate that the striking shine from the cleavage planes might have reminded the hominins of the shine of water in a puddle or a water hole. This

could then have evoked a positive connotation between the optical effect and water, which is so essential for life and survival. One can also speculate that the ephemeral and intangible phenomenon of reflection might have been understood by the hominins as a kind of shining path into a transcendental world, and perhaps it was celebrated by unknown ritual acts. Interestingly, the attraction to shiny things seems to be innate for various animate beings, as it is found not only in infants but also in a number of animal species such as, for example, magpies.

Finally, I would like to return to Juanma's plenary lecture at the IUCr Congress 2021 in Prague, in which he reported on the possible preferences of monkeys, and possibly infants, for regular and symmetrical patterns and his planned behavioral studies on them. For me, this will essentially be summed up in one question: is there an innate sense for symmetry? I have not found an answer myself, and I hope to get one from Juanma or other eminent experts. In doing so, I refer to two publications from the non-crystallographic literature in the strict sense. One was published in the German weekly DIE ZEIT on 9 June 2022 in an article by Christoph Drösser entitled *Was ist leichter zu zählen?* (*What is easier to count?*), where he reported on exciting debates between interested philosophers, psychologists, cultural anthropologists, cognitive researchers and other scientists. Ultimately, the question is whether there is an innate sense of numbers or whether the human understanding of numbers is a cultural achievement. It seems that the majority of these scientists think, and the article provides several examples to support this, that the sense of the natural numbers 1, 2, 3 and 4, maybe even 5, is innate, while everything else is in mathematics cultural appropriation (Menschenwerk), starting with the basic arithmetic calculation skills. Such an achievement can also be lost again if it is no longer needed. A recent example seems to me to be the widespread declining ability to do mental arithmetic, no doubt because of the ready availability of electronic devices.

Can the findings about innate number sense be transferred to symmetries? Is there possibly an innate sense of symmetry? To say it in advance, if there were such a thing, then this sense would not be equated with crystallographic symmetry concepts: the laborious learning of symmetry operations, plane, point or space groups and their complex relationships represents a cultural appropriation; through disuse one can lose this again. So there must be a more primal level from which one might hope to find something like an innate sense of symmetry.

In a chapter for *Symmetry 2 – unifying human understanding* (1989, edited by István Hargittai, Pergamon Press) Y.-M. Ha on pages 921–930 under the title *Symmetry in pictures by young Chinese children* describes the age-dependent development of the use of symmetry features in the paintings of Chinese children. The earliest recognizable symmetrical representations shown are observed in drawings by around 3-year-old children and can be interpreted as round, approximately radially-symmetric objects such as the sun or the silhouette of a human face. Later, these can be supplemented by mirror-symmetrically arranged eyes or ears, and stick figures with human-like attributes, such as outstretched arms and legs, also show mirror symmetry. The sequence of appearances of these early painted realizations of such patterns – and in later ages of even more complicated patterns – is certainly directed and controlled by the developmental process of the child's brain and motor development. However, it should be clear that these are active pictorial formations by young children who have learned these skills, not original passive preferences for particular patterns presented to them. So is there in humans – and in hominins? – hidden, innate abilities to recognize symmetry? Y.-M. Ha does not report on such studies and the question remains unanswered for me.

However, it is worth noting an interesting cross-relationship between the accepted natural number sense mentioned before, on the one hand, and the cleaved rhombohedra of calcite found by the *Ancient crystal collectors*. The (idealized) rhombohedron, and also the cube from which the rhombohedron emerges through distortion, and provided that the respective polyhedron is non-transparent, as is the case with the corroded crystals of the find, the eye of the viewer perceives either 1, 2 or 3 crystal faces. Is it by pure chance? Or did the hominins attach a meaning to that? We do not know. With all due respect to the hominins, I presume that they tended more to number mysticism than to an early kind of Haüy's theoretical approach. This question is open to various forms of speculation, which I would like to refrain

from.

But what about the 4? Of course we don’t know either, but it doesn’t seem obvious how this natural number should be found on the cleaved rhombohedra of the calcites. But had later relatives of the `ancient crystal collectors' within the genus Hominidae lived in the canton of Berne in Switzerland, they might have seen a sight such as that depicted by the painter Ferdinand Hodler (1853–1918) in his painting *Le Lac de Thoune aux reflets symétriques* (1909). It shows an almost mirror-symmetrical mountain range reflected in the still waters of the lake, so the painter had to depict four `symmetrically equivalent' mountains. The reader may wonder what this means. Of course, this has little to do with calcite, but the peculiarity of the number 4 becomes apparent. This picture is shown as a present for my friend Juanma, in order to congratulate him once again on receiving the Liebau Prize.



Ferdinand Hodler (Berne,1853–Geneva, 1918) “Le Lac de Thoune aux reflets symétriques” (1909). Reproduction with permission of MAH Musée d'Art et d'Histoire, Geneva, Switzerland (Inventory No. 1939-0036).

COMMENTARY

Crystal allure: a response to Depmeier's article



Juan Manuel García-Ruiz

I would like first to thank Professor Wulf Depmeier for writing a thoughtful, informative and overly generous *laudatio* on the occasion of the Waltrude and Friedrich Liebau Prize for the Promotion of Interdisciplinarity in Crystallography, awarded to me by the Deutsche Gesellschaft für Kristallographie (Depmeier, 2022). Working on the frontiers between disciplines is not an easy task. It is a zone not always appreciated by evaluation panels and science programs. I like to explore that zone. I have been a fan of crystallography since I was sixteen years old, an expert who knows its powerful diffraction methods developed during the XX century, one of humankind's most fascinating intellectual odysseys. I know about crystals, their fascinating properties, their birth and growth, and I apply this knowledge to everything I find interesting, beautiful and challenging. To be awarded for this is something unexpected that I receive with honor and happiness. I will not comment on the biographical aspects of the article except to inform the reader that the ESA headquarters announced today that the ExoMars mission that will transport the rover "Rosalind Franklin" to the surface of Mars is re-scheduled for 2028.

In addition to the *laudatio*, Professor Wulf Depmeier, Wulf, opens with a discussion on a couple of points I would like to comment on because it is also of interest to one of my current interdisciplinary investigations. I have devoted part of my research in recent years to studying the influence that the idea of crystals has had on art, an intellectual passion that I share with Professor Depmeier, a pioneer in this field. During my sabbatical in Germany this year, we shared many ideas and data; along with Professor Wolfgang Bach we visited the Wenzel Hablik Museum in Itzehoe, a small but historical town not far from Hamburg and Kiel, where Wulf lives. We discussed how these influences occurred at several stages of history/prehistory and what evidence we have for them.

The oldest of these influences is rooted in the earliest stages of the evolution of our minds before what we call consciousness emerged. Nowadays, it is considered that the first evidence of the symbolic thought of our species is none other than the collection of quartz and calcite crystals, a practice that started at least 780,000 years ago. There is plenty of archeological evidence for this practice, as described in the literature (García-Ruiz, 2018) and a previous article in this newsletter (García-Ruiz, 2021). In that article, I wondered if crystal morphology could be one of the reasons for the allure of crystals for our ancestors and modern humans. Professor Depmeier kindly discussed this issue in his article and proposed that another cause of the attraction of crystals for hominins could be the reflection of light by their flat faces, which is termed brightness or luster. This is an important issue because we need to know how deep in our minds is the attraction that we feel for crystals. We need to know in detail the reason(s) for the crystal allure and how it affected the development of our brain and our

understanding of the world, our social relations and our beliefs. Some could consider that this kind of investigation is hardly within the limits of what we consider science (Helliwell, 2018). We should recall that, despite the absence of scientific evidence, a large percentage of the population, irrespective of educational level, gender or regional origin, believes in the healing power of crystals. Sixty percent of the sales in mineral shops are related to this belief. I think it is neither ethically correct nor wise for rational scientists to fight these feelings. However, a serious investigation of crystal allure would explain why today so many people still believe in magic crystals. My research aims to send the message “you are free to trust in the magic properties of crystals, but we can explain why you are trusting, which is the origin of that belief, and to what extent that belief is reasonable”.

There is no doubt that optical properties such as brightness and transparency are among the main reasons why single crystals could have been attractive to our ancestors. Hominins were familiar with both optical properties because water, under certain circumstances, can have them, as Depmeier perceptively suggests. In fact, the word `crystal', coined in ancient Greece to name rock crystals and other transparent minerals, means frozen water. This etymology is proof of the relevance of optical properties in the conceptual relations of early humans with minerals. The solidity of crystals would make those optical properties even more charming. Quartz and other crystals would have been the only solid objects showing high transparency and light reflection that early humans would have encountered and handled.

However, brightness (*i.e.* light emitted by a reflecting surface) is not a passive property of the objects but an active one. Unlike shape or transparency, the light reflected by an object unavoidably draws our attention, bothers us, disturbs our vision. It is a call that makes us pay attention to the shiny object. Mineral sellers place sparkling crystals in strategic places on their sales tables and their most valuable crystals around them because they know that customers will be attracted to the shine and stop by. The glow of crystals was undoubtedly an important property in attracting hominin attention, but probably not enough by itself to make them valuable to be collected. Last fall, I started investigations to explain the allure of crystals for hominins with the help of a group of chimpanzees, the closest apes from which we parted about six million years ago and with whom we share many genetic and behavioral similarities. The results have not yet been published, but in correspondence to the beautiful gift offered by Professor Depmeier, the painting of Ferdinand Holder “Le lac de Thoune aux reflets symetriques” I wish to share with you in his honor some frames of a couple of the videos recorded during the investigation with the cooperation of Dr. Tomás de la Rosa, Guillermo Bustelo and Aden Bart; see the figures below.



In this series of frames, we see Ivan, a chimpanzee who picked one of the crystals of quartz that we deliberately located in their garden within a pile of pebbles. Chimps only selected the quartz and calcite crystals and left the pebbles in the

green. Here, Ivan has a transparent crystal of quartz of *ca* 3.5 cm in size in his left hand. He then brought the crystal very close to his eye and inspected it carefully. The numbers in the pictures indicate the time of the frame in the video. He repeated the actions several times. This episodic inspection lasted for more than 15 minutes. Ivan and the other chimps also did the same inspection of transparency inside the dorm and outside in the garden. These and other results of our investigation suggest that the mind of the chimps is prepared to identify and recognize crystals from other natural stones, value them and have a curiosity beyond the one driven by novelty.



Toti is shown here examining a large single crystal of quartz. That crystal was used in one of our experiments along with an irregular stone of similar size to compare their attractiveness for chimps. The two objects were exposed in the garden of the chimps on top of two pedestals. The preference for the interaction with the crystal was statistically obvious. In addition, the chimps took the crystal and transported it to their dorm, where they studied it for a couple of days until we managed to take the crystal back. Toti oriented the crystal to observe it from different angles, showing particular interest in the view parallel to the hexagonal axis.

Toti's attentive observation of the quartz crystal, rotating it in her hands and tilting her head to see the crystals with specific orientations, reminds me of the other question that Wulf asks in his article. Is there an innate sense of symmetry? In my opinion, based on paleo neuropsychological studies, the perception of symmetry and the production of symmetrical artifacts is a consequence of the evolution of hominid spatial perception-cognition (Coolidge & Wynn, 2020). This evolution included both developments in perceptual-cognitive abilities and developments in skill, but – unlike numbers (quantity), another subject discussed by Wulff – does not require language (Wynn, 2000). While there are studies on pattern recognition and preferences performed with the typical methods of cognitive psychology, I found especially informative archeological studies on hominins' tool production (Malafouris, 2021). These studies tell us that the cognitive requirements of stone knapping are within the abilities of apes, although at a very primary level. The earliest artifacts produced by hominids Mode I tool industry 2.5 million years ago do not exhibit clear symmetrical patterns. The earliest examples of hominid-imposed symmetry occur on tools termed bifaces or hand axes, which appeared 1.4 million years ago, and experienced a qualitative enhancement of symmetry around 500 thousand years ago, *i.e.* at the time when hominins started to collect crystals. To the best of my knowledge, behavioral studies on the preferences of humans

and apes for symmetrical patterns have never considered the attraction that crystals, the only 3D natural objects with Euclidean symmetry, exert on hominins, hominids and humans. Incorporating such information in these studies is important because it is a fact, not an assumption, a belief or a conjecture. Experimental studies devoted to explaining the details of the attraction will help us to understand it better and to answer new questions like, is our brain designed to prefer order? *i.e.* do we like crystals because crystals were among the first natural object to be collected? Or did we collect crystals almost one million years ago because our brain was already designed to prefer Euclidean order? Is the impact of crystals on culture due to the fact that they are firmly linked to the birth of art, symbolism and conscience? The future is open to those who wish to find the answers to these questions.

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HISTORY OF CRYSTALLOGRAPHY

René-Just Haüy and the birth of crystallography



Jean-Claude Boulliard, Delphine Cabaret, Paola Giura

In 1784, a small book entitled *Essai d'une Théorie sur la Structure des Crystaux* was published marking the beginning of modern crystallography. A crystallography that departs from being purely descriptive to using mathematics. A crystallography that predicts shapes and reveals molecules that would be debated for almost a century.

Its author, René-Just Haüy, a French abbot living in Paris, at almost 40 years old, began a scientific career focused on the study of crystals. His successes made him one of the greatest scientists of his time.

To mark the bicentenary of his death, this article presents the milestones of his unusual career in the troubled historic context of the end of the 18th century. The state-of-the-art knowledge of crystallography before Haüy is demonstrated. Then, Haüy's work is highlighted from the birth of a myth to that of a theory that made crystallography and mineralogy real sciences like physics and chemistry. Finally, without neglecting the criticisms of the German scientists, the heritage of Haüy's theory is developed with the works of Delafosse and Bravais.



Portrait of René-Just Haüy by Nicolas Gosse. Oil canvas © MINES ParisTech, Mineralogy Museum, Paris, France, photo D. Nectoux.

René-Just Haüy, an uncommon course

Haüy: one name, two brothers, two great men

René-Just Haüy was born on 28 February 1743 in Saint-Just-en-Chaussée, a small town located 100 km north of Paris. His parents were modest linen weavers. On 13 November 1745, they had another child, Valentin (Fig. 1, left and middle). Valentin is rather well-known outside of scientific circles for his work on behalf of blind people. A brilliant mind, he learned Latin, Greek, Hebrew and a dozen modern languages. Scandalized by the lack of consideration of society towards young blind people, he decided to act to improve their lot. In 1786, he founded what was to become the French 'Institut National des Jeunes Aveugles' (INJA). He made relief prints on paper that enabled blind people to learn to read. This new method inspired one of his students, Louis Braille, who invented the so-called Braille writing system.

René-Just Haüy is much less well-known. Like his brother, he showed keen intelligence, leading him to teach and preach. His attendance at the Royal Botanical Garden (the forerunner of the National Museum of Natural History) led to his interest in crystals and crystallography. After a long gestation period, this discipline began to emerge at the beginning of the 18th century and made significant progress in the description of minerals. Haüy revolutionized crystallography with a theory that, from success to success, made him one of the greatest scientists of his time.

The two Haüy brothers lived their last years together, in a certain degree of discomfort, and died in the same year, 1822, on 19 March for Valentin and on 1 June for René-Just. They are both buried in Paris in the Père Lachaise cemetery (Fig. 1, right).



Figure 1. Left: René-Just Haüy and his brother Valentin by A. Boilly. Engraving, XIXth century. Middle: statue of the Haüy brothers located in front of the city hall of Saint-Just-en-Chaussée (Oise, France). René-Just is watching a calcite prismatic crystal and Valentin is helping a blind child. Right: grave of the Haüy brothers at the Père Lachaise cemetery (60th division).

From church to crystals

Nothing seemed to predestine Haüy to all the activities he carried out. His path seemed to be all mapped out, but it was not.

From the first years of his life, he showed a certain disposition to piety that never left him. Because of his singular enjoyment of religious ceremonies and songs, coupled with his quick wit and intelligence, the prior of the Premonstratensian abbey of Saint-Just asked some monks to teach him some lessons. Impressed by the child's skills as young as six years old, the prior convinced his mother to move to Paris so that René-Just could receive a proper education. In 1749, the family moved to a street near the church of Saint-Eustache in the center of Paris. For a few years, he was a chorister at the Saint-Paul church (Faubourg Saint-Antoine). During his childhood years, he practiced singing, harpsichord and violin, and developed his talent for music. Then, with the help of recommendation letters written by the prior of the Abbey of Saint-Just-en-Chaussée, he obtained a scholarship to study theology at the Collège de Navarre (Fig. 2, left). He was tonsured at the age of 19. Two years later, he became regent of fourth grade in the same college where he taught grammar and where he also attended the lectures of the Academician Mathurin Jacques Brisson. This course led him to develop a real interest in physics experiments, especially in electricity and magnetism.



Figure 2. Left: College of Navarre. Engraving ~1848 © Musée Carnavalet, Paris, France. Middle: portrait of Louis Daubenton, attributed to A. Roslin, oil canvas, 1791 © Musée des beaux-arts d’Orléans, France. Right: wooden model of Haüy representing layer by layer crystal growth. Private collection.

At the age of 27, he was ordained a priest and then moved to the Cardinal Lemoine College where he taught Latin. He became friends with his colleague, the abbot Charles Lhomond (1727–1794), who had a passion for botany that he succeeded in sharing with Haüy. As the Jardin royal des Plantes (Royal Botanical Garden) was close to the Cardinal Lemoine College, Haüy and Lhomond visited it almost daily. During these visits, Haüy met Louis Daubenton (1716–1799), the collaborator of Buffon, the director of the Jardin (Fig. 2, middle). Daubenton introduced him to mineralogy and directed him towards crystallography, which was in development thanks to the work of Romé de L'Isle.

In 1779, at 36 years old, he submitted to Daubenton his personal work on the formation of garnet and calcareous spar crystals based on a layer-by-layer model (Fig. 2, right). The two memoirs he wrote of these minerals were read at the Academy in 1781 and received a favorable reception. A great career had begun...

From successes to perils

Haüy's first works quickly gave him a great reputation and an amazing rise in recognition. About two years after their publication, he was appointed to the Académie des Sciences, in botany, on 15 February 1783, as no place was available among the physicists.

The year after, he published his famous *Essai d'une Théorie sur la Structure des Cristaux Appliquée à Plusieurs Genres de Substances Cristallisées* (Fig. 3, left). In 1784, he retired as a teacher (regent) to devote himself entirely to crystallography. He was then 41 years old.

In 1785, under the advice of Lavoisier, Louis XVI promulgated a new academic status, and Haüy became assistant botanist in the class of Natural History and Mineralogy. He was then employed at the Academy's library.



Figure 3. Left: title page of the first book written by René-Just Haüy, published in 1784, one year after he became a member of the Royal Academy of Sciences. Right: divided standard kilogram, made by Nicolas Fortin between 1796 and 1799. Private collection.

The French Revolution brought him into new organizations that were recruiting scientists. For example, Haüy was appointed to the Temporary Committee on Weights and Measures and the Metric System (1793), where he participated with Lavoisier in the definition of the kilogram (Fig. 3, right). Furthermore,

he taught at the École Normale de l'An III (1794). He was also a member of the National Institute, which replaced the Academy of Sciences in 1795. That same year he was appointed curator and professor at the École des Mines.

The French Revolution was also a dangerous period. Indeed, Haüy was a refractory priest (one who refused to sign an oath of loyalty to the state and before the Pope) and was arrested on 12 or 13 August 1792. He was imprisoned in the Saint-Firmin seminary, located next to the Cardinal Lemoine College. Thanks to the tenacious intervention of Etienne Geoffroy Saint-Hilaire, his loyal student and friend who was totally frightened by the situation, Haüy was quickly released. Later, thanks to the revolutionary Eloi-Nicolas Lemaire, a professor at the Collège Cardinal Lemoine, he obtained a certificate of civism. Thus, Haüy escaped the September massacres; at Saint-Firmin, almost 80% of the prisoners were murdered on the morning of 3 September.

In 1801, with the help of the École des Mines, Haüy published the *Traité de Minéralogie*, his first major book. Success was not long in coming.

An imperial consecration

The First Consul, Bonaparte, had great esteem for Haüy. In 1802, he demanded his appointment as honorary canon of Notre-Dame de Paris. The same year, he agreed to his appointment as professor of mineralogy at the Museum of Natural History ('*jardin des plantes*'). In 1803, he asked Haüy to write a book on elementary physics for the mathematics classes in national high schools (Fig. 4, left). Napoleon Bonaparte was completely satisfied with the result, so he made Haüy a member of the Legion d'Honneur.

Until the beginning of the 19th century, the 20 French universities had four faculties, namely Theology, Law, Medicine and Arts. In 1808, Emperor Napoleon I founded the Imperial University with the aim of administering the whole French education system. The former Faculties of Arts were cancelled and divided into Faculties of Literature and Faculties of Mathematics and Physical Sciences. On 14 April 1809, nine chairs were thus created at the Faculty of Sciences of Paris (Sorbonne), including that of Mineralogy, which was offered to Haüy (see the schedule of the various courses opened in April 1811 in Fig. 4, middle). He accepted, on condition that he kept his post at the Museum and was assisted by Alexandre Brongniart (1770–1847). The creation of this first chair of Mineralogy at the Sorbonne represents the origin of the Laboratory of Mineralogy of Paris, which then became the Laboratory of Mineralogy and Crystallography of Paris (LMCP), currently called the Institute of Mineralogy, Physics of Materials and Cosmochemistry (IMPMC) of Sorbonne University.

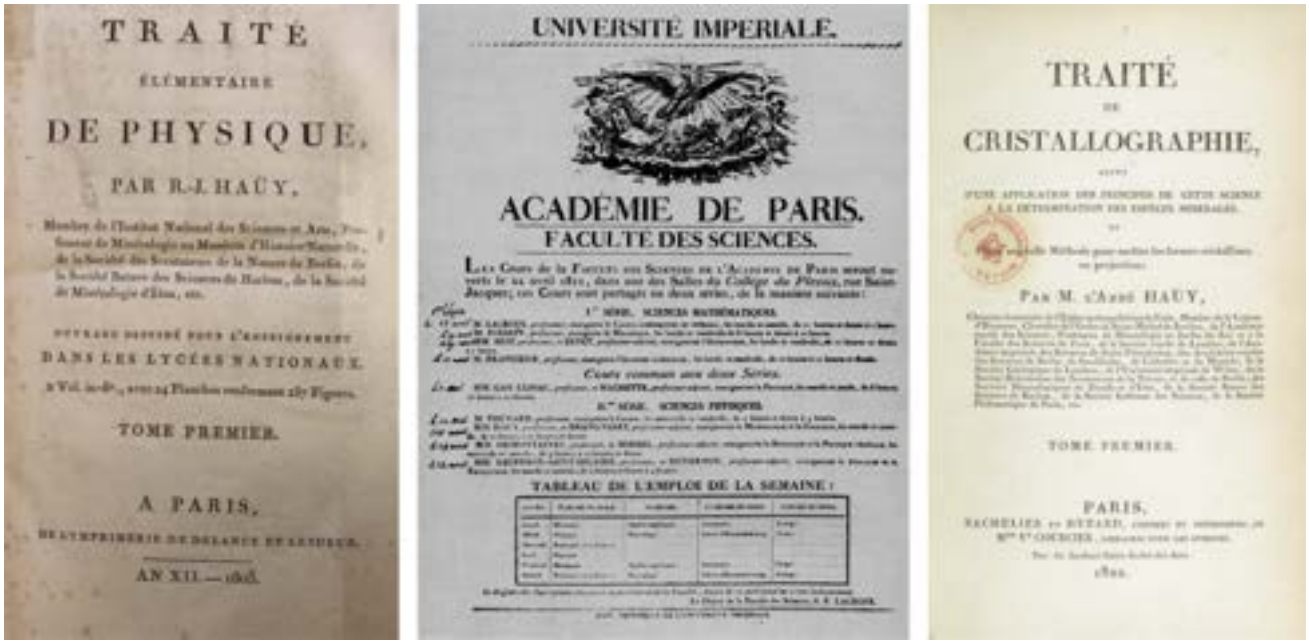


Figure 4. Left: title page of the *Traité de Physique* published in 1803. Middle: timetable for the first week of classes opened on April 22nd 1811 at the Faculty of Science in Paris (Sorbonne). Mineralogy classes were scheduled on Tuesdays

and Saturdays. Right: title page of the *Traité de Cristallographie* published in 1822.

From honors to honors to a mixed ending

On the title page of his *Essai* (Fig. 3, left), Haüy introduced himself as a member of the Royal Academy of Sciences, Professor of Humanities at the University of Paris.

Thirty-eight years later, his *Traité de Cristallographie* (Fig. 4, right) tells us that he is "*an honorary Canon of the Metropolitan Church of Paris*, *a Member of the Legion of Honor*, *a Knight of the Order of St. Michael of Bavaria*, *a member of the Royal Academy of Sciences*, *Professor of Mineralogy at the Jardin du Roi and at the Paris Academy of Sciences*, *of the Royal Society of London*, *of the Imperial Academy of Sciences of Saint Petersburg*, *of the Royal Academies of Sciences of Berlin*, *Stockholm, Lisbon and Munich*; *of the Geological Society of London*, *the Imperial University of Wilna*, *the Helvetian Society of Scrutineers of Nature*, *and that of Berlin*; *of the Mineralogical Societies of Dresden and Jena*, *the Batave Society of Sciences of Harlem*, *the Italian Society of Sciences*, *the Philomathic Society of Paris*, *etc.*"

What a career! And yet, at the end of his life, Haüy was somewhat embarrassed. He had lost part of the emoluments he had received under Napoleon's empire and shared his home with his niece and her husband, as well as his ruined brother.

On 1 June 1822, René-Just died as a result of a fall and an untreated fracture of the neck of a femur. His funeral took place on 3 June. The same year, 1822, the second edition of his *Traité de Minéralogie* and the three-volume *Traité de Cristallographie* were published.

Crystals before Haüy, a long gestation period

A name coming from the cold

The history of crystallography is marked by two minerals that have intrigued scientists and curious people by their shape and physical appearance.

The first is a variety of quartz, rock crystal, which is found in mountains, mostly as colorless and transparent crystals. The word 'crystal' comes from the ancient Greek word '*kryos*', meaning cold, from which krustallos is derived, which means clear ice. In the Ancient World, people often thought by analogy: *similar things had to share similar substance.* If we consider ice, for example, the first observations about its appearance are its transparency and its lack of color.

Quartz is a very common mineral, which makes up sand, sandstone, agates and chalcedonies. It exists in several varieties: when it is purple, it is amethyst; when it is yellow, it is citrine; when it is black, it is morion quartz; when it is grey, it is smoky quartz; and, finally, when it is transparent and colorless, it looks like ice and becomes rock crystal. Quartz also has another characteristic, it is often found with close geometric shapes. At the beginning of our era, Pliny the Elder (23–79) (see Fig. 5) had already noted this matter of fact and wondered in his *Natural History* (78):

"*It is not easy to understand why it has six angles and six faces, especially as the angles do not always have the same appearance. As for the polish of the faces, it is such that no art can equal it*."

This frequency of angles and faces has resulted in the gradual naming of crystals as 'all minerals with geometric shapes'. History dictates that quartz is also the mineral for which the first law of crystallography was discovered.



Figure 5. Left: quartz, Corinto, Minas Gerais, © Collection de Minéraux, Sorbonne Université. Right: imaginary portrait of Pliny the Elder. Engraving, XIXth century.

Calcite: an incredible variety, an incredible constancy

Calcite is the other major mineral in crystallography, first due to the spectacular variety of its natural crystal habits (Fig. 6). It appears in caves as stalactites, stalagmites or abundant aggregates. In mines, it is often found with numerous angular shapes. At the beginning of the 20th century, 2544 different shapes of calcite crystals were inventoried.

Calcite is also characterized by the shapes of its breaks (fractures), well-known to miners. These fractures show similar shapes, *i.e.* rhombohedra, a constancy that contrasts with the amazing variety of crystals and concretions.

As early as the 16th century, this constancy began to intrigue some minds. Nicolas-Claude Fabri de Peiresc (1580–1637), whose nickname was the prince of the curious, "*discovered near Aix* [...] *some rhomboid stones, either red or crystalline, of the talc species or transparent stone. These stones, found at Rians, are remarkable, in that when they are resolved into small pieces, each of these pieces retains the Rhomboid figure.*"



Figure 6. Calcite samples of different origins: Maharashtra, India (left), Bellecroix, France (middle), Frizington, Cumbria, United Kingdom (right) © Collection de Minéraux, Sorbonne Université.

Crystallography, the birth of a name

The heritage of antiquity, with Aristotle, was the idea that minerals did not have their own shapes; only plants and animals could claim them. Mineral forms were accidental: they had to be generated by the environment, the angular shapes of minerals being only particular cases. This idea persisted until the end of the 18th century, a time when the science of crystals was emerging. As Buffon (1707–1788) wrote: "*All the work of crystallographers will only serve to demonstrate that there is only variety wherever they suppose uniformity: their multiplied observations should have convinced them of this and reminded them of this very simple metaphysics which shows us that in nature there is nothing absolute, nothing perfectly regular. It is by abstraction that we have formed the geometrical and regular figures, and consequently we must not apply them as real properties to the productions of nature, whose essence may be the same in a thousand different forms*" (Buffon, 1783–1788).

On the other hand, some observers were disturbed by the frequency of similar angular shapes in certain minerals, such as quartz. Yet in the 16th century, the Dutch scholar Boethius de Boodt (1609) wondered about stones "*which seem to derive their accidental shape from the intrinsic essence*".

At the beginning of the 18th century, more and more scientists became interested in angular shaped stones. In 1723, the Swiss scientist Moritz Anton Cappeller (1685–1769), inspired by the increasing use of the term 'crystals' for these stones, coined the word 'crystallography' in the title of his book, in which he recognized nine main shapes among the crystals (Fig. 7).



Figure 7. Left: portrait of Moritz Anton Cappeler (1685-1769). Engraving, XIXth century. Right: engraving from *Prodomus Cristallographiae, de Crystallis Improprie sic Dictis Commentarium*, M. A. Cappeler, 1723.

Erring ways and success of a bad idea

One of the great challenges of the 18th century was to classify natural productions. The Swedish scientist Carl Linnaeus (1707–1778) or von Linné (after his ennoblement in 1762) is very famous for his work *Systema Naturae*, published between 1735 and 1770, where he classified animals and plants by species, families, orders and classes (Fig. 8, left). For minerals, he started with the idea that crystalline shapes were useful in their classification, but he did not obtain many results.

However, the Linnaeus idea was further developed by Romé de L'Isle (1736–1790), who presented it for the first time in his *Essai de Cristallographie*, published in 1772 (Fig. 8, middle): "*Instructed by the works of the famous von-Linné, how interesting the study of these angular forms of crystals could become... I followed them in all their metamorphoses with the most scrupulous attention; I compared the figures and the descriptions that the Swedish Naturalist had given with the originals that I possessed, I discovered several species that were missing; I cut and modeled in clay those that I had not been able to obtain in nature; finally I succeeded in forming a picture that presents the whole and the result of all that is known today on this subject.*"

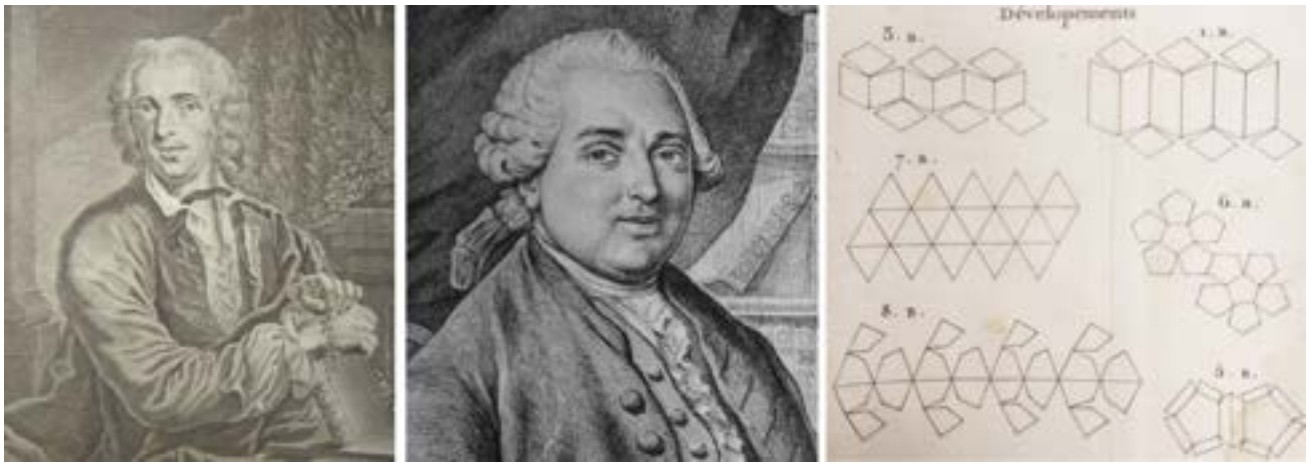


Figure 8. Left: portrait of Carl von Linné (1707-1778), Engraving adapted from *Philosophia Botanica*, 1751. Middle: portrait of Jean-Baptiste Romé de L'Isle (1707-1778) by P. Lélu, engraving, 1783. Right: engraving extracted from *Essai de Cristallographie*, J. B. Romé de L'Isle, 1772.

How geometry was introduced in crystallography

The description of crystals had been succinct for a long period, often based on what was seen at first sight. Sometimes, angles were emphasized. Most often, the face shapes were privileged, and 'square' and 'hexagon' were used to qualify angular shaped stones. Volumes were rarely considered.

In his *Essai de Cristallographie*, Romé de L'Isle began a systematic description of crystalline shapes (Fig. 8, right). He was much more precise than the crystallographers who had preceded him. He introduced and generalized the vocabulary of geometry. Then, polygons, polyhedra, rhomboids, prisms, pyramids and cubes definitely appeared in the vocabulary of crystallography.

From one crystal to another

In 1773, the Swedish chemist Torbern Olof Bergman (1735–1784) published his only article on crystallography, entitled *On the Shape of Crystals* (Bergman, 1785). Inspired by the plane fractures of calcite shown to him by his student J. G. Gahn, he showed with the help of drawings how to go from one crystal shape to another, starting from a primitive solid, a nucleus limited by faces. He assumed that crystal growth was the result of the apposition of polygonal layers (lamellae) whose dimensions can vary during the growth (Fig. 9). Using assumed truncated lamellae, he managed to describe how to go from one crystal to another.

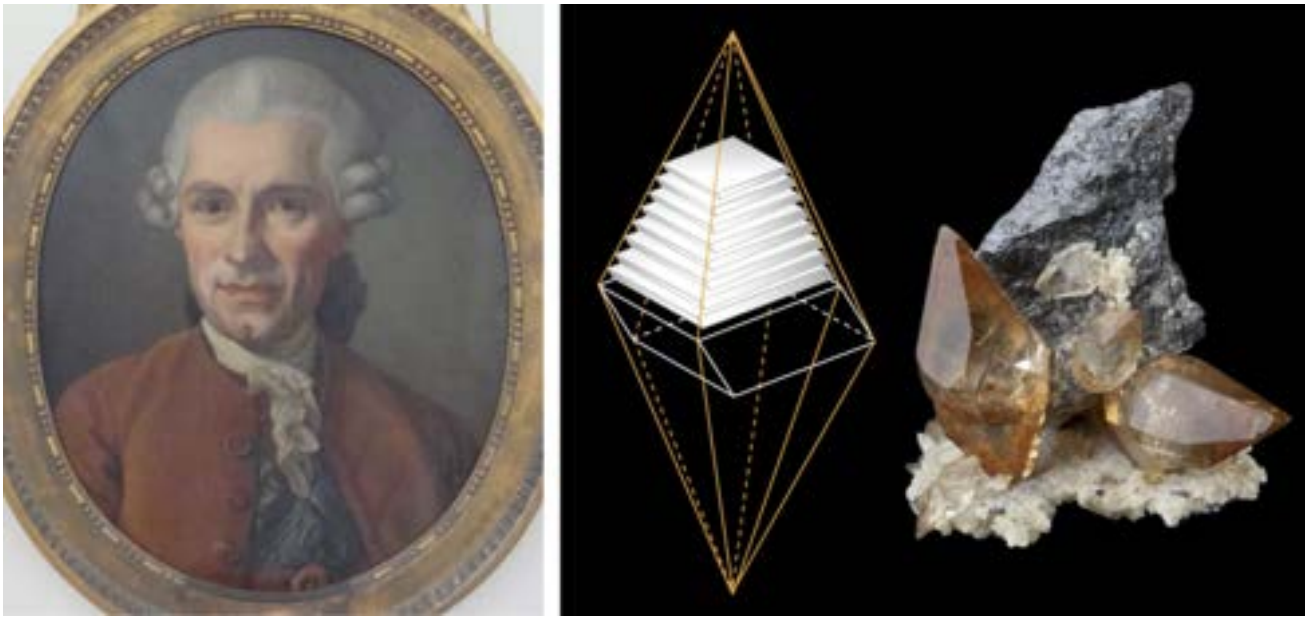


Figure 9. Left: portrait of Torbern Olof Bergman, by P. Kraft, Oil canvas, XVIIIth century. © Royal Swedish Academy of Sciences, Stockholm, Sweden. Right: illustration of the crystal growth model of a calcite scalenohedron using the apposition of polygonal layers (lamellae) onto a rhombohedron primitive solid. Calcite (Elmwood, TN, USA) © Collection de minéraux, Sorbonne Université, Paris, France.

Romé de L'Isle imagined that crystals were formed by the aggregation of integrant molecules, which are inaccessible to our senses, and stuck to the observation of crystals. By practicing plane cuts, called truncations, in his mind or in clay models, he confirmed the passage from one crystal form to another from a primitive solid (Fig. 10, top). He remarked that crystals could be sorted according to six primitive polyhedra: the cube, the tetrahedron, the octahedron, the rhomboidal parallelepiped (rhombohedron), the rhomboidal octahedron and the dodecahedron with triangular faces (Fig. 10, bottom).

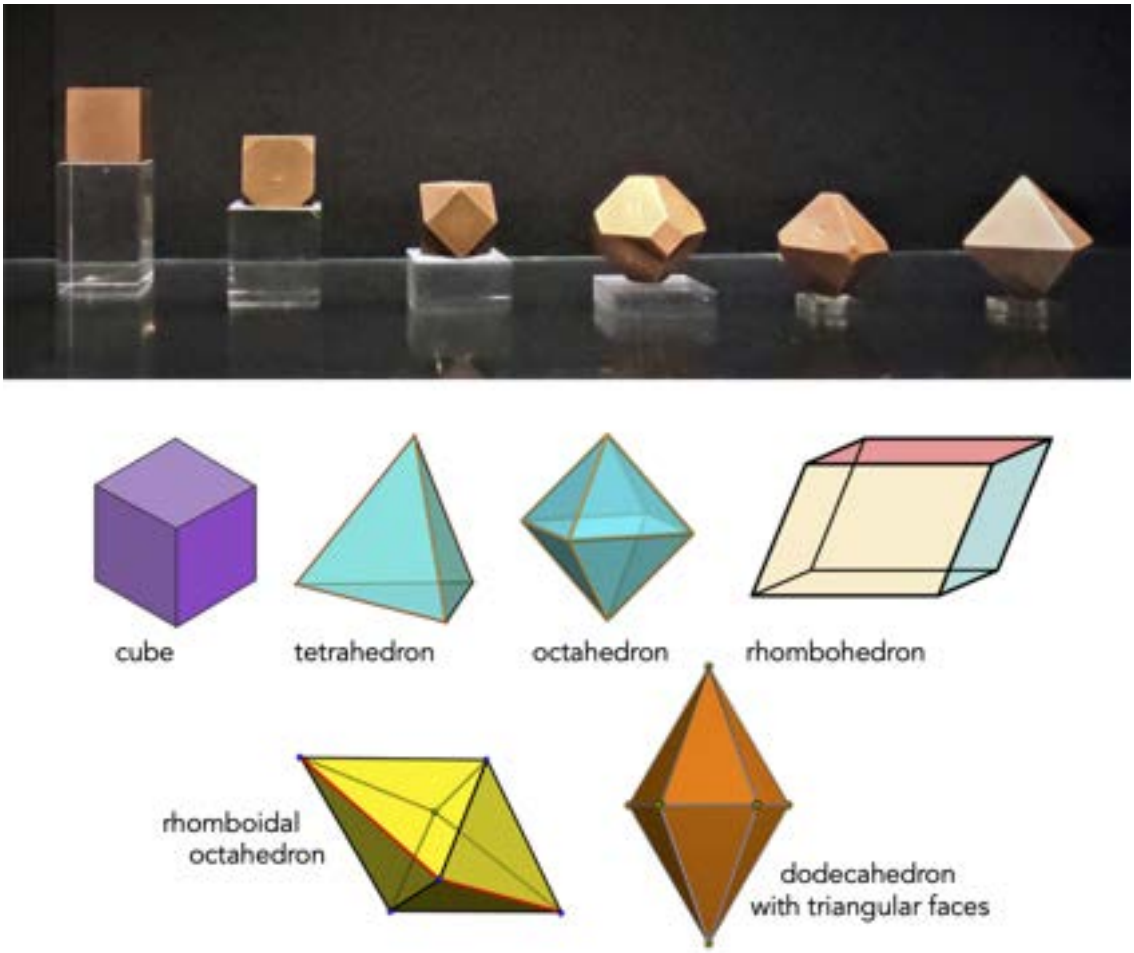


Figure 10. Top: successive truncations from the cube to the octahedron. Bottom: the six primitive polyhedral established by Romé de L'Isle. © Collection de Minéraux, Sorbonne Université, Paris, France.

How measurements were introduced in crystallography

To better illustrate the second edition of his *Cristallographie*, which was published in 1783, Romé de L'Isle had the idea to reproduce crystals of his collection in terracotta. He was helped, among others, by Arnould Carangeot (1742–1806), who wrote in March 1783 that he was "*a novice in crystallography*, [...] *despairing, after several unsuccessful attempts, of not being able to render with truth a very strange form of rock crystal*". He "*decided to cut out while playing with a card, the angle that two of the faces formed between them*. [...] *Once these two faces were cut, he was surprised to find the same angle on the two opposite faces, and so successively on the other faces of the same crystal*. *The experiment repeated on all the crystals of rock that he had at hand, and he recognized with satisfaction that the angles were constant*, [...] *whatever shape the crystal had*" (Fig. 11, left).

Carangeot conceived a goniometer for the angle measurements (Fig. 11, right). He concluded that "*any saline, stony or metallic substance, has a polyhedral form..., which varies only by truncations more or less strong, more or less multiplied, but whose angles are constantly the same in all crystals of the same species*". The law of constancy of dihedral angles was hence discovered. This is the first law of crystallography.

The most extraordinary thing about Carangeot's work is that for decades, even centuries, people had been wondering about crystalline shapes, seeing hexagons, squares and other polygons, speculating about their formation, but no one before him had ever had the idea of systematically measuring the angles between faces or the angles between edges.



Figure 11. Left: 120° angles in quartz crystals. Right: Carangeot goniometer (C. Basoche property), end of the XVIIIth century, beginning of the XIXth century. © Collection de Minéraux, Sorbonne Université, Paris, France.

The birth of a myth

In science, several chapters are mythological, a legend that illustrates their birth. Archimedes is said to have discovered the Archimedean upthrust in his bath and to have acclaimed it with a powerful "*Eureka, I have found it*!". The fall of an apple is said to have inspired Newton, resting under an apple tree, for his theory of gravitation.

Crystallography also has its myth: the broken calcite crystal of M. Defrance de Croisset. In his *Essai* of 1784, Haüy presented it as follows: "*An observation I made on a six-sided prism calcite spar, terminated by two hexagonal faces, suggested to me the fundamental idea of the whole theory in question. I had*

noticed that a crystal of this variety, which had detached itself by chance from a group, was broken obliquely, so that the fracture presented a clear cut... I tried if I could not make in this same prism cuts directed along other directions and after different attempts I obtained ... a rhomboid ... which occupied the middle of the prism. Struck by this observation, I took other calcareous spars, ... and I found the same rhomboidal nucleus."

Later, in 1823, Cuvier was more precise. He revealed to us that Haüy had the happy misfortune to drop a beautiful group of calcareous spar crystallized in prisms and that after having broken other crystals at his place he exclaimed "*Everything is found!*" (Fig. 12).

The authenticity of this event has not been proved but there is no doubt that Haüy knew the work of Bergman and Romé de L'Isle when he presented his first results to the Academy of Sciences. The anecdote of the broken calcite is, however, far from being forgotten, because it is part of those beautiful stories of science that one wants to tell and that a large consensus considers inelegant to contest.

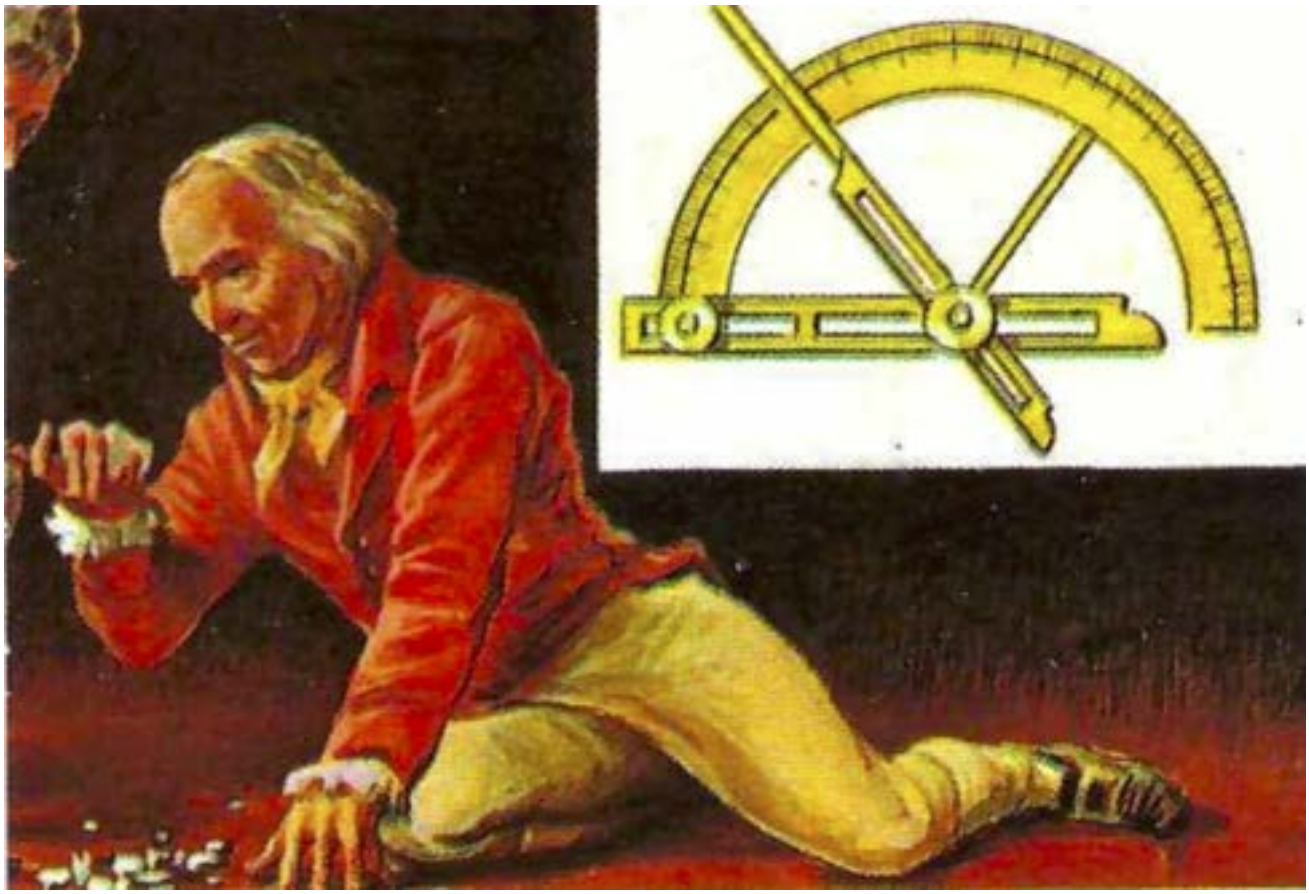


Figure 12. Postcard showing Haüy sitting on the floor observing the fragments of a group of prismatic crystals of calcite (calcareous spar) that, according to the legend, he accidentally dropped while he was in the cabinet of curiosities of Mr. Defrance, one of his friends. Private collection.

The birth of a theory: the primitive shape

"*The theory that I propose in this work is based on the agreement of observation with calculation, which I could not dispense with using, to treat, with some success, a matter where everything is, so to speak, proportion and regularity*." (Haüy, 1784).

To explain the different shapes of a crystal, Romé de L'Isle had imagined a primitive solid that was cut along specific planes, which he called truncations. It turns out that a certain number of crystals, such as calcite, can break along planes with precise orientations: this is what is called cleavage.

Inspired perhaps by the broken crystal of M. Defrance de Croisset, Haüy developed an experimental protocol. Instead of starting from a primitive solid, he had the idea to 'dissect' the crystals, using a hammer and a knife blade, by successively removing cleavage lamellae until the crystal shape remains

similar from one cleavage operation to the next. He called this shape the primitive shape. It is hidden in a crystal, but is constant for a mineral species (see Fig. 13).

From the repeated dissections applied to the crystals of his own collection and from the observations he made, Haüy concluded that there were the following primitive shapes: the parallelepiped, which includes the cube, the rhombohedron, the regular tetrahedron, the regular octahedron, the hexagonal prism and the dodecahedron with rhombic faces.



Figure 13. Left: calcite cleavage revealing the rhombohedral shape. Right: research of the primitive shape within a hexagonal prism and within a rhombohedron. © Collection de Minéraux, Sorbonne Université, Paris, France.

From the primitive shape to integrant and subtractive molecules

Haüy assumed that the mechanical division of a crystal into small solids has a limit such that any further division would distort the nature of the mineral substance. Haüy called these limit solids '*molécules intégrantes*'. The shape of these molecules is that of the primitive solid when it is a parallelepiped. This is the case for halite (sodium chloride crystals) with its cubic cleavages and, of course, for calcite with its rhombohedral breaks. In these situations, Haüy could deduce, by "*sine and cosine*", the possible shapes of the crystal.

From cleavage to cleavage, Haüy found three possible shapes of integrant molecules (Fig. 14, left and middle), namely "*the parallelepiped which is the simplest of the solids whose faces are parallel two by two, the triangular prism which is the simplest of the prisms and the tetrahedron which is the simplest of the pyramids*". Then, an issue arose because the possible crystal shapes in the last two cases could not be deduced.

Thus, Haüy introduced an appropriate group of integrant molecules resulting in a parallelepiped that he called subtractive molecules (Fig. 14, right).

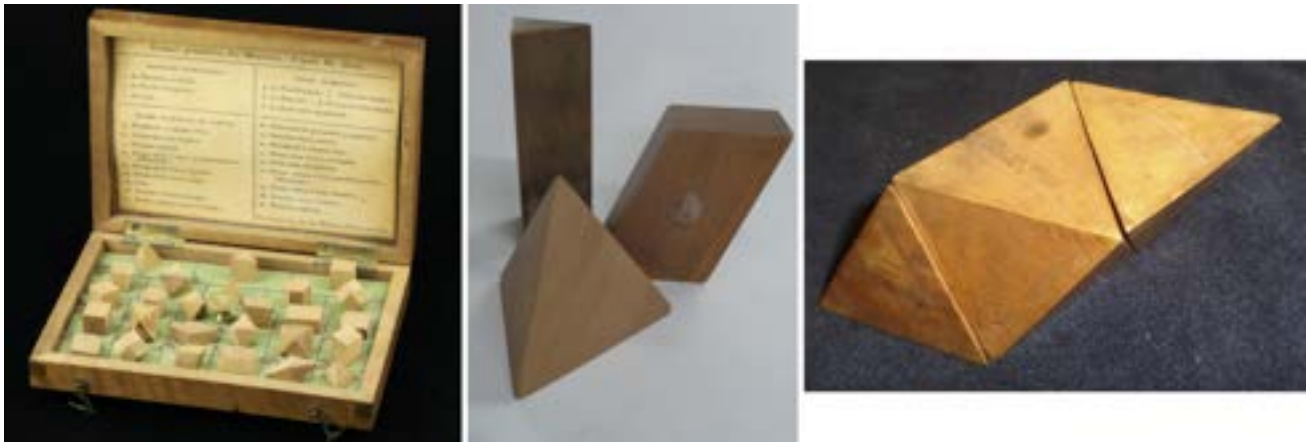


Figure 14. Left: set of wooden models of Haüy's theory made by Lambotin around 1805 © MINES ParisTech, Mineralogy Museum, Paris, France. Middle: the three integrant molecules of Haüy's theory. Right: a subtractive molecule built with two tetrahedra and one octahedron © Collection de Minéraux, Sorbonne Université, Paris, France.

The case of fluorite

Haüy was quickly confronted with a mineral that escaped his theory: fluorite. Indeed, "*in whatever way one goes about subdividing either the cube, the rhomboid, or the octahedron, one will always have solids of two forms, that is to say octahedra and tetrahedra, without ever being able to reduce the result of the division*."

In other words, the 'dissections' systematically led to octahedra and tetrahedra. Haüy's theory is based on the fact that there is one and only one shape of integrant molecule for a given mineral. It is thus necessary to choose in which polyhedron the nature of the mineral is and to suppose that the structure is "*as riddled with a multitude of vacuoles occupied, either by water of crystallization or by some other substance, so that if it were given to us to push the division until its limit, one of the two species of solids of which it is a question would disappear, and all the crystal would be only composed of molecules of the other form*".

Moreover, it is necessary to find a parallelepipedal shape in order to recover the octahedral or cubic morphology of fluorites using Haüy's theory (Fig. 15, left). Indeed, starting from a primitive solid with either tetrahedral or octahedral shape, Haüy's theory does not lead to either an octahedron or a cube (Fig. 15, middle). According to Haüy, the subtractive molecule of fluorite is a rhombohedron formed by an octahedron and two tetrahedra, each placed on one of two opposite faces of the octahedron (Fig. 14, right). Later, in 1943, Charles Mauguin suggested an interpretation of this subtractive molecule: when considering a calcium atom in the octahedron and one fluorine atom in each tetrahedron, it exactly corresponds to the CaF_2 chemical formula of fluorite (Fig. 15, right) (Mauguin, 1944).

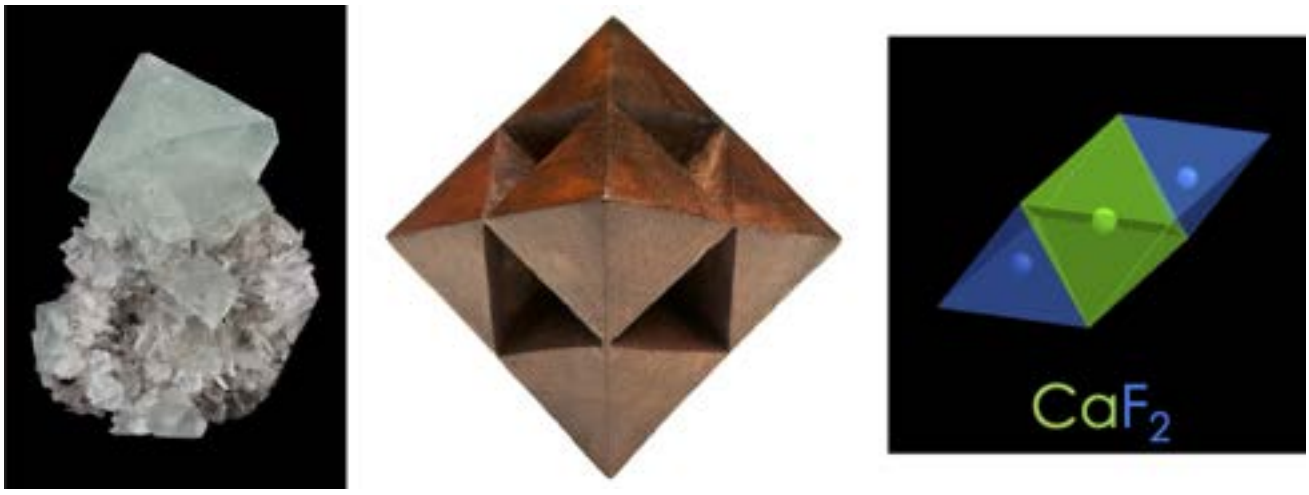


Figure 15. Left and middle: fluorite (Mundo Nuevo, La Libertad, Peru) and Haüy's wood model of a cube built from octahedra. © Collection de Minéraux, Sorbonne Université, Paris, France. Right: analogy between the subtractive molecule of fluorite (Fig. 14, right) and the polyhedral representation of the CaF_2 formula unit.

From the primitive shape to all shapes

Once the primitive solid was found, Haüy used it as an 'abstract' substrate with which he predicted the possible faces with the successive apposition of lamellae constituted by joined integrant or subtractive molecules. The dimensions of the lamellae were supposed to be constant or decrease one after the other in a row often, two sometimes, three more rarely, in one, two or three of the directions of the molecule.

Haüy established his 'laws of decrements' according to their orientation: 'decrements on the edges', parallel to the edges of the primitive solid, forming steps; 'decrements on the angles', parallel to the diagonals; and the other cases being 'mixed and intermediate decrements'. According to the relative dimensions of these molecules and these laws, all the most probable faces can be predicted (Fig. 16).

Until Haüy, the objective of crystallography was the description and identification of minerals. Haüy was the first to establish a complete theory: it is based on (i) a specific experimental protocol, (ii) observations that enable one to make hypotheses about molecules, (iii) the concept of a primitive solid, (iv) and the modeling of possible faces by stacking of lamellae and molecules according to simple rational laws of decrements.

Hence, with Haüy, crystallography was extracted from natural history and became a real physical science.

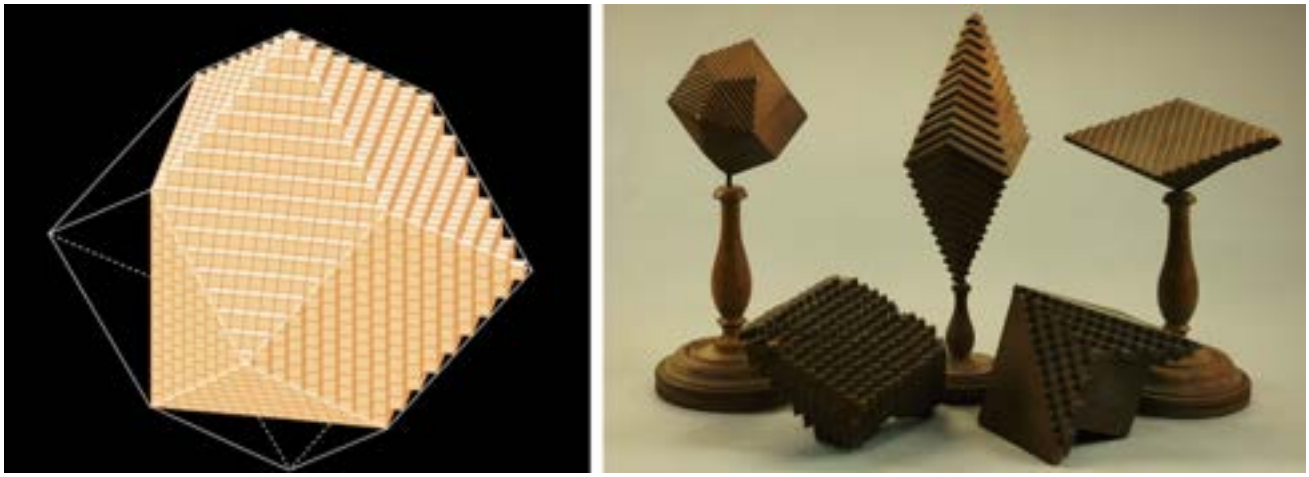


Figure 16. Left: decremented layers (lamellae) on the six faces of a cube leading to a rhombo-dodecahedral shape typical of garnet. Right: Haüy's wood crystal models illustrating the decrements laws © Collection de Minéraux, Sorbonne Université, Paris, France.

How the law of symmetry was introduced in crystallography

Haüy used the term symmetry several times in his early writings, such as the *Essai d'une Théorie sur la Structure des Crystaux*. He established a law later, in 1815. He presented it as follows: "*The laws of decrements whose actions on the edges and on the angles of the faces which finish the primitive shapes of minerals, ..., are subordinated to another law, to which I give the name of law of symmetry, ... Symmetry consists in the fact that the same kind of decrement is repeated on all the parts of the nucleus, whose resemblance is such that one can substitute one for the other by changing the position of this nucleus with respect to the eye, without it stops to present itself under the same aspect*". In 1822, in his great *Traité de Crystallographie*, he attributed to his law a great importance by affirming that it is "a *great law of crystallization, whose influence is communicated to the results of all the particular laws on which depend the crystal shapes. To give an idea of this, I distinguish two relative ways of being of the edges and angles of a primitive shape. Those which I call identical are one in the judgment of the eye: such are, for example, two opposite edges which have the same length and are included between faces equally inclined one on the other. The law of symmetry consists of the fact that the same kind of decrement is repeated on all the identical edges or angles, while those that are not identical may undergo another kind of decrement, or even remain free*."

Haüy physicist and gemologist

The work of Haüy is not restricted to the study of crystal shapes. Very early, during the writing of his first *Traité de Minéralogie* at the École des Mines de Paris, he became interested in the physical properties of minerals. He started with density. The *Traité* exhibits an illustration of a Nicholson hydrometer, an apparatus for measuring density, consisting of a cylindrical volume closed by two cones (Fig. 17, left). Haüy was also interested in the magnetism of minerals with a compass and in the static electricity produced by friction or by heating with a kind of compass equipped with an electrifiable ball at both ends (Fig. 17, middle).

Perceived as a physicist, the revolution asked him to work on the realization of the kilogram in cooperation with Lavoisier. Realized by Jean-Nicolas Fortin, the replicas of the standard kilogram were to

be distributed in all of France (Fig. 3, right). Under the request of Napoleon, in 1803, he wrote a book on elementary physics for the mathematics classes of the national high schools, which was re-edited in 1806 and 1820 (Fig. 4, left; Fig. 17, right). His skills were also used to design a book on the identification of gemstones once they had been cut. Published in 1817, this book marks the birth of modern gemology for many.



Figure 17. Left: Nicholson hydrometer, XIXth century. Middle: mineralogy compass, beginning of the XIXth century. Right: engraving from the *Traité Élémentaire de Physique* by Haüy. © Collection de Minéraux, Sorbonne Université, Paris, France.

Numerous discoveries

Crystallography allowed Haüy to differentiate between minerals close to each other by their physical appearance and their chemical composition. This is how he reassessed the definition of Schorl, currently a species of black tourmaline (Fig. 18, left). Indeed, the name "*Schorl was given to more than fifteen substances, all very different, among which was also hornblende. Thus, it was given to Tourmaline, to a variety of feldspar in small and usually white crystals, and to the `Croix de Bretagne' stone, [...] This species, the most badly defined that perhaps existed in natural history, was like a meeting (sic) of all the minerals that one was embarrassed to classify. One called them Schorls, because one had to do something with them. I tried to unravel this mess; I even substituted the name of amphibole for that of Schorl, which was vague and meaningless, and which had to be punished for all the errors it had caused in Mineralogy. I have restricted this name of amphibole to Hornblende; I have kept that of Tourmaline; I have called pyroxenes the volcanic Schorls*".

Another success concerns the zeolites of the alumino-silicates, which have similar appearance and chemical formulas and which boil and give off water vapor when heated! In Haüy's time, the word zeolite designated a mineral. Haüy showed that actually they were minerals: stilbite, chabazite, mesolite (Fig. 18, right) and analcime. For stilbite, he distinguished two varieties, which were recognized in 1822 by H. J. Brooke as two species: stilbite proper and heulandite.



Figure 18. Left: schorl and topaz, Gilgit, Pakistan. Right: mesolite, Poona, Maharastra, India. © Collection de Minéraux, Sorbonne Université, Paris, France.

Finally, Haüy published the first description of nearly 40 minerals. Nine of them have kept the name he gave them: actinote (1801), amphibole (1797), anatase (1801), apophyllite (1808), axinite, epidote, dioptase (1797), kyanite (1801) and stilbite (1796).

Decline and revival

New discoveries

The criticisms of Haüy's theory, those that question it the most, originate from the discovery and confirmation of three phenomena: hemihedry, isomorphism and polymorphism.

Hemihedry

Exactly when Haüy stated the law of symmetry, he was aware that there were counter-examples. Some crystals, such as tourmaline, present prisms where the extremities do not respect symmetry: one is pyramidal and the other flat (Fig. 19, left and middle). Haüy saw only an apparent anomaly. In 1819, the German crystallographer Christian Samuel Weiss (1780-1856) demonstrated the generality of this phenomenon and gave it the name of hemihedry. This embarrassed Haüy.

Isomorphism

At the end of 1819, the German scientist Eilhard Mitscherlich (1794-1863) noticed that "*some different elements, combined with the same number of one or more different elements, affect the same crystalline form*" (Mitscherlich, 1822). As he obtained a large number of favorable results, he postulated that bodies "*of the same crystalline shape can crystallize together in any proportion*". This phenomenon is called isomorphism (Fig. 19, right). Frequently encountered, this was an issue for Haüy. Indeed, his theory was based on the fact that any mineral results from the stacking without voids of similar molecules. How then to explain a mineral with two different molecules? Haüy did not know how to answer this question and adopted a hostile, almost sectarian, attitude.



Figure 19. From left to right: elbaite (flat extremity), Pala, Californie, USA; elbaite (pyramidal extremity), Malkhan, Zabaykalsky Krai; and rhodochrosite (calcite isomorphe), N'Chwaning, Northern Cape, South Africa © Collection de Minéraux, Sorbonne Université, Paris, France.

Dimorphism and polymorphism

Dimorphism corresponds to the possibility that two or more minerals have the same chemical formula. From the beginning of the 19th century, this situation was known.

Martin Heinrich Klaproth (1743-1817), for example, demonstrated that aragonite has the same composition as calcite. This situation, in disagreement with Haüy's theory, was quickly confirmed by many chemists.

Finally, Haüy conceded, without much conviction, "*that it is not impossible that one would not be forced to place in distinct species minerals which would contain the same principles united between them in the same ratio, if the diversity of the reciprocal functions exerted by these principles determined one in the most remarkable properties of the minerals in question*."

Criticism of Haüy's measurements

All his life, Haüy used the goniometer of Carangeot, the best accuracy of which being one-tenth of a degree. However, Haüy took certain liberties by presenting angular values with an accuracy of one second of arc (1/3600°). These values were not always in agreement with the measurements presented by other scientists. Indeed, as early as 1809, William Wollaston (1766-1828), Professor at Cambridge, developed a goniometer based on light reflections on the faces of a crystal. Its accuracy, around one minute of arc (1/60°), demonstrated the errors of Haüy's measurements, errors that he never admitted. At the end of his life, Haüy saw his influence diminish and his theory more and more questioned.

The continuous vision of matter

Another source of criticism concerns the foundations of Haüy's theory. The very hypothetical concept of integrant molecules, subtractive molecules and primitive shapes was contested.

At the beginning of the 19th century, crystal models based on the stacking of similar particles were not new. However, they were criticized by mineralogists, especially German mineralogists, who preferred a continuous description of matter. Therefore, they abandoned molecules and turned to geometry and, in particular, to the operations of symmetry that Haüy had seen but not developed enough. As Ernest Mallard (1833-1894) would later write "*Geometry, introduced as a master in science, brought with it its theories and its procedures; Haüy's painful calculations were replaced by elegant and rapid calculations*" (Mallard, 1879).

German mineralogists were much interested in the optical properties of minerals. They also established systematic descriptions of crystals. This allowed them, from 1808, to classify crystals into six, four, then finally seven systems. These systems are subdivided into `subsystems', called `classes', defined by point symmetry groups or by an orientation symmetry group. The two first determinations of all possible groups were made by the German crystallographers Frankenheim M. L. in 1826 and Hessel J. F. C. in 1830. They were unknown and almost forgotten, but were rediscovered later by Auguste Bravais (see https://www.iucr.org/news/newsletter/volume-27/number-1/auguste-bravais,-from-lapland-to-mont-blanc) in 1851 with what can be considered as a revival of Haüy's theory.

Delafosse and Bravais: the revival

The task of rescuing what could be saved from Haüy's theory naturally fell to his closest student, Gabriel Delafosse (1796-1878) (Fig. 20). It took him about 20 years to start to work on it. In his theory, published in 1840, he made the difference between physical molecules and integrant or subtractive molecules: "*in the interior of the crystal, the molecules are symmetrically spaced, so as to present as a whole a sort of staggered configuration, or more exactly the image of a continuous lattice with parallelepipedal cells. Haüy's integrant molecule is nothing more than the smallest parallelepiped formed by neighboring molecules, marking its corners; or, if you like, it is only the representation* [...] *of the cell of the crystal lattice. It is therefore perfectly distinct from the physical molecule, which can have* [...] *a completely different shape*".

Unfortunately, Delafosse's model was not really successful.

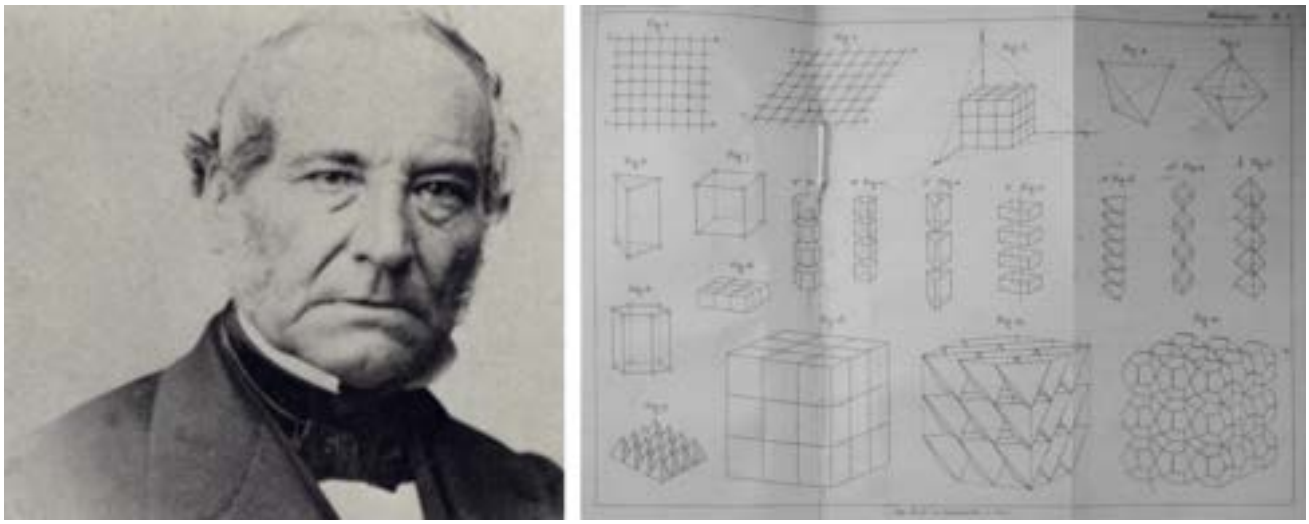


Figure 20. Left: Gabriel Delafosse, photography by Ch. Reutlinger, 1864. Right: crystallographic models by Delafosse (mineralogy courses, 1848).

Things began to change in 1850 and 1851 with Auguste Bravais (1811-1863), who developed Delafosse's intuitions mathematically (Fig. 21). The results are numerous: from the demonstration of possible symmetries to the inventory of point symmetry groups, to the seven Bravais systems, the 14 Bravais lattices, and the first theories on hemihedry, face stability and twinning (defects associating two crystals). Almost unnoticed, the work of Bravais was to be recognized later, as Mallard wrote in 1879: "*M. Delafosse and M. Bravais thought that there was better to do than to reject, in order to substitute a sterile geometry, the theory of Haüy, so intimately penetrated by physical reality. Thanks to their work, we can now give to the science of crystals a solid and wide enough base to carry the whole edifice*".

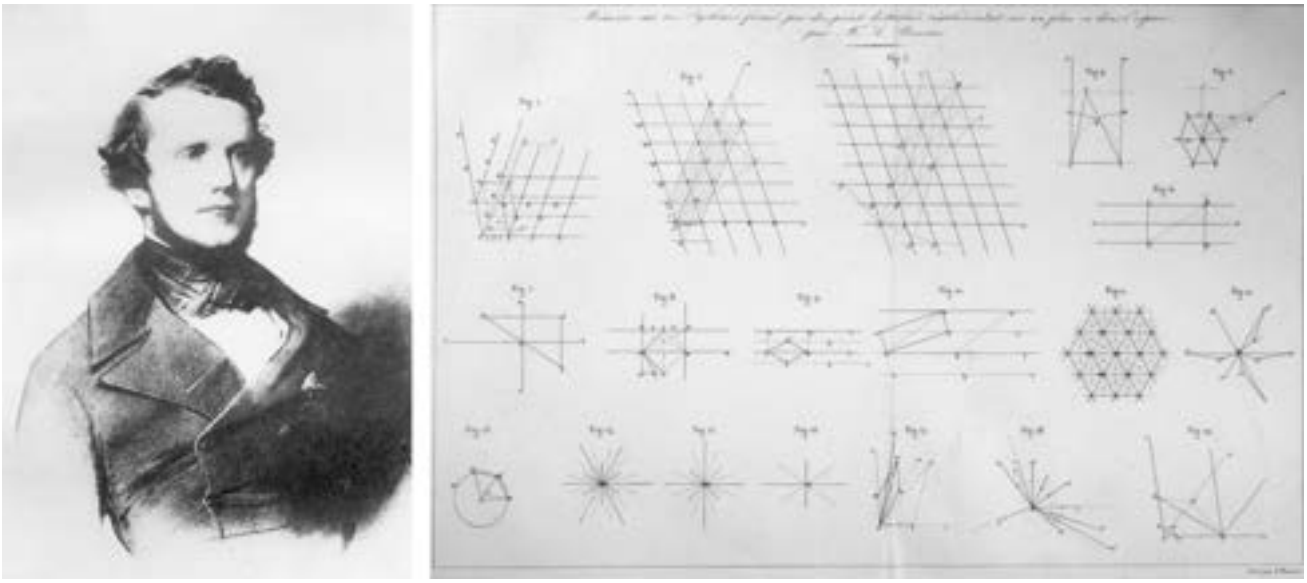


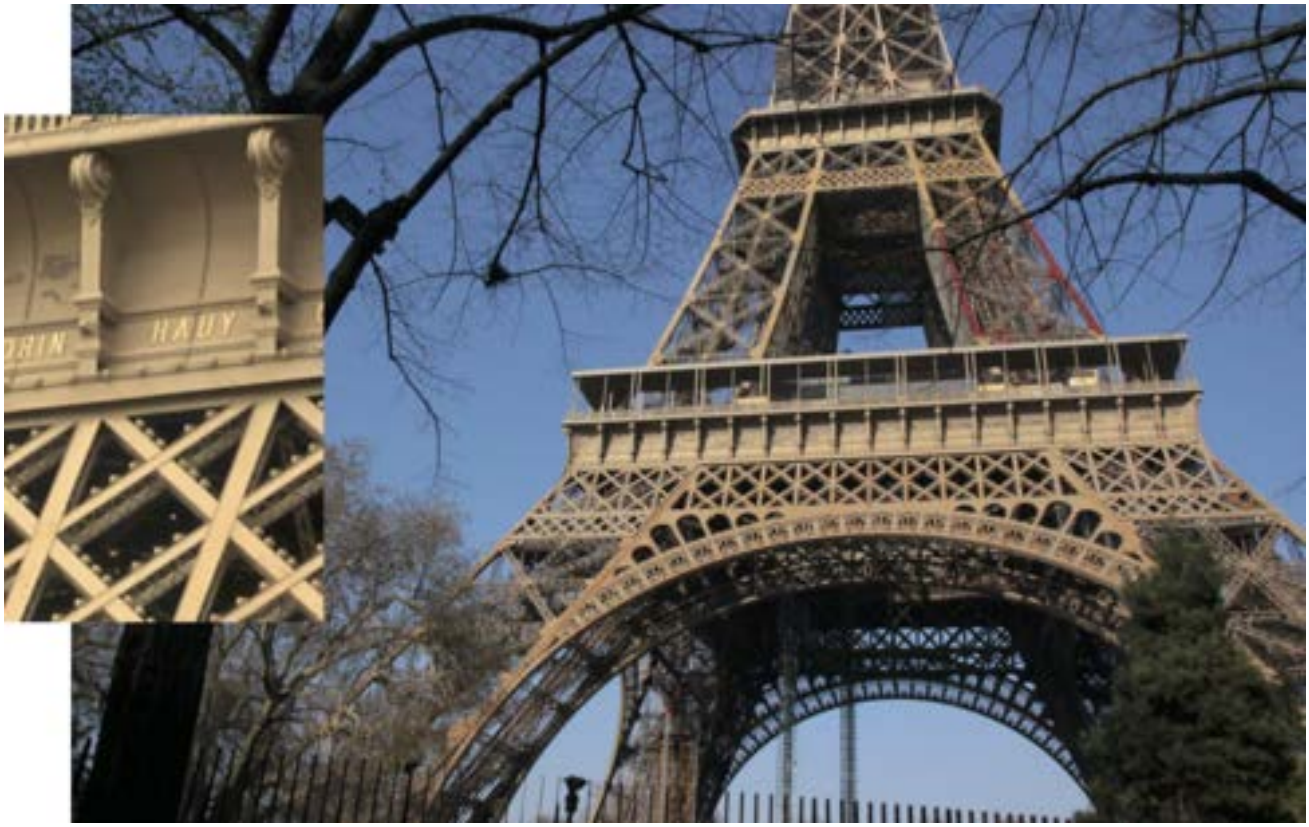
Figure 21. Left: Auguste Bravais, in *Les Contemporains*, N. 588, 1904. Right: first theoretical schemes of lattices in *Mémoires sur les Systèmes Formés par des Points*, Auguste Bravais, 1849.

Concluding remarks

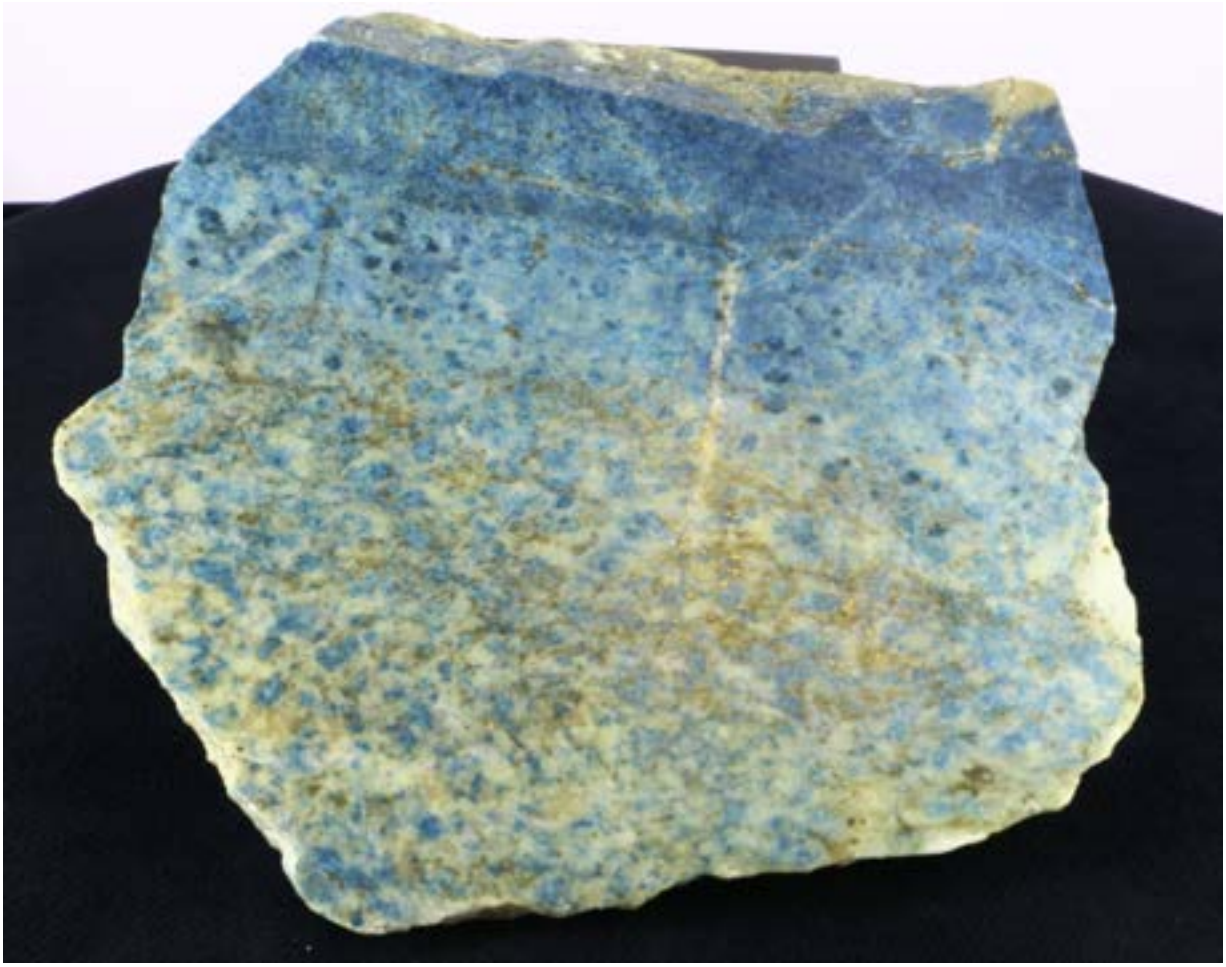
The 18th century, the century of the Enlightenment, gave primary importance to reason and science. Newton's discoveries enthused philosophers like Voltaire. Mathematics described the order of the world. Apart from mechanics, astronomy and optics, few sciences at that time used mathematics. At the end of the century, a theory of crystals demonstrated how inorganic matter, which was supposed to have no form of its own, could have perfect geometrical shapes that could be calculated mathematically. The impact is substantial and Haüy is considered as a Newtonian!

His crystallography heralded a 19th century in which science was triumphant. It opened up new horizons in mineralogy, optics and chemistry, and then in the last part of the 19th century, in the physics of materials. It also introduced symmetry, one of the most important concepts in physics, which allowed Pasteur to discover molecular dissymmetry and Curie to discover the principle of symmetry.

The discoveries made during the 19th century should not let us believe that there was no resistance. The theories inspired by Haüy were not fully accepted until the discovery of X-ray diffraction in 1912. The work initiated by Romé de l'Isle and Haüy then found its completion with the X-ray diffraction experiments of Bragg, father and son. And a new era began for crystallography...



On the frieze on the first floor of the Eiffel Tower, Haüy can be read among the 72 names of scientists and engineers that Gustave Eiffel had inscribed in gold letters because they honoured France between 1789 and 1889.



Haüyne, Afghanistan © Collection de Minéraux, Sorbonne Université, Paris, France.

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HISTORY OF CRYSTALLOGRAPHY

The end of an era at NIST



From left: Judy Stalick, Tony Santoro and Ted Prince in front of the 3rd generation (and current) 32-detector BT-1 instrument shortly before the instrument was placed into operation, likely in the late 1980s.

Brian H. Toby

In preparation for the NIST (then NBS) Reactor producing neutron beams starting in 1969, the science leader, Jack Rush, assembled a top-notch team of scientists that included crystallographers Ted Prince, Antonio (Tony) Santoro and, just a bit later, Judy Stalick. With the passing of Ted, Tony and Judy, I'd like to put a few words in remembrance of what was likely at one time the most respected neutron crystallography team in the USA. I was fortunate that after Ted officially retired (but still came to work each day), I was able to work with them.

It may have been chance that the reactor started just as Hugo Rietveld's work was published. The team was a very early adopter of his technique. I can recall Judy more than once telling me how gracious Hugo was on the occasions they met. I had the good fortune to experience this myself.

Ted died a few years ago. Tony died about a week ago. Judy died this morning, after much more than a decade with severe pain and disability. I'll write a bit about each of them individually.

Ted was a crystallographer's crystallographer. He was an expert on so many different aspects of crystallography, but perhaps above all he was a leading authority on the math and statistics we use. In fact, it was Ted who proved the correctness of the Rietveld technique. Crystallographers prior to Rietveld would chain a fit for integrated intensities of individual powder diffraction peaks together with a structural fit, by using those output intensities as input to single-crystal software. With that approach, they would see very different standard uncertainties (then called e.s.d.'s) in comparison with the values obtained from Rietveld fits. This from their view indicated that something was wrong with Rietveld's technique. The "Rietvelders" argued that chaining least-squares fits was invalid. Ted demonstrated that chaining least-squares fits together serially is perfectly valid statistically, provided that the covariance matrix from the first fit is used as weighting in the second fit — something not possible in standard single-crystal software (as weights are input as a vector). When Ted wrote software that allowed this, he showed the s.u. values then agreed with the Rietveld values. QED, the Rietveld technique gives correct answers.

Ted was very proud to have gotten his crystallographic education in the UK; not a common thing for a US undergrad to pursue in the 1950s, at a time when the country was rebuilding from WWII. My father (who grew up in London during the WWII bombings) finished his Queen Mary College undergrad degree around then and came to Canada for his graduate work. Ted would sometimes mention different happy

experiences he had in those years, but the one story I remember best was when he told us how impressed he was at the time to be introduced to Rosalind Franklin (1920–1958) when she came to see the lab where he worked. Back then crystallographers knew who she was and what she had done, even if the rest of the world was yet to learn it.

Ted was the editor for the initial edition of Volume C of *International Tables of Crystallography* and its first revision. He asked me if I would then take over for the second revision. I could not imagine ever finding the time for that, but now wonder how he managed. Ted's book, *Mathematical Techniques in Crystallography and Materials Science*, is considered a classic in the field and nearly 20 years after its 3rd edition was released is still available on the Kindle. I will warn the reader that while I go back to this text often, I do budget at least a few hours per page. Ted assumed his readers know a lot. Larry Finger told me that when he retired and gave away his library of crystallography texts so that he and his wife could fit into a mobile home, Ted's book was the only one he retained. Ted and Larry were also well known for their fine crystallography package, which included a Rietveld code customized to the 5-bank and later 32-bank BT-1 instrument at the NIST reactor.

Tony came to the US from Italy after his education. Tony was loud, opinionated, blunt and so, so much fun to spend time with. On one occasion, when I was discussing with him the classic work of Cagliotti from the 1950s, he corrected my pronunciation of the name and then added "and he was quite an SOB" but in slightly more colorful language. When I was asked to be the crystallography team leader, while still in my early 30s, I found it very daunting to supervise someone who was a world-level practitioner and also about the same age as my parents. Tony was never anything but gracious and kind towards me. In fact, at one point I came to him saying that the end of the fiscal year was close and this was a good time to put in a request for purchases, as the beloved benevolent despots (and I mean each of those three words for Mike and Jack) who ran the reactor always kept some money in the budget in case of unseen problems, but needed that to be spent before the books closed. So, smaller quick purchases might fly through if put in at the right time. Tony asked me if he could get his first PC and a Fortran compiler and then told me that I was the first person in his many years at NBS/NIST who had ever asked him if he wanted to order something. He got the PC and g77 before the end of the day.

Tony loved to walk, commuting by Metro and bus from DC to the front gate of NIST, where he then walked a mile or so to the Reactor and did the reverse in the evening. Just once, on a cold rainy day, he accepted a ride from me. Another favorite memory was while at the 2005 IUCr Congress (Florence), Tony invited me to his apartment in Lido di Ostia. However, he had a bad experience in the Rome train station, and he insisted on meeting my train and escorting me to Ostia lest the same happen to me. He also insisted I should sleep in his bedroom while he slept on the couch, as it would be too noisy for me to sleep otherwise. Alas, with the non-stop partying all around us all night, even with his room and earplugs, the sound levels were still more than I could manage.

Ted, Tony and to a lesser extent Judy, were crippled in their work by a decision at the NCNR in the very early 1990s to move all computation and data analysis from a VAX computer to Unix machines. It was true at the time that Unix machines offered much better performance for the buck, but almost all crystallographers were using VAXes in those days and very little software was available for any other platform. Each was very comfortable with the VAX/VMS OS and found switching to Unix bewildering. Once they no longer had VAX access, Ted and Tony gave up doing Rietveld refinements themselves. Ted moved to more theoretical work and Tony switched to problems where he could use a pocket calculator, until about a decade later when he got that PC. Judy struggled along with Ultrix but was never comfortable with it. The NCNR continued to use VAXes to run instruments for at least another five years at that point, but the loss of effectiveness for crystallography vastly outweighed the high cost of a small microVAX. What a waste.



Ted Prince and Judy Stalick at the 2nd generation five-detector BT-1 instrument.

Tony hired an assistant scientist, Qingzhen Huang, more-or-less as a postdoc, despite Qing not having the Chinese equivalent of a PhD. Qing was a terrifically productive scientist and became a world-class expert in magnetic crystallography. At one point I was told by someone outside NIST that Qing was also the most prolific publisher of Rietveld results in the world. This was doubly impressive to me, as magnetic crystallography is not easy and even for non-magnetic materials, neutron data collection might require days/sample. One would expect a synchrotron or even lab scientist to have access to more data, but the truth is that Qing did excellent work and a number of notable synthesis experts knew that and sent their samples to Qing. With time, Qing's expertise and productivity was recognized by the NCNR and he became an independent full-fledged member of the team. Qing was of great help to me as I started to learn about magnetic scattering and was always ready to step in to help users run samples at BT-1.

Judy was a superb but a more practical crystallographer, in comparison with Ted and Tony. Ted Prince is credited for the design of the 3rd generation (32-detector) BT-1 instrument, which still offers the highest resolution neutron diffraction in the US ~30 years after it was initially deployed. (Sad that it has seen no major updates since!) However, it was Judy who made that instrument happen, working with engineers and technicians to get it done and commissioned. She also never stopped tinkering with the instrument to improve performance. For example, by convincing a bunch of us to work on pressing and aligning Ge(311) and Ge(733) crystals, two seldom-used monochromators were replaced with capabilities that greatly enhanced the range of the instrument by providing significant wavelength shifts from the initial design. Later she figured out that use of a "zero-blade Soller collimator" would provide ~60' collimation, doubling the speed of measurements at the cost of some resolution, and that mod would be pretty simple to install — by replacing one of the two "off" positions in the neutron shutter with that open collimator to offer a third collimation option. Cheap and highly effective! (See for yourself here.)

Judy had been a grad student of Jim Ibers and had been back then "very married" (in the words of someone who overlapped with her) to another chemistry grad student. I can recall Judy saying that she

would take breaks at her desk in Jim’s lab and read a novel or newspaper. Feeling very confident in her work, she shocked the other students that she felt no need to hide what she was doing when Jim came into the lab. Jim clearly respected that too. Following her husband’s hire at a faculty position in Virginia, she wanted to find a position nearby that would also allow her to start a family and took a job I feel was below her level, working on the NBS*CrystalData database. Despite an arduous commute, she felt NBS would be good for her overall goals, albeit perhaps not very professionally ambitious. As congestion, construction and for that matter her health issues got worse, she dropped to working a 30-hour week sometime later. In her CrystalData job, Judy was pivotal in the design of the first computerized data storage format (then called AIDS*83, later renamed as PDF-2 for some reason) for storage of both the JCPDS (now ICDD-JCPDS) and the NBS database, along with data entry software for the folks who abstracted from the literature. She would tell me how the ICDD had to be talked into using the computerized format. By that time, the ICDD was marketing a PDF-2 product on the recently-invented CDROM platform; it was already clear that computerization had saved the ICDD from obsolescence. After just a short period with CrystalData, Jack noticed Judy’s talents and recruited her to join the reactor staff. It was at the NCNR where her talents could be more fully recognized.

Judy specialized in intermetallic systems, but like everyone else in the neutron field, also did plenty of oxide crystal structures. She never lost the NBS credo that anything published from there had to be 100% above any critical dissent — even to comma placement — but she also never gave up on any project. She was willing to keep picking up a project again and again to get it to “done." I can recall one intermetallic with a huge cell that she revisited perhaps a dozen times over 15+ years.

A remembrance of Tony Santoro by Jeffrey Trossen, NCNR Technical Staff Member

I will greatly miss Dr Tony. I first met him in 2013 in the breakroom as he was eating his favorite snack, dragonfruit. I sat near him and asked him what it is that he does, what kind of a scientist he was. From that point forward when I saw him, I would ask him, "Hey Dr Tony, what's new?" This happened repeatedly over the weeks and months, and I think I overdid it because it seemed to annoy him, so I cooled it. But one day, meeting him in the break room he said:

"Hey Jeff, what's new?" (beating me to the punch, I guess). "Oh," I replied, "I'm almost done with book number four."
"You read books? What book is it?"
"It's one of my books. I have written three, now I'm almost done writing number four."
Tony's eyes widened with astonishment. "You write books?"
"Well, yes, I do. Would you like to see book one? I have a copy at my desk."
"YES!" he said.
I came back to the break room and handed it to him. "This is my first book in a series. I . . ."
Tony, with his eyes wide and his mouth open rifled through the pages looking at it up and down, waving the book in the air as though he were feeling its weight. "Why … this changes EVERYTHING!"
"What do you mean?" I asked. “How does it change everything?"
"Well," he shrugged, "I thought you were simple minded!"
"Uh, gosh. Um … thanks … I think."

Several weeks later he gave it back to me and said that he enjoyed it and asked for book 2. A couple weeks later, book 3. A week later, book 4. Later, after I finished book 5, I handed it to him. When he read it, he told me that he'd been too busy to read on Saturday, so he started it at 3 pm on a Sunday and finished at 5 am the next morning.

All I can say is that Dr Santoro was Superman. He had read for 14 hours straight through and didn't put it down until he was done. Evidently Dr Santoro loved books. He mostly liked to read autobiographies and history, especially World War Two because as a young man he'd lived through it in Italy. When he finished book 6, he told me that it was the best science fiction he'd ever read. I asked him what other science fiction he had read, and he answered "None. I don't read science fiction." So, I guess that since

he read all six books, it was a compliment.

I will definitely remember Dr Santoro with a smile.



The scooter provided by NIST that allowed Judy to get around Building 235. She was provided with a special parking spot in front of the building (hers was the only non-government vehicle allowed to drive on that section of road). Photo thanks to Peter Gehring.

Alas, if being a woman scientist and the expected roles for women in the 1980s were not enough of a handicap, she also had to face several others. Judy lived with crippling back pain and operations and drugs to treat that, at one point getting methadone treatment for addiction to prescribed pain meds. Her professional visibility was undercut by her inability to travel to meetings, as family responsibilities and the long period of pain that followed a plane flight prohibited travel. Sadly, if her life was not already demanding enough, Judy’s then husband left her when her son Jon was a pre-teen. That shortened Judy's commute, but left her as a single parent. She was apparently very effective in that. Jon has grown into an impressive human being, who was a devoted caretaker over the past two decades as his mom disabilities only compounded. To the credit of the NIST Center for Neutron Research’s management, she was offered amazing levels of physical accommodation that allowed her to keep coming into work until just a few years ago. She loved her work and the NCNR community and gave it up only when there was no other possibility.

I came to NIST originally as a facility user when employed at Air Products, so I could use the newly upgraded BT-1 for zeolite studies. I felt very much to be Judy’s student in CW neutron diffraction; I had done TOF neutron PDF work with Takeshi Egami and Jim Jorgensen before, and some, but not a lot of Rietveld. I was shocked when Jack suggested that I should consider applying for the job Ted was leaving, since I could not envision anyone appropriate to fill his shoes and certainly not me. I don’t remember how I managed to put together a seminar, as I could not talk about any of the work I did for Air Products (or perhaps being vague was good), but I got the offer. Unlike my prior terrible industrial job at Union Carbide (Rest In Pieces), Air Products had been a great place to work and I felt a lot of loyalty until a

massive layoff not long before the interview, so my wife Diane, then 13 month-old son Jason and I left Allentown for Potomac as quickly as we could, living in temporary housing while house hunting. For what it's worth, I don’t think a single one of my coworkers from back then remained at Air Products long enough to retire. Only a few left voluntarily. Employee loyalty is overrated unless reciprocated.

I continued to learn from Judy once her coworker. I’d like to hope she learned from me too. She would have been the team leader if she wanted the role. Instead, she had to put up with me as her supervisor, but she also did not hesitate to tell me on occasion how to do my job. I listened and learned.

My final project at NIST came from my belief (still held) that the best thing one can do with a thermal beam from a reactor is to build a Laue diffractometer. (Some triple-axis folks might disagree.) I infected Tony with that belief and together we worked on Laue diffraction geometries together as I built a prototype instrument without any funding. It was a fun project. I wish it had gone farther.

I spent a decade at NIST. It is now just a few years short of two decades since I left. The NCNR was an environment filled with top-level scientists who (perhaps unusually) were almost all gracious, caring and collaborative. In all the places I have worked, that environment was unique, and I still miss it. But even more, I miss the collaboration and learning with Ted, Tony, Judy and Qing. Perhaps my arrival was the beginning of the end there, but at least during my professional lifetime, I don’t think any other American institution can claim to have employed three crystallographers of that stature. I personally owe them a debt that I cannot repay; I will just try to pay it forward. Farewell and thanks, Ted, Tony and Judy.

Postscript: In the week or so since I wrote this, I have found myself listening over and over to the tape that I made of a concert I organized for the late Stan Rogers (some Canadians will recognize the name) while a grad student. It is a comfort as much as it also reopens a deep feeling of pain. I suspect that as I process the loss of people who meant so much to me, and flirt with thinking about my own mortality, I want to remind myself of how many wonderful things I have had the chance to do. I wish the same to all. Brian

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OBITUARY

Václav Janovec (1930–2022)



Jiří Hlinka

Václav Janovec, Czech physicist and crystallographer, passed away in Prague, Czechia, on 16 February 2022. Václav was one of the founders of the Czechoslovak ferroelectric research school and a world-renowned enthusiastic advocate of group theory approaches in structural phase transitions. He formulated foundations of the symmetry theory of domain boundaries in terms of layer groups.

Václav Janovec was born in 1930 in Pěčín, a small mountain village in the north-eastern part of Czechia. Despite the political turbulences during World War II and the installation of the Communists as a single ruling party in 1948, he completed high school in Klášter nad Orlicí in 1949 and was admitted to studies at Charles University.



Václav at the time of receiving his "matura" qualification.

His university professor Václav Petržílka, author of outstanding Czech textbooks on electricity and magnetism, introduced him and his classmate, Jan Fousek, to the publications of A. von Hippel on barium titanate and proposed to him to start work on this subject. For his diploma work, Václav investigated X-ray diffraction of barium titanate single crystals under an applied electric field. Both Václav and Jan graduated in 1953 and were offered to work in the newly established Laboratory for Experimental and Theoretical Physics, which had its premises in the lofts of the historical building of Charles University, where many years ago, Albert Einstein was to read his lectures. Václav started there by designing a set-up for measuring ferroelectric hysteresis loops in butterfly-type single-domain crystals of $BaTiO_3$ grown from flux by the Remeika method. The theoretical part of his PhD thesis was published in the *Czechoslovak Journal of Physics* in 1958 [1], and it contained a theoretical derivation of the thickness dependence of the coercive field, nowadays known as the Kay–Dunn–Janovec law [2,3].



Young Václav at work.

In 1960, Václav Janovec became the first head of the ferroelectric group, the same group that later became the Department of Dielectrics of the Institute of Physics of the Czech Academy of Sciences. Subsequently, Václav Janovec alternated in the leadership of the Department with Jan Fousek. They both were keen on the strong involvement of the Department in international collaborative activities. In the summer of 1966, at the occasion of the first International Meeting on Ferroelectricity, they managed to bring scientists from many countries on both sides of the cold-war polarized world to Prague. Václav was lucky to receive a postdoctoral scholarship from the National Research Council of Canada, allowing him to stay in the laboratory of J. A. Morrison in Ottawa from 1964 to 1966, and he also profited from a later invitation to the laboratory of W. Känzig at ETH Zürich in 1975.

Václav was known for being a great speaker and teacher, insisting on well-formulated scientific terms, well-posed questions and correct chains of arguments. Václav taught at Charles University and had an

influence on several generations of his colleagues in the Department of Dielectrics. After his formal retirement, he was invited to read lectures at multiple places all over Europe and visited, for example, his collaborators at the Universities of Dijon, Karlsruhe, Montpellier and Rennes. In 1995, he was promoted to professor at the Technical University of Liberec. There again, together with Jan Fousek, he advised his young colleagues, and he was also read courses on thermodynamics, statistical physics and tensor calculus to undergraduate students till 2008. In the last dozen years of his life, Václav was again a prominent and very active emeritus member of his Department of Dielectrics at the Institute of Physics of the Czech Academy of Sciences.



With J. Fousek considering collaboration with Czechoslovak industry.

Václav Janovec’s main research interests covered thermodynamics and symmetry aspects of structural phase transitions. His best-known publication is a joint paper with J. Fousek, in which they summarized the rules for identifying all permissible planar ferroelectric walls [4]. Nevertheless, Václav's natural inclination towards complete coverage of a subject by considering all possible symmetry aspects of the problem can be found already in his early publication devoted to the generalization of the Pippard relations for ferroelectrics [5]. Some of his theoretical works went on for years, for example, that on a complete enumeration of macroscopic crystallographic symmetry reductions induced by irreducible representations. The resulting tables, completed together with his colleagues V. Dvořák and J. Petzelt in 1975, are still being used [6]. Václav Janovec also contributed to the theory of incommensurate structures (for example, [7]). The most groundbreaking contribution of Václav Janovec was formulated in his publications devoted to the symmetry of domain walls [8–10]. There were other interesting subjects he worked out, for example, together with J. Fuksa, V. Kopský, J. Přívratská, J. Erhart, Y. Ishibashi, G. Godefroy, P. Saint-Gregoire, W. Schranz and in particular with D. B. Litvin [11–16]. For many years Václav also served on editorial boards of several international journals, in particular *Ferroelectrics*, *Ferroelectric Letters* and *Phase Transitions*. Since the 1990s, he was an active member of the team that edited A. Authier’s Volume D of *International Tables for Crystallography* entitled “Physical Properties of Crystals”.

In particular, he contributed to all four chapters of its third part “Symmetry aspects of phase transitions, twinning and domain structures”, coedited with P. Boček, Th. Hahn, H. Klapper, V. Kopský, J. Přívratská, J. F. Scott and J. C. Toledáno [17].

Václav was an extremely kind companion. Many of his scientific collaborators knew that he was a skilled violoncello player and a real lover of classical music, as well as of tennis, literature, computer science and good food. Until his last days, he was surrounded by his beloved family. His impressive calm and kind character were encouraging to all of us who had a chance to meet him, and this pleasant experience will remain with us.

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OBITUARY

Ian Munro – father of synchrotron radiation in the UK (1937–2022)



A photograph of the NINA Synchrotron Radiation Facility team taken a few hours before the final switch off of NINA on 31 March 1977. From left to right: Pat Ridley, Iggy McGovern, Bill Smith, Tony Bourdillon, John West, John Beaumont, John Morton, Ian Munro, Paul Brint, Samar Hasnain, Jeff Worgan, Robert Pettifer, Tom Short, Joan Bordas, Ken Lea and Tony Cox.

Samar Hasnain

It was Sunday afternoon, 29 September 1974, when I arrived at Manchester Airport, the year in which the ‘air bridges’ connecting passengers direct from the aircraft to the terminal had become operational at Manchester. A smiling face full of welcoming enthusiasm, so typical of Ian Munro, recognised me and came forward with his positive style so that I did not have to wonder or worry if there would be someone there to meet me. I soon discovered that I was not going to the student accommodation but to his home, where I stayed for a whole week. I was moving from my mother’s home in Karachi to Ian’s home in Didsbury – both full of love – home from home.

During the daytime through the week, he devoted a lot of time introducing me to the department colleagues and the tea room, helping sort out my accommodation in Owens Park and opening my bank account (almost 50 years later, I still have the same account). In the evening, we would travel from the university to home in his VW van, where he and Joan would rustle up dinner for the four kids (Robert, Elizabeth, Neil and Janet) and me. What a man! Caring, warm, loving and above all, a modern family man, sharing duties of the kitchen and everything in the days when it was not the norm.

During the next three years, initially as a PhD student then as a PDRA, I joined Ian Munro in his Synchrotron Light Project, which he had established in 1973 at the Daresbury Laboratory, in the village of 'Alice in Wonderland'. He had taken a bold action upon his return from a sabbatical in Canada to write a letter to the Director of Daresbury, Alec Merrison, in 1967, to obtain his support to explore the properties and use of light from an electron synchrotron that had been commissioned in 1967 for a different scientific purpose (particle physics). His vision, enthusiasm, ability to bring people together and endless energy resulted in him obtaining twice the funding he had requested, allowing him to establish two beamlines rather than just one. When I arrived in 1974, there were already teams from Reading, Oxford, Bristol and the famous MRC Laboratory of Molecular Biology in Cambridge. Teams from Leicester and Warwick soon joined this amazing project.

While we were immersed in the new exciting science made possible by this new tool, Ian, with other senior science leaders, was working on a way to get a more ambitious project approved, as he knew that

the parasitic synchrotron light facility was going to close in a few years. In 1976, we learned that the closure would be sooner than even Ian had expected only a couple of years before. It happened on 1 April 1977 with the highly positive news that the UK's Government Science Research Council had decided to build the world's first dedicated purpose-built Synchrotron Light Source (later to be known as the SRS) at Daresbury. On 31 March 1977, he worked with the troops until late in the evening before returning home to Didsbury. The next morning, we had a closing ceremony for the old NINA facility and the announcement of the start of the construction phase of the SRS. Ian duly turned up, enthused, and thanked the troops and made us all happy. It was only later that we discovered that Ian had spent the rest of the late evening of 31 March with his father, who lived a few doors away from his home. His dad had passed away during the night as if he knew the importance of Ian's presence at Daresbury on 1 April 1977 at 11 am. Ian was an exemplary leader.

After the closure of NINA, Ian took the opportunity to spend a year at the Stanford Synchrotron Radiation Project (SSRP, but now SSRL) in California from September 1977 (see Box 1). Here, Ian set up a new experimental facility through his ingenuity and persuasion in a Sears garden shed (nothing fancy but a world's first) installed on the roof of the Stanford Positron Electron Accelerating Ring (SPEAR), and published a seminal paper (Munro *et al.,* 1979) with the world-renowned biochemist Lubert Stryer.

Box 1. From Keith Hodgson, Stanford (with input from Piero Pianetta and Herman Winick)

After the operations of the NINA Synchrotron Radiation Facility (SRF) in Daresbury were concluded in 1977, Ian took the opportunity to spend a year at the SSRP in California. After arriving at the SSRP in August 1977, Ian continued his pioneering development and applications of synchrotron radiation (SR) for time-resolved optical excitation and emission studies. As the lead scientist, and with support of the SSRP staff, Ian set up a new experimental station in a Sears garden shed installed on the roof of the SPEAR storage ring (see first photo below). To celebrate the first light, Ian arranged for a bagpipe player and provided Scotch and haggis and drinks on the occasion of the successful commissioning of the station. Ian and collaborators pursued innovative experiments that took advantage of the unique properties of SR, including its brilliance, broad energy bandwidth and polarization.



Ian Munro (third from right, wearing a tie) with SSRP Director Seb Doniach (second from left) and other involved SSRP scientific and technical staff in front of the experimentation station built on top of the SPEAR storage ring for time-resolved studies. Herman Winick took the photo.



Keith Hodgson presenting a photo of his time-resolved instrument picture on the occasion of the 25th year celebration of the SRS.

In September 1978, he returned to Daresbury, working to make the SRS – which became operational in 1980 – not only the world's first but also the leading light to the world's scientists. Many leading researchers from across the world became regular visitors and friends of Ian, Daresbury and the UK. Two of these collaborations are worth mentioning: one with the Soviet Union through the Royal Society agreement with the Academy of Sciences, and the other between the Science Research Council (Daresbury Laboratory was one of their laboratories) and the Japanese Ministry of Education, Science and Culture. The second of these led to a close relationship with the Institute for Molecular Science (IMS) in Okazaki (see Box 2).

Box 2. From Nobuhiro Kosugi, Director of KEK IMSS, Japan

The UK–Japan Scientific Cooperation started in the areas of space science, biotechnology and molecular science through the *aide-mémoire* signed in 1982. Noting the success in developing co-operative research activities, SERC and Monbusho [the Japanese Ministry of Education] agreed to continue co-operative research activities and expand the areas through the *aide-mémoire* in 1990 and in 1993. In molecular science, Daresbury Laboratory and the IMS in Okazaki were key institutes and Ian Munro and Hiroo Inokuchi were key persons for more than 20 years, focusing on the important areas of molecular science linked with SR, lasers and supercomputers applied to atomic, molecular, optical and materials sciences. This agreement embraced many different universities, various research institutes and SR facilities (SRS, UVSOR, Photon Factory and SPring-8) in the UK and in Japan. Ian organized various UK–Japan N+N meetings and took care of many young visitors from Japan at the Daresbury Laboratory, for example, in 1984, Takao Namba (initiated infrared spectroscopy using SR) and Nobuhiro Kosugi (1993 successor to Hiroo Inokuchi as Director of UVSOR).

Ian stayed several times in Okazaki and enjoyed Japanese cultural activities with his local friends. As seen in the photo below, Ian played a leader of the samurai squad of the Ieyasu Procession Festival in the cherry blossom season of 1987, as Okazaki Castle is famous for being the birthplace of the founder and first shogun, Tokugawa Ieyasu, of the Edo Shogunate period. While Ian was working as guest professor at the IMS in 1998, Hiroo played a vital role by helping to minimize the consequences to Ian of a massive, life threatening, brain hemorrhage. His last visit to the IMS was in 2015 to attend the memorial symposium for the late Hiroo Inokuchi.



Photos from Ian's time in Japan. Bottom right: Ian and his wife, Caroline, having dinner in Okazaki with their Japanese friends.

Many of the researchers in the UK benefited from his vision, enthusiasm and support. Several became Fellows of the Royal Society as a result of their work at the SRS (see Box 3). Before his retirement, the SRS achieved another world's first, the first Nobel Prize given to work based on synchrotron X-rays, to Sir John Walker, marked by the *Journal of Synchrotron Radiation* through a special issue on Synchrotron Radiation and Structural Biology in July 1999.

Box 3. From Sir Richard Catlow, FRS, former Foreign Secretary of the Royal Society

I remember Ian with both gratitude and affection for the support and encouragement he gave me when working at the SRS in the 1980s. Together with Alan Chadwick and Neville Greaves, I was one of the early users of the extended X-ray absorption fine structure technique in materials chemistry. And, although this was not Ian's scientific field, he saw the value and significance of our work. Even more important was the help during my four years as a joint appointee between Keele University and the Daresbury Lab, with the role of helping to develop the powder diffraction facilities. There were many difficulties, but working with Phil Pattison, Andy Fitch, Bob Cernik and others we achieved a great deal and Ian's support was crucially important. The synchrotron community owes a great deal to Ian's broad-minded enthusiasm which, coupled with his humour, made him a great colleague.

There are many stories that I can tell, but here I offer only three short ones. During the NINA SRF operation, Ian would always come back in the evening whenever we had a dedicated time. Quite often, he would make coffee/tea from the office building located 100 yards from the experimental hall and bring several cups balanced on a tray. One wet evening, he came into the experimental hall and saw some frogs. His 'save the frogs' instinct prompted him to immediately open the big shutter doors designed to receive large equipment and let the frogs out. Later on, Ian was horrified to discover that these were special frogs that had been imported from Hungary by Hugh Huxley and Wasi Faruqi for the very

important work of understanding how muscles work (Huxley & Holmes, 1997) (see Box 4).

Box 4. From Wasi Faruqi, MBE [MRC, Laboratory of Molecular Biology (LMB)]

Starting in ~1971 our motivation for using SR was in the hope of achieving much higher fluxes than were available with laboratory-based X-ray sources. The driving force for the science behind this project was Hugh Huxley's long-term project aimed at unravelling the molecular details of muscle contraction. It was expected that higher fluxes would hopefully, with SR, allow rapid time-resolved imaging of living muscle fibres to follow the course of structural changes on a millisecond time scale. The organisation of the SRF, where the 'parasitic' beams provided photons for the experimenters, was organised by the Daresbury Laboratory committee chaired by Ian Munro with Jeff Worgan as Secretary. Our camera, based on a double focusing mirror monochromator, was quite an elaborate undertaking for LMB, containing components from King's College London and the National Physical Laboratory – shown in the photo below. The whole assembly needed quite an effort on the part of the local mechanical workshop to mount the camera and the electrical wiring for all the stepper motors and other electronics – all done with Ian's blessing!



Another story relates to an incident that occurred on the South Beamline of the NINA SRF, where numerous exploratory X-ray experiments were conducted, which often required new installations and changeover. It was the beamline where muscle diffraction had a permanent installation (Box 4), whereas others such as protein crystallography, white-beam topography and energy-dispersive powder diffraction experiments required putting things together for a particular experiment, which sometimes called for a hectic pace of work (Box 5). Ian would join in helping to assemble the components, partially to see that the exploratory experiments got the best chance but also to share in the excitement of new results from these experiments (see Box 5). During one such exercise, technicians were working on some installation on the mezzanine floor while the scientist and engineers were putting things together for the experiment, going in and out of the southern experimental hall. To try out the experiments with the beam, they

searched the area and locked up the hall, soon to discover an electrician running out and breaking the emergency exit – he had been working on the mezzanine, which Ian and his colleagues had forgotten to check.

Box 5. From Mike Glazer, Oxford University and co-founder of Oxford Cryosystems

In 1974 I was working at the Cavendish Laboratory Cambridge when I was approached by a young researcher called Joan Bordas. He had just left the Cavendish to work at the NINA synchrotron in Daresbury. He told me about this interesting X-ray source and suggested we could work together to explore what can be done with it. So, we began a programme of trial experiments, the first one being to show how to study a phase transition using white-beam topography. This was when I first met Ian Munro in Daresbury. He helped us to continue to try different experiments. At that time, all that we had in the hall (referred to as the South Beamline) was an empty room and a beam pipe: any equipment or mountings had to be built from scratch, often using things like books on which to place detectors. Lining up was rather hit or miss and required many attempts. Ian was very useful here in seeking whatever he could find to enable us to work.

In 1975–1976 we tried to use an Li-drifted solid-state detector (this was the first at a synchrotron), and Ian actively helped us to do this. I recall that the detector was placed on a pile of lead bricks plus some books in order to get it in line with the X-ray beam. We soon found that in order to not saturate the detector we had to attenuate the beam dramatically so that the source appeared to be weak, and to do this we mocked up a collimator out of lead blocks. In the end, we were able to get a good set of diffracted intensities from rat-tail tendon (I don’t recall where we got this from). We were able to show that the peak intensities obtained were meaningful, which led us to measure energy-dispersive powder diffraction peaks. The rat-tail work was written up and published in *Nature* (Bordas *et al.*, 1976). The paper seemed to attract a lot of attention, although personally I thought that what we had done was rather trivial!

In early 1976 we were all invited to a Royal Society Conversazione to show off the work. The Daresbury media machine swung into action and produced a load of glossy brochures and an exhibition stand. I remember the then Prime Minister, Harold Wilson, coming along to chat to us. I mentioned to him that later that year I would be going to Jesus College Oxford, where he had been an undergraduate. He replied that he would buy me a beer next time he was there. I am still waiting. Anyway, my recollection of working with Ian Munro was a lot of fun and a lot of laughing, especially when we were trying so hard to line up the detector with no extra equipment.



From left to right: Mike Glazer, Samar Hasnain, Charlie Bugg, John Helliwell and André Authier on the occasion of the IUCr Congress and General Assembly in Seattle, WA, USA, in 1996. Ian Munro played an important role in supporting and encouraging the launch of the *Journal of Synchrotron Radiation* (JSR), of which he was one of the founding co-editors.

From John Helliwell, Manchester

My first encounters with Ian were at SRF and then SRS. I imagine that it was Ian, as the head of SRF, who wisely assigned the highly experienced SR scientists Joan Bordas and Jeff Worgan to work closely with me as I was totally inexperienced at Daresbury, or any synchrotron. Ian in his 1998 look-back overview in the *Journal of Synchrotron Radiation* (JSR) spoke favourably about how my efforts had worked out. Always encouraging, Ian could nevertheless be incisively critical, as he was when he reviewed my time-resolved diffraction book, also in JSR.

The final story relates to a visit by my group in February 1986 to the Photon Factory in Japan. Ian was visiting another laboratory in Japan in Okazaki at the time and decided to come to the Photon Factory in Tsukuba, whose director at the time decided to throw a party in Ian’s honour. To our surprise, it followed karaoke, which was very fashionable in Japan then, but we had not yet come across it in the UK. As we were very few from the UK compared with the Japanese contingent, we were joined by a couple of senior visitors from Germany. The Japanese party and us had to alternate. Initially, we did pretty well, but soon we started running out of material. Ian, thinking on his feet, suggested singing *God Save the Queen* – the German colleagues joined in happily. We could finish the party with our heads held high.

On a personal note, his return to Daresbury in 1978 was good fortune for me. I had gone to Germany in September 1977 when Ian had gone to sunny California. I came to the UK in September 1978 *en route* to emigrating to the USA. Ian persuaded me to stay in the UK and take up one of the job offers there. I took up a PDRA position in Manchester Chemistry and Medical Biophysics departments with David Garner and David Hukins – the rest is history – all of which is owed to Ian Munro sharing lots of joyful time, whether experiencing getting a tailor-made suit for Ian (who normally did not wear a suit) or getting a special tailor-made wedding dress for his second wife, Caroline, with the master tailor doing the fitting trial in the

comfort of her hotel room. It has been the greatest privilege of my life to know Ian Munro and to be able to call him my true mentor and friend. Thank you, Ian, for looking after me and many others who came across you. Ian – you are rightly regarded as the Father of Synchrotron Radiation in the UK and will be remembered so for many years to come.

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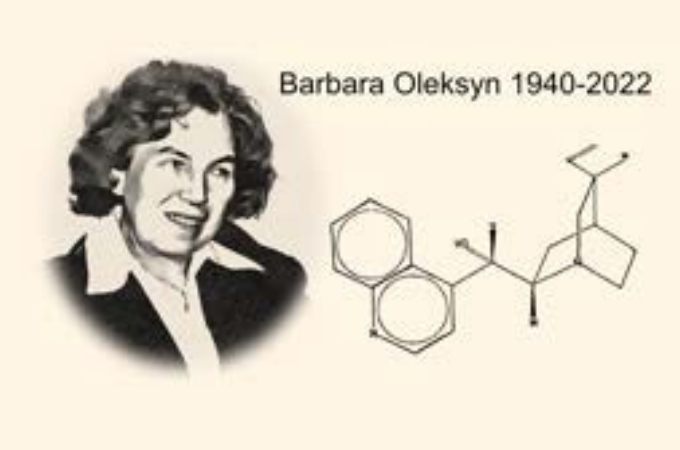
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Samar Hasnain is Max Perutz Professor of Molecular Biophysics at the University of Liverpool, UK, and was Editor-in-Chief of IUCr Journals from 2012 to 2018.

OBITUARY

Barbara J. Oleksyn (1940–2022)



Katarzyna M. Stadnicka, Paweł Serda

Barbara Jadwiga Oleksyn, crystallographer, retired professor of the Jagiellonian University in Kraków, died on 26 October 2022 at the age of 82. Barbara was born on 1 July 1940 in Lwów – then a Polish city under soviet occupation – now Lviv, Ukraine. She was a daughter of Dr Krystyna Oleksyn (*née* Dajewska), known for her research of Tatra waters and soils, and Zdzisław Oleksyn, a chemist, murdered by the German Gestapo in 1941. After the end of the Second World War, Barbara's family moved to Kraków, Poland, within the framework of repatriation.

Barbara studied chemistry at the Jagiellonian University and received her MSc in 1962, when she began to work in the field of crystal chemistry and crystal physics as assistant to Professor Józef Chojnacki (1913–1975), an outstanding Polish crystallographer of the time. While doing research and teaching students, she prepared her PhD thesis and defended it in 1972. In 1988 she received her degree of *doctor habilitatus* for the dissertation entitled "Crystal chemistry of *cinchona* alkaloids and related compounds". The full title of professor was granted to Barbara Oleksyn by the President of the Republic of Poland in 2002.



Barbara Oleksyn, or rather as known to us as Basia, was the author of numerous publications devoted to the analysis of the relationship between crystal/molecular structure and biological activity. She specialized in the crystal chemistry of antimalarial drugs, particularly *cinchona* alkaloids. She participated in the WHO Antimalarial Programme. In 1983, the Editor of *International Tables for Crystallography* Volume A, Theo Hahn, asked Basia to write a review of the first edition of this volume. The review was published in *Acta Crystallographica* B**42** and A**43** in 1986 and 1987, respectively. In 2001 she was one of the main organizers of the 20th European Crystallographic Meeting (ECM-20) in Kraków.

Basia was also known for her activity in the IUCr Commissions on Small Molecules (now Structural Chemistry) and Crystallographic Teaching. She was a member of the Polish Chemical Society – being in 1993–1997, the Chairman of its Kraków Branch, the Crystallography Committee of the Polish Academy of Sciences, and the Polish Crystallographic Association. At the Jagiellonian University, Basia was a Deputy Dean of the Faculty of Chemistry (1996–1999) and Head of the Crystal Chemistry and Crystal Physics Department (1981–1983, 1991–1997).



Basia with Jerome and Isabella Karle.

Basia was a teacher and mentor to a number of generations of chemists and crystallographers. She was a person of great kindness and wisdom, loving the truth, guarding tradition, always ready to help and care, combining modesty with personal dignity and auto-ironic humour, implacable in her views, but always willing to listen to another.

Katarzyna M. Stadnicka and Paweł Serda are at Jagiellonian University, Kraków, Poland.

Note added by Mike Glazer

I was deeply saddened to hear of the death of Basia, whom I have known for many years during visits to the Jagiellonian University. She was a lovely person and a good friend. I recall many times being invited to dinner at her apartment in Kraków which she shared with her mother, who was a soil scientist. I was intrigued to meet there another soil scientist, Professor T. Komornicki, who despite having never left Poland, spoke English far better than I. Discussions at the dinner table were always entertaining.

PRESS RELEASE

Kirara service for high-quality protein crystal growth in microgravity



The microgravity environment of space is an ideal place to study complicated protein crystallization processes. In space, gravity and convective forces do not get in the way of crystal formation, allowing crystals to grow larger, with a more rigid, ordered, near-perfect structure compared with those produced on Earth.

The unique microgravity laboratory and environment of the International Space Station (ISS) can be used to support the development of novel drugs that could treat viral outbreaks or antibiotic-resistant bacteria.

Kirara, the Protein Crystal Growth & drug discovery support service using high-quality crystals grown in microgravity, is a low-cost crystallization opportunity using the ISS. The service uses an original small incubator unit developed by our partners at Japan Manned Space Systems Corporation (JAMSS) and accommodated inside the ICE Cubes Facility on the ISS.



Kirara offers a unique end-to-end service where a microgravity and crystallization expert determines the ideal crystallization conditions for the user and users are offered several options for returning their crystals for terrestrial testing – including having the same experts that set up the experiment performing post-flight analysis (*e.g.* X-ray diffraction on the crystals), if requested.

All deliverables and intellectual property rights obtained belong to the customers.

The Kirara protein crystallization service has had three successful missions already. During the first mission in December 2019, seven pharma companies and research centres participated and the first ever cellulose synthesis by enzyme in microgravity took place. On Kirara#2 in December 2020, the Kirara service was used to investigate Veklury, a redemsivir-based medicament for treating COVID-19, from InnoStudio Inc. and CycloLab Cyclodextrin C&D laboratory Ltd. And in December 2021, Kirara#3 exposed to microgravity the research of five different customers from pharma/agbio companies and research institutes from three different continents: Asia, US and Europe.

A fourth launch of Kirara is currently under preparation, with a following mission being already planned.

The service providers are calling for samples for the upcoming launches, and they are not strictly limited to proteins, as shown through the examples of previous missions.

If you're interested in the upcoming launches, let's discuss right away!

ICE Cubes/Space Applications Services contacts:

Dr Hilde Stenuit: hilde.stenuit@spaceapplications.com

Andrei Sapera: andrei.sapera@spaceapplications.com

Learn more here.

Find out how microgravity can boost research in a variety of sectors and fields of activity.

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