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President's Letter – Fall 2024

Santiago García-Granda

The summer and early autumn of 2024, like every year between congresses, has been a period of implementation of the changes and transformations resulting from the decisions that were taken at our last General Assembly, a period in which the continuation of the scientific debate is transferred to the Regional Associations.

The IUCr Executive Committee, the Finance Committee and our Commissions and Committees have been working in their respective areas with a specific focus on our next global meeting in Calgary, Canada in 2026.

The administrative heart of our Union, in Chester, is behind all of this activity, keeping the activity of the Union orderly in the service of global structural science. This involves maintaining the momentum of our editorial force, which is so important for the maintenance of scientific programs, support for young researchers and the promotion and dissemination of structural science through our 'Open Labs', and for the establishment of new infrastructure in the most disadvantaged regions. Among these are the initiatives in the LAAAMP environment for building new light sources and the Laboratories for Structural Science in Benin and Jamaica. Vice-President Graciela Diaz is the IUCr representative on the LAAAMP Executive Committee.

Following the implementation of more frequent Executive Committee meetings, taking advantage of the ability to meet online, with bimonthly face-to-face meetings, the Finance Committee has adopted the same model, while incorporating two advisors with profiles that complement those of its statutory members. Ilia Guzei and Ed Mitchell, who were already advising the Finance Committee on its decisions, have now been incorporated as advisors.

The Finance Committee is doing a good job in containing expenses consistent with fulfilling our mission and obtaining the maximum return on our investments.

Given the importance of the various dissemination projects throughout the world and in order to provide a channel for response to requests for support, the Executive Committee has created an Advisory Committee to evaluate, in an agile and fair manner, the various requests for support; this committee is chaired by the Past-President.

I have had the opportunity to attend and participate in various meetings and congresses of the Regional Associations. Last July in Denver, after the meeting of the Executive Committee and the Finance Committee, where we had the opportunity to discuss the preparations for the 27th General Assembly and Congress in Calgary, we were also able to exchange projects with the Council of the American Crystallographic Association during its 74th meeting.

Later, at the end of August, the meeting of the European Crystallographic Association (ECM34) took place in Padova in combination with the meeting of the European Powder Diffraction Conference (EPDIC18), a very fortunate combination that had not occurred since 2010 at the Darmstadt congress.

At the end of September, I had the opportunity to represent the IUCr at the meeting of the Latin American Crystallographic Association (LACA) in Montevideo.

All of these meetings of our Regional Associations have been extraordinarily satisfactory, not only in the high quality and variety of the research that was presented, but especially in the high proportion of young researchers, the initiatives to increase the influence of women scientists and the growing connection of structural science with society and sustainability.

Unfortunately, this year I shall miss the Asian Crystallographic Association (ASCA) meeting, which takes place at the beginning of December in Kuala Lumpur, Malaysia, but I will be at the African Crystallographic Association meeting in Algeria in April 2025 and will be present at the 2025 ASCA meeting.

As a consequence of the generational changes in our Chester office, Louise Jones has been promoted to the new position of Head of Publishing Operations, and we have recruited a new person to fill the position of Head of Publications. Kezia Bowman is now responsible for the publication of this Newsletter, in addition to her other duties.

An important step in the incorporation of new blood into the IUCr has been the first meeting of a group of young researchers in structural science, this meeting was attended by young scientists proposed by the five Regional Associations, together with our CEO Alex Stanley, Louise Jones, Manfred Weiss and myself. This inaugural meeting was highly satisfactory and inspiring for the future of the IUCr. A calendar of actions was designed for the full operation of this group and for its gradual incorporation into the various bodies and commissions of the IUCr before its formal approval at the 27th General Assembly. This movement and its success will be fundamental for the future of the International Union of Crystallography and the maintenance of our leadership in structural science.

The International Science Council (ISC) Elections Committee presented a shortlist of candidates for renewal of the ISC Governing Board. The list of candidates promoted by the IUCr, together with the rest of the Unions making up the ISC, had relative success, with some candidates from the Unions' list being included in the final shortlist. Nevertheless, our candidate Hanna Dabkowska was excluded, and the presidency and some other positions were reduced to only a single candidate. This lack of capacity to elect the general assembly results in an obvious democratic deficit and a consequent deterioration in the public image and in the legitimacy of representation, and to a deficit in the confidence of the associates, in particular of the Scientific Unions.

The Nobel Prize in Chemistry 2024 was awarded to the researchers David Baker, for his work on computational protein design, and Demis Hassabis and John M. Jumper, for their work on the AlphaFold tools for protein structure prediction using artificial intelligence. This award is also a great encouragement to the many of you who work in this field, and particularly the members of the Biological Macromolecules Commission.

The International Programme Committee (IPC) for the Calgary congress is now being formed, and it is very important that the Commissions are able to nominate the most scientifically appropriate persons, so that the IPC is a true reflection of the diversity that characterizes our International Union, in particular in gender, geography and age.

At the beginning of next year the IUCr award call for nominations (the Ewald, Bragg and Struchkov Prizes) will be announced. The committees are being decided and the rules are being revised, and for the maximum success of the prizes it is important that the community is prepared to nominate the most outstanding researchers, particularly in areas and sectors that have not been recognized by past awards.

As usual, I end this letter with profound gratitude to all those who form and make our organisation work, the Regional Associates, the IUCr Commissions and Committees, Editors, Co-editors, referees and authors of our journals, our Chester staff and all individual crystallographers, women and men.

Thanks to IUCr Newsletter Editor Mike Glazer and his team, welcome to Kezia, and thanks to all contributors for making possible, as in every quarter, a new quarterly issue that continues to be the reference communication for our community.

Many thanks to all for contributing to maintaining the momentum of the IUCr, wherever they are in the world.

Enjoy practicing structural science!

Editorial

Mike Glazer

This summer, I had the pleasure of attending the European Crystallographic Meeting held in the beautiful city of Padova. As always, an excellent opportunity to meet old friends and to make some new ones. I always enjoy visiting Italy, and we took this opportunity to do some touring after the meeting: Bologna, Verona, and Venice. After all that sunshine and heat (and not to forget the food!), it came as a severe letdown to return to a wet and grey Britain.

The meeting was very well attended, and many interesting talks were given. We have a report on the meeting, see ref. One fun thing was the Science Slam, sponsored by Stoe & Cie, in which a number of contestants presented topics in a novel and entertaining way to a non-expert audience. The audience then judged these in terms of how loud the applause was. The winner was the indomitable Bill Clegg, who chose to sing his contribution to the tune of Mozart's Horn Concerto number 4 (K495), 3rd movement, but in the style of Flanders and Swan (https://en.wikipedia.org/wiki/Flanders_and_Swann). I could not resist asking Bill to let me have a copy for the IUCr Newsletter, and so, for your enjoyment, here it is ref. Do have a go at singing along with the script. The music can be found at https://www.youtube.com/watch?v=VHbLV7G4vno. Who says crystallographers are not fun people?

Chirality, sometimes called "handedness," is a special type of symmetry that can be found in many surprising places. Think of the direction in which, say, a screw turns, left or right? It can also be confusing witness the number of times one sees pictures of the DNA molecule in the media, where the sense of hand is incorrect, i.e., left-handed helices rather than right-handed. Another interesting fact is that there has historically been much confusion about what is meant by the terms left-handed or right-handed in the science of optical rotation. This is where polarised light has its polarization rotated through an angle when passing through certain media (liquid or solid). This phenomenon was first reported by François Arago in 1811 and since then has been studied extensively. Louis Pasteur, in 1848, famously showed that the sense of rotation in certain tartrate crystals was correlated with their external morphology or shape, thus linking optical rotation to the chirality of the molecules within. Since optical rotation was known in fluids of biological origin, it was a small jump to understand that chirality was a major feature of living organisms! However, difficulties arose regarding whether one should consider the sense of rotation for light viewed from the source of the light, as originally used by physicists, or from the point of view of the observer, as used by chemists. The result was that one could often not be certain when reading scientific manuscripts on optical rotation as to which frame of reference the author was using. Very confusing. This was not resolved until relatively recently when the chemists' convention was universally adopted. You can read much more about this fascinating type of symmetry in this article by Istvan and Magdolna Hargittai ref.

You will undoubtedly have seen that the Nobel Prize in Chemistry this year has been awarded to David Baker, Demis Hassabis and John Jumper for their astonishing work on the use of AI. John Helliwell talks about the importance of their work in determining protein structures (ref).

The success of this International Newsletter is such that the IUCr has decided that it should be published six times from next year instead of four. This will, of course, mean extra work for the staff at Chester, especially for Kezia Bowman, who only recently joined the IUCr.

Finally, it gives me great pleasure to note that, for once, we have no obituaries this time!

Oxford

Protein design and folding prediction endorsed by the Nobel Prize for Chemistry 2024

By John R Helliwell, Department of Chemistry, University of Manchester M13 9PL.

I have written before in the IUCr Newsletter [1] on the breakthrough made in protein folding prediction by Google DeepMind's AlphaFOLD [2] and on the PDBe (Protein Data Bank Europe) facilitating availability for users of some 200 million AlphaFOLD predicted proteins [3]. Protein folding prediction was one of the decades-old grand challenges of science. Since my student days, I have been fascinated by the physics-based hunt for the Gibbs free energy minimum, which must be the protein 3D structure identified by Anfinsen's protein denaturation and renaturation studies [4]. However, it wasn't energy minimum methods that solved it; it was a combination of learning from protein sequences and precise protein experimental structures carefully curated in databases [5]. These AI and ML ((artificial intelligence and machine learning) methods based on big data are applied to many different prediction challenges in science and, more widely, in society. The continued wish for a physics-based energy minimum approach has led to further debate on whether the protein folding challenge has been solved [6, 7].

On October 9th, 2024, the Nobel Prize for Chemistry was awarded [8]: -

"David Baker has succeeded with the almost impossible feat of building entirely new kinds of proteins. Demis Hassabis and John Jumper have developed an AI model to solve a 50-year-old problem: predicting proteins' complex structures. These discoveries hold enormous potential."

Protein design is a reverse procedure than protein fold prediction, which involves designing a protein structure and determining the amino acid sequence that would produce that designed protein. This is a fantastic breakthrough by David Baker and his coworkers at the University of Washington in Seattle. The first of these was published in 2003 [9], see Figure 1. As remarked by the authors of [9]:-

“The ability to design a new protein fold makes possible the exploration of the large regions of the protein universe not yet observed in nature.”

They also recognised the potential for a sweeping change in protein crystallography phase determination :-

“Remarkably, a strong molecular replacement (MR) solution to the phase problem was found with the use of the design model. (So) the design model was quite close to the true structure: Even the small deviations of NMR solution structures from X-ray crystal structures can make molecular replacement searches fail. “

Figure 1 The first designed novel globular protein fold by David Baker and coworkers confirmed with a 2.5Å X-ray SAD (Single wavelength Anomalous Diffraction) phased crystal structure, PDB code 1QYS [9]. Figure prepared by me using CCP4MG [15].

Why did I not write about it [9] these past 20 years in the IUCr Newsletter? I certainly admired it, but I imagined it as mainly about molecular biophysics, at that time. Meanwhile, the protein fold prediction I could always see, if fully solved, would have a massive impact on my efforts in protein crystallography phase determination using tuneable synchrotron radiation. This was a topic that Dorothy Hodgkin drew my attention to in 1975 when she received a pre-print from the SSRL (Stanford Synchrotron Radiation Laboratory) via Sir Ron Mason of the seminal work of Keith Hodgson and colleagues there [10]. Indeed, we are approaching the fiftieth anniversary of that momentous paper, and a special issue of articles in the Journal of Synchrotron Radiation is underway [https://journals.iucr.org/s/services/specialissues.html], endorsed, of course, by Keith Hodgson himself.

An interesting feature about this year's Nobel Prizes in Chemistry and Physics was a seeming coordination of topics with the Physics Nobel Prize announced the day before to John J. Hopfield and Geoffrey E. Hinton [11]: -

"for foundational discoveries and inventions that enable machine learning with artificial neural networks."

The Nobel Prize in Physics led to comments on TwitterX that the Prize had been hijacked by computer scientists. The Nobel Committee explanation, seemingly to anticipate such criticisms, had already emphasised that the Hopfield contribution was statistical physics and that Hinton's contribution involved a so-called

Boltzmann machine. Interestingly, the applications of the Hopfield and Hinton methods emphasised in the main press conference were things like interpreting medical imaging data and particle physics data. It seemed to carefully exclude protein folding prediction. However, in the detailed explanation and interview of the Nobel Physics Committee specialist after the main announcement event, he cited application of their methodology in that domain.

So, what next for the two domains of protein prediction and protein design? Google DeepMind, who are based in London, recently launched its AlphaFOLD3 software for predicting biomolecular interactions, including proteins, nucleic acids, small molecules, ions and modified residues [12]. For the domain of protein design the list of impressive applications described by David Baker in the telephone interview at the press conference already includes a designed protein suitable for incorporation in a nasal spray against the covid-19 spike protein and a designed protein sensitive to environmental pollutants. As was remarked in the Nobel Chemistry Prize ceremony subsequent discussions, the limit is not the possibilities but our imagination.

In my own tweet about it on TwitterX (@helliwelljohn) I wrote: -

"Hearty congratulations to all three Laureates. Both domains, protein design and prediction, are fantastic breakthroughs. Hearty thank yous too to the great care of the sequence data bases and of the PDB experiments' structures database. @rcsbPDB @PDBeurope @PDBj_en"

Where are we today in my view as a protein crystallographer then? Recently I was asked this by the ESRF communications office, who were writing a piece about the 30 years of user operation at the ESRF since it came online, "since I had been involved in the ESRF since the early days". I replied that: in the mid 1980s I led the ESRF MX (macromolecular crystallography) Working Group and wrote the MX sections for the ESRF Foundation Phase Report (Red Book) [13]. Since then MX crystals have got ever smaller, that tuneable wavelength resonant scattering phasing got supplanted by AlphaFold2 about 4 years ago, that CryoMX (at 100K) is getting more and more supplanted by room temperature MX, that structural dynamics (including time resolved MX) keeps growing in importance rather than structure determination per se, that neutron MX is growing in importance and that X-ray wavelength tuning for site specific metal or ion determination in MX remains very important. Then, for the future using the new ESRF Extremely Bright Source upgrade of 2 years ago, it will be dominated by the physiological relevant MX and structural dynamics (time resolved) MX studies. Of course another major breakathrough is that crystallisation failures of large complexes now have a different way forward with cryoEM."

Inherent in this personal assessment for the ESRF communications office is that predictions of protein folds have somewhat elaborated into predictions and designs of protein structures including complexes, not 'only' folds. Thereby the emphasis for the experimental protein crystallographer is apparently shifting to being determining structures closer to the conditions of the living cell itself be it temperature or pH. For example my colleagues and I just this week published a body temperature (37°C) study of a protein with a bound rhenium theranostic compound seeking a truly physiologically relevant structure [14]. I also note that in an unusual move the EuroXFEL have promptly announced the day after the Nobel Prize that David Baker is one of their users, stimulating my thinking that he is moving into the design of protein structure and dynamics. Clearly, close fit predictions to the current predominantly 100K database entries of protein structures is one thing. But the need is with us for an expanded number of experimental structures at a wide range of physiologically relevant conditions if there is to be attempts at a close fit of predictions to the living cell situation. Of course, any protein 3D structure prediction or design has to be experimentally validated by crystallography, cryoEM or NMR spectroscopy.

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ETERNAL CHIRALITY

Istvan Hargittai and Magdolna Hargittai

Chirality as a phenomenon in Nature has always been present. As a concept in science, it has been around for some time. It began as a curiosity, then became a fundamental component in scientific research, and today, it is a crucial consideration in medicine. It is important in crystallography, though not always recognized explicitly; for example, it does not appear in the Subject Index of the excellent Historical Atlas of Crystallography [1].

From left to right: Homochiral pair of hands: Auguste Rodin, "The Cathedral," Rodin Museum, Paris; Heterochiral pair of hands: tombstone in the Jewish cemetery, Prague; Legs: detail of the sculpture "Wave," by Kay Worden, Newport, Rhode Island. Photographs by the Hargittais.

The main thrust of our research careers has been determining and modeling molecular structures. We were not concerned with chirality when using gaseous electron diffraction to determine internuclear distances because the same set of internuclear distances characterizes both chiral versions. However, chirality has fascinated us due to our broader interest in symmetry [2−4]. This essay surveys a set of selected examples of chirality.

Many objects, both animate and inanimate, have no symmetry plane but occur in pairs that are related by a symmetry plane. They are each other's mirror images but cannot be superimposed. This is called chirality or handedness from the Greek word for hand, cheir (χέρι). Above, we present examples of a homochiral pair, a heterochiral pair of hands and a heterochiral pair of feet—the concept could be called just as well "podality" (from pódi—πόδι). The phenomenon belongs to the more general concept of dissymmetry, which signifies the absence of certain symmetry; in the case of chirality, it is the absence of a symmetry plane.

Chiral pair: J. S. Bach, “Die Kunst der Fuge,“ detail

Not only material objects can have handedness: here is a beautiful example in Johann Sebastian Bach's (1685−1750) "The Art of the Fugue".

Immanuel Kant: stipple engraving by J. Chapman, 1812 (Wellcome Collection)

The German philosopher Immanuel Kant (1724−1804) wrote about the puzzle of the isometric left and right hands that cannot be made to coincide in space. He called the non-superposable mirror images "incongruente Gegenstücke" (incongruent counterparts) [5].

D. François J. Arago and Jean Baptiste Biot: lithographs (both: Wellcome Collection)

In 1811, D. François J. Arago (1786−1853) described the optical activity of quartz crystals. Some rotated the plane of polarized light in one direction, while other quartz crystals rotated it to the same extent but in the opposite direction. [6]. This discovery was one of Arago's many discoveries in several areas of science. For one of them, on the magnetic properties of substances not containing iron, he received the most prestigious Copley Medal of the Royal Society (London) in 1825.

In 1812, Jean Baptiste Biot (1774−1862) discovered the optical activity of quartz crystals [7] and observed that some solids, even when dissolved in water, showed the same effect. Biot's genius manifested in his conclusion that the effect is a molecular property. It was then left to Louis Pasteur (1822−1895), decades later, to understand the correlation of dissymmetric crystals and the optical activity in solution. Chirality and optical activity have been intimately related, and laevo-active (L) and dextro-active (D) chiral substances have been distinguished. Optical activity does appear among the entries in the Subject Index of the Historical Atlas of Crystallography [1]. Indeed, it is a more general concept than chirality. If a molecule or a crystal is chiral, it is necessarily optically active, whereas the converse is not true. There are symmetry classes of crystals that are non-enantiomorphous yet may exhibit optical activity.

Louis Pasteur's bust in front of the central building of the Institut Pasteur, Paris, and his models as exhibited there. Photographs by the Hargittais

What Pasteur did in this connection in 1848 may be called the reverse experiment. He crystallized sodium ammonium tartrate from a solution he prepared from the optically inactive salt. He obtained crystals of two kinds, which were each other's mirror images. One of the two was identical with the crystals of the naturally occurring optically active tartrate—a product of the fermentation of wine. But the other, its mirror image, had never been seen before. Pasteur separated the two forms by hand. Tartrate was a lucky choice because manual separation is rarely possible. In his next experiment, Pasteur dissolved the two kinds of crystals separately in water, and the two solutions showed optical activity of the same magnitude but opposite in direction. The old Biot presented Pasteur's findings of crystal and molecular dissymmetry (today, we prefer the term chirality) to the French Academy of Sciences. Biot realized the magnitude of Pasteur's discovery, so he had Pasteur first to demonstrate it to him in the laboratory before reporting about it to the Academy. When Biot could see with his own eyes the experiment, in Pasteur's words [8]: "very visibly affected, the illustrious old man took me by the arm and said, 'My dear child, I have loved science so much throughout my life that this makes my heart throb.'"

Pasteur's discovery had broad implications. J. Desmond Bernal (1901−1971) pointed out that it arose at a meeting place of three great distinct disciplines: crystallography, physics, and chemistry. In his treatise "Molecular Asymmetry" [9] Bernal charted the developments that could be related to Pasteur's discovery. Here and already once above, the term "molecular asymmetry" figures whereas the term "molecular dissymmetry often occurs in describing chirality. It is a little confusing, so we better define them: asymmetry means the complete absence of symmetry and dissymmetry means the absence of certain symmetry. Accordingly, in this case, indeed, dissymmetry and asymmetry could be used interchangeably. When Bernal discusses the significance of Pasteur's discovery, he reaches back to other classics of science, to R. J. Haüy, J. F. W. Herschel, J. J. Berzelius, and Auguste Bravais He shows how they contributed to the development of the concept and to the development of X-ray crystallography in the early 1910s.

William Thomson, Lord Kelvin: photograph by Harry Herman Solomon (Wellcome Collection)

Lord Kelvin (1824−1907) wrote [10]: "I call any geometrical figure, or group of points, chiral, and say that it has chirality if its image in a plane mirror, ideally realized, cannot be brought to coincidence with itself."

Statue of Marie and Pierre Curie in the Marie Curie Garden, Paris 5—Latin Quarter; photograph by the Hargittais; and "Chiral Pierre Curie" by and courtesy of the graphic artist Istvan Orosz [3]

Pierre Curie (1859−1906) formulated the most general and fundamental concept related to symmetry that involves dissymmetry, including chirality: "c'est la dissymétrie qui crée le phénomène" (dissymmetry creates the phenomenon) [11]. A phenomenon is expected to exist and can be observed only if certain elements of symmetry are absent from the system. A forerunner of this concept was put forward in 1833 by Franz E. Neumann (1798−1859) in his studies of the physical properties of crystals: "The physical properties of crystals always conform to the symmetry of the crystal" [12].

Hans Erni's ex libris bookplate for Vladimir (Vlado) Prelog with a dedication to one of the present authors (courtesy of the late Vladimir Prelog). A peculiar feature of this drawing is that the two hands appear inverted due to the two arms being crossed [13]. Erni made other versions of this drawing in which the two hands appear non-inverted.

The emergence of stereochemistry could be a direct consequence of Pasteur's discovery. Its birth was in 1874, that is 150 years ago [14, 15]. The basic concepts were proposed by J. H. van 't Hoff (1852−1911) and J. A. Le Bel (1847−1930). Van 't Hoff published a booklet, La Chimie dans l'Espace (Chemistry in Space). Viktor Meyer (1848−1897) first used the term stereochemistry in 1890. The idea of extending the description of materials structures into the third dimension reaches back at least to Johannes Kepler in the early 18th century [16] and John Dalton in the early 19th century [17] in their discussions of the stacking of the building elements in water and ice. Still, even as late as 1956, the distinguished crystallographer Albert F. Wells (1912−1994) felt the need to stress that the description of "the three-dimensional arrangements of atoms in crystals was an integral part of structural chemistry" [18].

Hierarchy of molecular isomerism ([2], p. 100)

The possibility that chirality leads to two different versions of the molecules of the same substance causes a well-defined isomerism in molecular structures. This is shown in the scheme summarizing molecular isomerism. According to Vladimir Prelog (1906−1998), Hans Erni's ex libris, shown above, contains all three basic paraphernalia necessary for dealing with chirality. They are human intelligence, a pair of left and right hands, and two enantiomorphous tetrahedra [19]. Prelog was a corecipient (with John W. Cornforth) of the 1975 Chemistry Nobel Prize "for his research into the stereochemistry of organic molecules and reactions."

Returning to the multitudes of the consequences of Pasteur's discovery, it brought about the realization that biologically important substances occur in one of the two possible versions in living organisms. The Nobel laureate biologist George Wald (1906−1997) noted: "No other chemical characteristic is as distinct of living organisms as is optical activity" [20]. The great question is: How did it start, and how was one version of the two possibilities chosen? Already, Pasteur contemplated this, and Vladimir Prelog called this a question of molecular theology in his Nobel lecture titled "Chirality in Chemistry" [21]. Prelog gave his own definition to chirality: "An object is chiral if it cannot be brought into congruence with its mirror image by translation and rotation. Such objects are devoid of symmetry elements which include reflection: mirror planes, inversion centers or improper rotational axes."

Left-handed and right-handed helices at the Monastery in Zagorsk (left), and in a church in Paris (right). Photographs by the Hargittais

The philosopher and theoretical physicist Lancelot L. Whyte (1896−1972) extended the definition of chirality: "Three-dimensional forms (point arrangements, structures, displacements, and other processes) which possess non-superposable mirror images are called 'chiral'" [22]. This extension made it convenient to describe chiral point groups, such as chiral molecules, and space groups, such as left-handed and right-handed helices. One of us (IH) discussed the possible origin of handedness in biological macromolecules in 1998 with Nobel laureate Ilya Prigogine (1917−2003), who said [23]: "Some people had proposed that the preference of left-handed amino acids may be related to electroweak interactions which stabilize very slightly the left-handed

amino acids. Indeed, bifurcations are very sensitive to very small differences of energy. If the transition goes very slowly over years, then even such small differences in energy will introduce a slight effect in favor of one of the two amino acids." The polymath science historian Stephen F. Mason (1923−2007) did a great deal of pioneering studies on biomolecular homochirality and on the recognition of the electroweak origin of biomolecular handedness (see, eg, in [24]). The handedness of the biologically important helices has a vast literature.

At the birth of stereochemistry, it was impossible to tell when there was a molecule that could exist in two mirror image forms, which isomer was which—whereas there was no way to establish the absolute configuration. The organic chemist Emil Fischer (1852−1919) took the bold step in 1894 of arbitrarily assigning an absolute configuration to sugars [25]. There was a 50% probability that he might be right. Luckily, he was, which could be established only in the early 1950s when the crystallographer Johannes M. Bijvoet (1892−1980) and his team determined experimentally the sense of molecules [26]. Their technique was revolutionary but tedious because for each new molecule the chemical relationship with the initial one had to be established for which they had determined the absolute configuration. Prelog succeeded in simplifying the procedure a great deal.

In conclusion we mention two remarkable stories in connection with molecular handedness.

Dorothy L. Sayers, 1925, publicity photo from her American publisher; in the public domain (File:Sayers-whose-body-image.png - Wikimedia Commons; downloaded March 28, 2024)

In Dorothy L. Sayers's (1893–1957) detective story, The Documents in the Case, an expert identifier of wild mushrooms dies of poisoning. The question arose: was this death a consequence of accidental poisoning or even suicide, or was it foul play, i.e., intentional poisoning—murder? The analysis of the toxin in the victim's body showed the presence of only one of the two possible versions of the poisonous molecule, pointing to a man-made product, ergo, murder. Sayers had a co-author for this book, Robert Eustace (pen name of Eustace Robert Barton, 1869–1943). He was a physician and himself a prolific author whose plots often included references to scientific innovation. He probably provided the scientific basis for Sayers' detective story; everything presented in the story was correct, even from today's perspective. Sayers's book has been kept in print ever since it appeared in 1930. The date of the original publication is significant as it was anticipated by decades by the current legislation that rigorously prescribes chiral purity for pharmaceutical products. Pharmacology necessitated this legislation because the physiological impact of left-handed and right-handed versions of the same molecule may vastly differ. This is not what Sayers's story exposed. It exposed some physiological relevance of chirality, which was sufficiently pioneering to deserve our appreciation [27].

We present a few examples of differences in the properties of chiral versions of the same substance. We list the names of the substances with selected properties of the right-hand/left-hand versions in that order:

Ethambutol, treats tuberculosis/causes blindness

Penicillamine, treats joints/is toxic

Naproxen, reduces inflammation but risks heart disease/is toxic for the liver

Propoxyphene, pain reliever (Darvon)/cough medicine (Novrad). Note that the names of these two medications are each other's mirror images.

Asparagine, bitter/sweet

Carvon, caraway smell/spearmint smell

Limonene, Lemon smell/orange smell

Computer drawing of thalidomide molecular structure (courtesy of Ilya Yanov) and Frances O. Kelsey, 2000, in her office at the U.S. Food and Drug Administration. Photograph by the Hargittais

A tragic example was the thalidomide case − N-phthaloyl-α-aminoglutarimide (its model is shown above). It was known as Contergan in Europe. Originally, it was marketed as a sedative in the late-1950s. It was given to pregnant women suffering from morning sickness. The drug was marketed as a racemate (i.e. consisting of

both chiral molecules) and by the early 1960s, many birth defects in Western Europe were associated with Contergan. Slowly, the correlation between its consumption and the occurrence of birth defects was recognized, and it was finally withdrawn from the market. Eventually, it was understood that one of the two chiral versions of thalidomide was teratogenic; the other was harmless. The tragedies occurred worldwide except in the Soviet bloc, where it was not available, and the United States, where the Food and Drug Administration (FDA) had never approved it. A young and conscientious official of the FDA, Frances O. Kelsey (1914−2015) [28], resisted approval and demanded more and more tests and thorough investigations. Her work contributed to establishing a regulatory regime—the Kefauver-Harris Amendments of 1962 and the Investigational New Drug Regulations of 1963. Today, and for some time this has been the case, in the European Union and elsewhere, molecules that may have two enantiomeric versions may be marketed for medicine only in the version that has the desired effect. This has resulted in a huge industry of chiral separation.

On the one hand, this has added to the costs of medicine, while, on the other hand, it has saved enormous amounts of substances that are not consumed and wasted. For fairness, we add that chiral separation would not solve the problem of thalidomide causing birth defects because the harmless version rapidly converts into the other version in the organism. Note also that thalidomide has other beneficial uses in medicine, but it should never be administered to expectant mothers.

Here, we make a big jump to allude to the enormous significance of chirality—or, more generally, dissymmetry—on a universal scale. In 1960, there was less than a half-page note in Nature [29] in which the physiologist John B. S. Haldane (1892−1964) returned to Pasteur in the wake of the recent discovery of parity violation. Haldane's starting point is T. D. Lee and C. N. Yang's discovery [30], which led to the acceptance of the notion of the asymmetrical universe. Pasteur first enunciated this [31], and Haldane quotes him in the French original. Here, we provide the quote in English translation (courtesy of Alan L. Mackay): "It is inescapable that dissymmetric forces must be operative during the synthesis of the first dissymmetric natural products. What might these forces be? I, for my part, think that they are cosmological. The universe is dissymmetric, and I am persuaded that life, as it is known to us, is a direct result of the dissymmetry of the universe or of its indirect consequences. The universe is dissymmetric." (emphasis in the original)

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A Crystallographer's Concerto

Words by Bill Clegg (in the style of Michael Flanders and Donald Swann's "Ill Wind")

Music by Wolfgang Amadeus Mozart: Horn Concerto number 4 (K495), 3rd movement: https://www.youtube.com/watch?v=VHbLV7G4vno

Written for the 'Science Slam' entertainment session at ECM34, Padova, 2024

I made a new compound and needed its structure

But spectroscopy doesn't tell me enough.

Now X-ray diffraction will give me a picture

So I can be sure that I made the right stuff.

Tutti

For crystal growth, I had to dissolve it and let it cool.

Upon my oath! It's incredibly boring to see.

But to my surprise, and in front of my eyes,

A crystal did grow to useful size.

Oh, what a pain of learning to cope

With peering for hours down a microscope!

But that was yesterday, and now today

I looked for diffraction effects.

There were the spots, but they didn't fit a lattice.

What on earth does it mean?

Single crystals give patterns without a flaw.

Oh, could it be a twin?

Yes indeed! Now I need

Clever software to find me a twin law.

Next integrate

And corrections apply to sigma and I.

Then I can use direct methods in structure solution.

If that doesn't work, I'll try flipping the charge

To look for electrons and their distribution –

Molecular fragments that I can enlarge.

Tutti

What a joy! Finding atoms in a Fourier,

Hydrogens showing up in a difference map.

This is easy, I learnt how to do it at Erice

With SHELX, or OLEX, or some other app.

Now everything's found, the structure is sound.

It's time to start the tricky part –

The first refinement round.

Now, I urge: please converge!

Away now we go with our least-squares refinement,

Constraining, restraining, and weighting it all.

The model gives data approaching alignment

With measured diffraction; the R factor's small!

Tutti

It's looking fine; the goodness of fit is precisely 1 –

A pleasing sign! Shout out loud: I'm on cloud nine!

Now on the screen the structure is seen,

No more density showing between.

A lovely molecule – it's really cool!

I'll show it at ECM.

I'll devise a surprise

And I'll snaffle the main poster prize!

I just need a nice diagram

Showing the molecules in the cell

And ellipsoids to prove I am

Not just a fraud.

Cadenza

And then publication – the very best journal,

Attracting citations all over the place.

My new reputation will blossom eternal,

I'll enter the database!

Tutti

I'm getting excited! I should wait till later,

My fingers are flying around.

I've just hit DELETE and I've lost all my data

And made an unprintable sound! #***!

And now comes the moment I dread,

Those crystals are looking quite dead.

I'll have to use powder instead!!!

EPDIC !!

SIG4 (ECA) Distinguished Publication Award 2024

Stéphanie Kodjikian (SIG4 co-chair), Tatiana Gorelik (SIG4 chair)

The "Distinguished Publication Award 2024," presented by the Special Interest Group on Electron Crystallography of the European Crystallographic Association (ECA SIG4), recognizes the most outstanding paper published in 2023. This award celebrates significant advancements and applications in the field of electron crystallography. Candidate publications were evaluated based on several criteria, including innovation, complexity, high-quality research with a focus on electron crystallography, broad scope, and impact on the community. The jury was made up of internationally renowned experts in electron crystallography. SIG4 extends its thanks to them for their engagement and professionalism.

This year's winner is the paper titled "Accurate structural models and absolute configuration determination using dynamical effects in continuous-rotation 3D electron diffraction data" by Paul B. Klar, Yaşar Krysiak, Hongyi Xu, Gwladys Steciuk, Jung Cho, Xiaodong Zou, and Lukas Palatinus, published on April 20, 2023, in Nature Chemistry 15, 848−855 (https://doi.org/10.1038/s41557-023-01186-1).

Klar et al. describe a method for analysing continuous-rotation 3D electron diffraction (3D ED) data for routine structure analysis across a broad range of materials, including minerals, framework structures, and organic compounds. The paper introduces the concept of "virtual frames" to calculate integrated intensities using the dynamical theory of diffraction. This approach is then applied to the dynamical refinement of crystal structure models using 3D ED data from 19 different compounds. The authors demonstrate that this refinement approach, which accounts for the multiple scattering of electrons, is clearly superior to the commonly used kinematical refinement, which neglects multiple scattering. Along with reducing noise in Fourier maps and improving overall agreement between measured and calculated intensities, dynamical refinement reveals structural details more clearly, such as hydrogen sites and guest molecules. A key focus of the paper is the determination of the absolute structure of chiral compounds, demonstrated by successfully assigning the correct handedness based on 3D ED data from 58 chiral molecular crystals.

The jury was particularly impressed by the wide-reaching impact of the work, as the results were based on data from 10 different transmission electron microscopes across various laboratories. This impact is further underscored by the paper's nearly 50 citations as of September 2024.

We congratulate the winners and look forward to future developments in the field of electron crystallography.

Gwladys Steciuk (left) and Paul Klar (right) at ECM34, Padua, Italy, August 2024.

Interview with Dr Julia Contreras-García

Author not stated in source

This interview with Dr Julia Contreras-García, President of the "Women in High Pressure" organisation, is part of the "Women in Crystallography - a video series" a project of the GIG03 (General Interest Group on Education in Crystallography of the ECA) and funded by the Royal Society of Chemistry within the framework of the "Inclusion and Diversity Fund". Dr Contreras-García discusses her research on electron density and its applications in understanding chemical bonds and predicting properties like superconductivity.

She shares the origins of the "Women in High Pressure" group, which was founded in response to the lack of female representation in the European High-Pressure Committee. The group began by creating an online database to ensure visibility for women in the field. Over time, the initiative grew through events at conferences and the creation of "Women in Crystallography" t-shirts you can see at conferences today. This initiative has already started funding its first recipients.

Dr. Contreras-García encourages students and postdocs to sign up for the Women in High Pressure database, emphasising the importance of building awareness of gender biases and becoming part of a supportive community for women in science.

Link video clip:

https://youtube.com/clip/Ugkxe0z69Gn6OdjCmuIYx8asVB_dm6rqIq9C?si=S4mHTuSiGTJWXO6P

Video: https://www.youtube.com/watch?v=FLUfjYV0yUI

European Crystallographic Meeting 34, Padova, Italy, 26-30 August 2024

Jan Dohnalek, ECA

During the last week of August the crystallographic community met in the medieval city of Padova to discuss the latest developments and results in the field of crystallography (https://www.ecm34.org/). The Congress welcomed more than 800 participants who contributed in 43 microsymposia spanning from quantum crystallography over applications in material and biological sciences to teaching and crystallography in art, accompanied by about 700 posters. The plenary lectures were given by Kristina Djinovic on the molecular architecture of muscles and by Jonathan Wright providing insights into imaging single crystals in powder samples. The most significant developments in the key directions of instrumentation, computational tools and application of crystallographic approaches in various branches of research were presented in 16 keynote lectures. The social program offered amongst others the Science Slam, a great concert of classical music in Palazzo Liviano, a public lecture “Einstein and Me” by Gabriella Greison, a students’ mixer, and an unusual experience in the form of a conference dinner in one of the historical city squares. This Congress was complemented by seven satellite events, including the European Young Crystallographers Satellite Meeting or the special event Crystallography in School promoting teaching of crystallography with school science teachers. The organizing committee chaired by Gilberto Artioli and Giuseppe Zanotti with the help from the chairs and co-chairs of the individual microsymposia managed to prepare a great event with exciting topics, excellent speakers, and plenty of space for social and scientific interactions. The crystallographic song “A musical account of a rather unfortunate trainee crystallographer” by Bill Clegg on the music by Wolfgang Amadeus Mozart performed in the Science Slam and for great success also during the closing ceremony was a treat to all crystallographers enjoying apart from science also good music and fun.

Five crystallographic prizes have been awarded during the Meeting. The Max Perutz Prize to Prof. Mariusz Jaskólski, Adam Mickiewicz University in Poznań, accompanied with his lecture “A path paved with crystals”, the Erwin Felix Lewy Bertaut Prize to Daniel Mazzone, Paul Scherrer Institute, Villigen, and the Alajos Kálmán Prize to Piero Macchi, Politecnico di Milano. Two newly established prizes have been awarded for the first time: The Lodovico Riva di Sanseverino prize in recognition of notable contributions to the dissemination of crystallography in the field of education at all levels to Claire Murray, Freelance Scientific Researcher in Germany and the George M. Shledrick prize to a non-tenured researcher for outstanding scientific contributions in the field of structural sciences to Marta Morana, University of Florence. Find more information about the ECA prizes here https://ecanews.org/prizes/.

Eleven poster prizes, supported by companies, IUCr Journals, CCDC and others, appreciated the best poster presenters, in specific fields of research, instrumentation development or at the start of their career.

The previous Executive Committee of ECA finished its term and a new Committee has been elected by the ECA Council. Achievements of the outgoing Executive Committee were appreciated by the Council and some Committee members have been re-elected into their new roles. Dr. Arie van der Lee (Université de Montpellier) has become the new President of the European Crystallographic Association. The ECA Council has approved the organization of the European Crystallographic School 11 in Stockholm, June 21-27, 2026 and of ECM37 in Athens, August 2028.

Photo of M. Jaskolski

The Max Perutz Prize awardee prof. Mariusz Jaskólski during his lecture A path paved with crystals.

Photo of Ex Comm

Some past and new members of the Executive Committee of ECA. From left to right: Marijana Đaković, Delia Haynes, Andrew Maloney, Arie van der Lee, Andrea Ienco, Consiglia Tedesco, Klaudia Hradil, Chiara Massera, Jan Dohnálek, on screen: Antonia Neels, Maria José Sanchez Barrena.

9th European Crystallography School (ECS9)

Author not stated in source

Laboratoire de Cristallographie, Résonance Magnétique et Modélisations

Nancy, 24th – 30th June 2024

The ECS9 was held in Nancy (France), at the site of the Faculté des Sciences et Technologies of Université de Lorraine, as an in-presence event. In this edition, the school targeted the improvement of crystallographic skills for young scientists (PhDs, post-docs, Master students) working in different fields (chemistry, physics, material science). The lectures and practical sessions covered all aspects from basic structure analysis to understanding of chemical bonds, bonding interactions and structure-properties relationships in materials, with a focus on single crystal X-ray diffraction and structure analysis. Consequently, the program was organized in the following 5 main scientific sections, with lectures on the fundamentals in the morning and practical sessions with applications and tutorials in the afternoon:

An introduction to X-Ray Diffraction (XRD) theory

Structure determination and analysis

Packing and interaction analyses

Using aspherical models of the electron density distribution

Crystallography under constraints.

The 18 speakers (9 international, 9 local) plus 3 sponsors (industrials) gave 8 fundamental lectures and 7 practical sessions during which at least 2 tutors were present for guiding and helping the participants. In order to guarantee a reasonable tutor-to-participant ratio, especially for the practical sessions, our laboratory of crystallography (CRM2) was heavily involved with 9 speakers/tutors. Most of the lecturers were present and available for the participants during the whole week, enabling further specific discussions and informal exchanges between lecturers and attendees, during and after presentations. Additionally, coffee breaks and two poster sessions helped significantly to develop discussions.

This school brought together a total of 62 (30 F, 32 M) participants of 25 different nationalities, coming from laboratories of 22 countries.

ECS9: Lecture (top) and practical sessions with hands-on structure solution and refinement.

Thanks to industrial (STOE, Rigaku, Bruker, Dectris, Cristal Laser) and public sponsors (Region Grand Est, Metropole of Nancy, City of Villers-les-Nancy) as well as local support of the Université de Lorraine registration fees could be proposed at very low rate (350 € for PhDs and postdocs, and 450 € for other people). Registration fees covered participation in courses and materials used, overnight stays, lunches and coffee breaks during the school, as well as the gala dinner and excursion. In consequence, the school attracted a lot of interest and the 50 available places (constrained by the capacity of the computer room for the practical sessions) were sold out already one month before the inscription deadline. In order to enable a maximum of interested young scientists to participate we accepted a total of 62 inscriptions (out of a total of 78 pre-registrations recorded at the closing date of inscriptions).

Thanks to the support of IUCr, ECA, and the French Crystallographic Association (AFC), we could offer 17 bursaries/travel grants for a total of 8784 €. The 17 laureates of the bursary came from 14 countries from Europe, Europe-Central Asia, South Africa, North Africa and South America. Additionally, we waived the fee for 2 students and 2 Italian students were directly supported by the Italian Crystallographic Association (AIC). Finally, two poster prizes of 100 £ and 100 € were awarded during the school, sponsored by the CCDC and CRM2, respectively.

ECS9: Group photo before school dinner at the Château Mme de Graffigny.

2nd High-Pressure Single-Crystal X-Ray Diffraction Summer School

Dominique Laniel, Elena Bykova, Maxim Bykov, Leonid Dubrovinsky, Natalia Dubrovinskaia

The 2nd High-Pressure Single-Crystal X-Ray Diffraction Summer School was held at the James Clerk Maxwell Building of the University of Edinburgh (Edinburgh, Scotland), from July 22nd to July 26th 2024 (https://indico.ph.ed.ac.uk/event/282/overview). The School was supported and approved by the IUCr, through the IUCr Commission on High Pressure. A total of 30 participants from fifteen countries and four continents attended the full week. These participants were provided an accommodation at the University's Pollock Halls. The School was such a vibrant success that we will hold another one next summer, but this time in Frankfurt (Germany)—and certainly upcoming years as well, making it an annual event.

Group picture taken during the School, with participants and lecturers present. The picture was taken in front of the Centre for Science at Extreme Conditions (CSEC) of the University of Edinburgh.

The intent of the School was to train young and established scientists in the recent methodological advancements in high-pressure single-crystal X-ray diffraction. These new developments enable solving and refining crystal structures from tiny micron- to submicron-sized crystallites confined in diamond anvil cells up to pressures of multiple hundreds of gigapascals (GPa). An overview of the necessary fundamental theoretical and methodological principals, including diamond anvil cell preparation, strategy of experiments, laser-heating, introduction to software and SCXRD, were covered through lectures. These were accompanied by thirteen hours of hands-on sessions, where participants were divided into five small groups of six individuals, each with its own instructor, and guided through step-by-step tutorials and examples. At the end of the School, participants were able to perform basic high pressure SCXRD experiments, as well as data processing and interpretation. The lectures and hands-on tutorials were given by a total of nine experts, including three from the United Kingdom, five from Germany and one from the United States, with a woman-to-man ratio of 4:5.

To maximize discussions between participants as well as between participants and lecturers, snacks, lunches and dinners were provided onsite for the complete duration of the School. All participants were requested to bring a poster presenting their research, which were shown and displayed during two poster sessions. Moreover, extracurricular activities took place during three evenings, namely a whisky tasting, a walking tour of Edinburgh and a ceilidh—a traditional Scottish group dancing.

During the last day of the School, the IUCr awardees were given their certificate. The participants were also requested to fill out an online survey to gauge their satisfaction and identify aspects to improve for next editions of the School. Overall, their response was overwhelming positive. Indeed, all 28 participants that took part in the survey said they would recommend the School to others, while 64.3% and 35.7% rated their overall impression of the School as "Excellent" or "Good", respectively. Among all surveyed aspects, the one with the least positive feedback was meals and refreshments, for which 75% of the participants were either "Very satisfied" or "Satisfied", but 25% were "Neutral" or "Dissatisfied". In the future, a different catering company will be used.

Questions and pie chart representations of the answers obtained from the survey filled out by 28 participants at the end of the School.

Given the increasing importance diamond anvil cell single-crystal X-ray diffraction of polycrystalline samples methodology, as well as the very positive feedback received from participants, we are confident that new

participants will attend the next edition in Frankfurt (Germany), which will undoubtedly be just as successful. Looking forward to summer 2025…!

IUCr Young Scientist Awardees (l-r): Benedito Donizeti Botan Neto (Universitat de València, Spain), Xuejing He (University of Tokyo, Japan), Almudena Inchausti Vallés (Complutense University of Madrid, Spain) and Natalia Sacharczuk (Adam Mickiewicz University, Poznań , Poland).

International School on Fundamental Crystallography: Seventh MathCryst School in Latin America - PERU 2024

Justiniano Quispe

The seventh edition of the School of Mathematical Crystallography in Latin America was recently held from August 12 to 16, 2024, at the Facultad de Ciencias Físicas. Universidad Nacional Mayor de San Marcos in Lima, Peru (https://www.even3.com.pe/e/ISFC2024-7MathCrystS). This school is part of a series of fundamental crystallography schools that began 17 years ago at the University of Havana, Cuba, and since been held biennially in various countries across South America, Central America, and the Caribbean. The first school took place in 2007 in Havana, followed by Montevideo, Uruguay in 2010; Uberlândia, Brazil in 2012; La Plata, Argentina in 2014; Havana, Cuba again in 2016; and Bogotá, Colombia in 2018. Unfortunately, the global impact of the SARS-CoV-2 pandemic led to the delay of subsequent schools. The successful realization of the 7th MathCryst School in Latin America marks a significant milestone, signaling the reactivation of this series after more than five years of inactivity.

Inauguration of 7th MaThCryst School in Latin America. From left to right Dr. Arbelio Pentón, Dr. Leopoldo Suescun, Dr. Massimo Nespolo, Dr. Justiniano Quispe, Dra. Marisel Espinoza, Dr. José Niño, Dr. Ángel Bustamante, Mg. María Luisa Cerón, Dr. Mois Arroyo, Dra. María Cristina Nonato y Dr. Carlos Landauro.

The primary objective of this school was to provide training and education to Latin American students and young researchers on the fundamentals of crystallographic symmetry, with a focus on the application of mathematical and computational tools in various fields. Additionally, the school aimed to encourage collaborative work through interaction and the exchange of ideas between course participants and renowned researchers.

Dr. Massimo Nespolo uses the ball to keep the attention of all students.

This year´s school attracted 82 participants, including 64 students with a notable representation from Peruvian institutions. The participants came from countries such as Peru, Ecuador, Colombia, Philippines, Cuba, Brazil, Germany, Spain and France. Efforts were also made to promote gender diversity, achieving a 33% participation rate for women. It is noteworthy that this is the second time the school has been organized by a participant from one of the previous editions.

The inauguration on the first day was led by university authorities from the oldest university in the Americas, founded in 1551. Present were Dr. José Niño Montero, Vice-Rector of Research and Graduate Studies; Dr. Ángel Bustamante Domínguez, Dean of the Faculty of Physical Sciences; Dr. Justiniano Quispe Marcatoma, President of the Organizing Committee; Dr. Marisel Espinoza Suárez, representing the local organizing committee; and Mg. María Luisa Cerón Loayza, who served as the coordinator for gender equality and diversity. The opening lecture, titled “X-ray Crystallography: From Material Science to Drug Discovery,” was delivered by Dr. Maria Cristina Nonato. Subsequently, the lecturers Dr. Massimo Nespolo and Dr. Mois Aroyo presented on various topics including symmetries in crystal families, lattice systems, and crystal systems. On the second and third days, they continued to explore the properties of space groups and their descriptions in the International Tables for Crystallography, incorporating exercises and in-class interactions. They also demonstrated the use of mathematical and computational tools to access crystallographic symmetry information from the International Tables for Crystallography databases.

Dr. Mois Aroyo teaching Space groups and their description in International Tables for Crystallography.

On the fourth day, professors Dr. Arbelio Penton, Dr. Maria Cristina Nonato, and Dr. Leopoldo Suescun covered topics such as Crystallographic Calculations in Reciprocal Space, Introduction to X-ray Diffraction, and Diffraction Symmetry: Space group determination. A poster session was held on the same day, featuring 15 works selected by evaluators from the local committee. Awards were given to the two best posters, which were evaluated by a jury of the school's professors based on their academic relevance.

On the final day, Dr. Gemma de la Flor joined online from Germany for a dynamic session in which students explored various applications of the International Tables-Online server and the Bilbao Crystallographic Server. The closing lecture, delivered by Dr. Maria Cristina Nonato, was titled "Fragment Screening by X-ray Crystallography: An Important Tool to Develop New Therapies Against Infectious Diseases." The week concluded with the presentation of the "School Proceedings" by Dr. Justiniano Quispe, summarizing the events of the week, followed by a musical performance featuring piano and violin by musician Rafael Huaroto Santillán.

Authors and co-authors in the poster session happy to show their work to the attendees

Dr. Allan O. Junio from the Philippines secured first place in the poster session, while Dr. Yonathan Parra from Ecuador earned second place.

The success of this school was largely due to the collaborative efforts of the IUCr Commission on Mathematical and Theoretical Crystallography, in coordination with local Peruvian researchers, and the support of institutions such as International Union of Crystallography (IUCr), National Council of Science, Technology and Technological Innovation (Concytec), the National Program for Scientific Research and Advanced Studies (Prociencia), the Center for Technological, Biomedical, and Environmental Research (CITBM), the Latin American Council of Physics (CLAF), Thermo Fisher Scientific, and the Peruvian Society of Physics (Soperfi).

(Local organizing committee)

25 August 2024

26th Heart of Europe Bio-Crystallography Meeting

Markus C. Wahl

The 26th Heart of Europe Bio-Crystallography Meeting (HEC26) took place from September 26 to 28, 2024, in the historic city of Kraków, Poland. Hosted by the group of Sebastian Glatt and Przemysław Grudnik from the Małopolska Centre of Biotechnology, Jagiellonian University Kraków, the event gathered a vibrant community of structural biologists from across Central Europe. The meeting was attended by structural biology experts from numerous research groups, and the participation of scientists from Austria, the Czech Republic, Germany, and Poland contributed to the lively exchange of ideas.

A total of 121 participants registered for this year's meeting at a spectacular venue, the monumental Forest Hotel on the hill of Przegorzały. The program included 50 talks: the "HEC Lecture" by Arwen Pearson, University of Hamburg, Germany, introductory lectures by three new HEC Groups, 17 scientific talks, and 25 flash talks by PhD and Master's students, as well as four sponsor talks. The opening session featured presentations from the three new HEC groups headed by Krzysztof Brzeziński and Miłosz Ruszkowski from the Institute of Bioorganic Chemistry Polish Academy of Science and by Michał Szymański from the University of Gdansk, Poland.

Over the course of the three-day program, fascinating research into the molecular mechanisms of biomolecules and their complexes as well as updates on state-of-the-art structural biology methods were presented. A highlight of the event was the HEC Lecture, delivered by Arwen Pearson, who captivated the audience with an overview on recent advancements in time-resolved macromolecular serial crystallography.

Participants at the 26th Heart of Europe Bio-Crystallography meeting in Krakow, Poland.

Several companies (Arinax, CGF Biotec, Cytiva, Dectris, Dunn, Formulatrix, Jena Bioscience, NanoTemper, PHCbi, Proteros, Rigaku, Sarstedt, Selvita) participated in the event, generously supporting the meeting

through presentations and sponsorships. Their involvement introduced the latest technological advancements to the structural biology community.

The meeting awarded prizes for outstanding presentations. Jana Skerlová from the group of Pavlína Maloy Řezáčová, Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, won the “HEC Prize” for the best full talk, with Evangelia Nathanail (group of Oliver Daumke, Max Delbrück Center for Molecular Medicine) and Mathias Schenk (group of Miriam Linnert, Fraunhofer Institute for Cell Therapy and Immunology) also being recognized for their excellent contributions. David Speck from the group of Patrick Scheerer, Charité - Universitätsmedizin Berlin, received a special distinction. The prize for the best flash talk was awarded to Duc-Anh Nguyen from the group of Milton Stubbs, Martin-Luther-Universität Halle-Wittenberg.

HEC26 Prize winners: Duc-Anh Nguyen (second from left), Mathias Schenk (third from left) Evangelia Nathanail (third from right), and David Speck (second from right) with organizers Przemysław Grudnik (left) and Sebastian Glatt (right). Jana Skerlová, who was awarded the prestigious “HEC Prize” for her outstanding presentation, was unable to participate in the group photo.

A social afternoon offered opportunities for relaxed discussions amidst nature, on a guided hike to Piłsudski Mound, and science, on a tour of the SOLARIS Synchrotron. The lively HEC Party at the Forest Hotel on Friday night created a warm and festive atmosphere, encouraging both formal and informal exchanges well into the evening.

Recreational hike to the top of Piłsudski Mound (left) and visit at SOLARIS National Synchrotron Radiation Centre (right)

The success of HEC26 sets the stage for the 27th Heart of Europe Bio-Crystallography meeting, which will take place in Halberstadt, Germany, from September 25 to 27, 2025, and will be organized by the group of Markus Wahl, Freie Universität Berlin. We look forward to another inspiring gathering next year.

12th Training Course on Symmetry and Group Theory (A Student’s Perspective)

James Steele

Group photo of the 2024 English basic course.

I first heard about this course from a colleague, an experienced experimentalist in diffraction-based characterisation, at the end of a long day of working together on a structural refinement that was proving troublesome. Like many PhD students in solid-state chemistry, or condensed matter physics (the same thing in my opinion), I had studied x-ray diffraction, and a small amount of group theory through the lens of molecular symmetry, during my undergraduate degree. “Excellent!” I thought, “I am fully prepared to tackle complex structural characterisation of novel materials and their phase transitions, based on symmetry relations, group theory, and space groups…” Of course not.

When I started my PhD, I had a limited grasp of what a space group even was. Rietveld refinements were a wonderous black box that you fed data, then marvelled at the structure that popped out (which was, more often than not, an unphysical mess). Programs such as TOPAS, GSAS, and FullProf are incredibly powerful and valuable tools to the experimental structural scientist. However, they are infamously poor at dealing with symmetry, particularly in the hands of a student with limited understanding of the underlying concepts.

“Garbage in, garbage out.”

This is of course, not for lack of trying. There are numerous resources (both online and in print) for the learning of crystallography. However, these can often seem impenetrable, riddled with confusing conventions, field specific jargon, and mathematics one may not have encountered in many years (if at all). Further, experimentally focused research groups don’t necessarily have theoreticians on hand, or experimentalists with the specific expertise (or free time) required to build up the knowledge and confidence of new students. This

often adds up to make crystallography seem insurmountable to the budding crystallographer, and is one of the main reasons I was so excited when I heard about this course.

The training course on symmetry and group theory has run for many years now, primarily in Japanese, but additionally in English since 2019, in response to the demand shown by students who are not native Japanese speakers. Primarily, the course was motivated by the many obstacles commonly faced by early career researchers, owed to the somewhat limited crystallographic training provided by (already busy) undergraduate curricula. The course is hosted at the High Energy Accelerator Organisation site in Tsukuba (KEK), and is provided free of charge.* It is sponsored by the Crystallographic Society of Japan, the Institute of Materials Structure Science, and supported by many other Japanese scientific societies and associations. From 2019, it has been certificated as a common lecture by SOKENDAI (The Graduate University for Advanced Studies). All lectures and exercises are delivered by Professor Massimo Nespolo (Université de Lorraine, France).

Unlike any other course I have previously studied, which required students to make unsatisfying concessions, accept axioms without explaining how they arise, and learn relations by rote, Professor Nespolo starts truly from first principles, with basic algebra. This lays necessary foundations, which are built up procedurally, and developed throughout the course into a rich understanding, with many satisfying relations that become apparent as more advanced concepts are introduced. Further, the opportunity to participate in frequent guided exercises, where the taught concepts are explored in greater detail, allows participants to really absorb the content of the course and solidify their understanding. The condensed nature of the course facilitates a breadth of topics to be taught, starting from the required fundamental algebra, building to point/space groups and their constituent properties from a geometric/graphical perspective. This then facilitates understanding of the physical meanings of the following crystallographic calculations via matrices, and how all of this adds up to macroscopic properties and phase transitions in the materials which are the subject of our research.

Participants receive certificates for completing the course.

I look forward to applying what I have learned regarding fundamental crystallographic symmetry, and group-subgroup relations, to solving the remaining novel structures throughout the Na1-xNiO2 phase-space, and would gladly participate in the advanced course (provided my Japanese improves over the next few years)! I strongly recommend this course to any other students who have struggled to understand the underlying crystallographic concepts which inform the necessary decisions required to devise physically meaningful (and symmetrically sensible) Rietveld refinements for novel structural elucidation.

James Steele is a PhD student co-supervised by Prof. Siân Dutton and Prof. Dame Clare Grey at the Cavendish Laboratory and Yusuf Hamied Department of Chemistry (University of Cambridge, UK).

* It is unfortunately not currently possible to provide financial support for travel, which is probably the main factor limiting participation by students outside of Japan. I was fortunate to receive a professional development grant from my funder (EPSRC NanoDTC), without which I could not have taken part in the course.

Inaugural MSI Crystallography Workshop at Howard University with the University of the District of Columbia and NSF's ChemMatCARS

Timothy R. Ramadhar, Yu-Sheng Chen, Raymond J. Butcher, Steven P. Cummings, Xueqing Song, Matthew V. Tirrell, Richard B. Fenner

Engaging the next generation of synchrotron X-ray crystallography researchers is of the upmost importance to sustain and build the future of this critical field. The universities that train experimentalists and the national facilities that harbor the infrastructure for cutting-edge research recognize their roles and responsibilities to grow the crystallographic discipline. Exploring partnerships between minority-serving institutions (MSIs) and national facilities can establish pathways to support this effort. These partnerships also promote further diversification in science, technology, engineering and mathematics (STEM), leading to a stronger national workforce.

Participants at the first MSI Crystallography Workshop in Howard University, Washington, District of Columbia, USA

This first-of-its-kind workshop was co-organized by HU, UDC, and NSF's ChemMatCARS and was funded by a National Science Foundation Partnerships for Research and Education in Chemistry (NSF PREC) Planning Grant. Timothy Ramadhar (HU and NSF PREC Planning Grant Principal Investigator) and Yu-Sheng Chen (University of Chicago and leader of the NSF's ChemMatCARS Advanced Crystallography Program) collaborated in organizing this workshop. While planning an agenda that would engage attendees, Ramadhar and Steven Cummings (HU and NSF PREC Planning Grant co-Principal Investigator) also ensured that attendees would be well nourished with catered meals throughout the entire workshop.

Welcoming remarks were delivered by Ramadhar, Xueqing Song (UDC) and Raymond Butcher (HU and NSF PREC Planning Grant co-PI). Both Song and Butcher provided background and current information on the UDC Division of Science and Mathematics and the HU Department of Chemistry, respectively. Matthew Tirrell (UChicago and NSF's ChemMatCARS PI) presented a history and overview of the NSF's ChemMatCARS facility along with the beam time application process. Butcher subsequently introduced single-crystal X-ray diffraction and discussed his collaborative research on spin crossover complexes with Greg Brewer (Catholic University of America). Chen concluded the morning session by presenting details of NSF's ChemMatCARS Advanced Crystallography Program and its technical capabilities.

Jennifer Swift (Georgetown University) presenting a scientific lecture on biogenic uric acids

Tieyan Chang (NSF’s ChemMatCARS) showing attendees how to integrate reflection data in Bruker APEX

Practical sessions on analyzing data from single-crystal X-ray diffraction experiments were held after lunch on the first workshop day. Pierre LeMagueres (Rigaku Americas Corporation) gave a virtual presentation introducing attendees to crystallographic data processing using CrysAlisPro. This software is used for the in-house Rigaku Synergy single-crystal X-ray diffractometers at HU and UDC that were funded by the National Science Foundation Major Research Instrumentation grants program (HU: DMR-2117502 (PI Ramadhar), UDC: CHE-2117621 (PI Song)). Next, Tieyan Chang (NSF's ChemMatCARS) gave a walkthrough on processing crystallographic data using the Bruker APEX software, which is used extensively at the beamline. In the sessions for CrysAlisPro and APEX, attendees learned how to perform reflection indexing, reciprocal lattice examination, integration, absorption correction, and space group determination. Jinxing Jiang (NSF's ChemMatCARS) discussed SHELX and Olex2 software programs, which can be used together for structure solution, refinement, finalization, and visualization. Before dinner, the practical sessions concluded with a hands-on tutorial where smaller group attendees had the opportunity to solve and refine sets of X-ray diffraction data collected at the NSF's ChemMatCARS beamline.

After the first day, all attendees were strongly encouraged to put what they learned into practice and apply for beam time at NSF's ChemMatCARS.

The second day featured an extensive listening session with undergraduate and graduate students at HU and UDC followed by a farewell lunch. Students had the opportunity to share their journey in STEM, noted why they chose to attend HBCUs, and presented ideas about how to increase student recruitment and retention in science. The workshop organizers left this session with valuable insights on ways to develop an impactful partnership between HU, UDC, and NSF's ChemMatCARS for a future submission to the NSF PREC grant program.

The organizers are in the planning stages of hosting another crystallography workshop this year at NSF's ChemMatCARS, which is being equipped with new capabilities along with a second beamline via a canted undulator to utilize a brighter X-ray beam (approximately 1,000-fold at most energies) afforded through the recent Advanced Photon Source upgrade. Improvements to the Advanced Crystallography Program as a result of the upgrade include the ability to perform small-molecule serial diffraction, resonant diffraction applicable to all transition elements for element-specific location and redox states, and high-throughput processing of microcrystalline samples through automation involving the use of a data collection robot that can be accessed via mail-in service.

This workshop was financially supported solely by the National Science Foundation through a PREC Planning Grant (CHE-2334957). The NSF's Chemistry Division (CHE) PREC program is dedicated to fostering, establishing, and enhancing collaborations between MSIs and CHE-supported facilities, centers, and institutes. Its main goal is to increase recruitment, retention, and degree attainment among underrepresented groups in chemistry. The program concurrently aims to boost outstanding research and educational initiatives that reinforce these partnerships. Underrepresented minorities supported through this program include Blacks or African Americans, Hispanics or Latinos, American Indians, Alaska Natives, Native Hawaiians, Other Pacific Islanders, and persons with disabilities. The PREC Planning Grant program that has funded this workshop aims to catalyze collaborative partnerships with CHE-supported facilities, institutes, and centers to facilitate the creation of competitive proposals for the PREC program in future solicitations. NSF's ChemMatCARS, a CHE-supported center, has established scientific partnerships with several MSIs. NSF's ChemMatCARS is supported by the Divisions of Chemistry and Materials Research of the National Science Foundation under grant number CHE-1834750.

International XRD excites: Non-Ambient XRD and Beyond Symposium

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Graz University of Technology and Anton Paar hosted the 1st International XRD excites Symposium

In July 2024, Anton Paar and the Institute of Inorganic Chemistry at Graz University of Technology successfully hosted the first edition of the XRD excites: Non-Ambient XRD & Beyond Symposium. More than 90 participants from over 20 countries gathered in the Austrian city of Graz for the meeting.

The event brought together an array of users from the field of X-ray diffraction (XRD) and non-ambient XRD, with the aim of encouraging multidisciplinary cooperation and an open exchange of experience between renowned scientists, young scientists and industry professionals. In this unique setting, researchers with different scientific backgrounds – ranging from materials science, crystallography, geology and mineralogy to energy storage and conversion – got together, learned about their individual progress and challenges in the application of non-ambient XRD and other areas, and sparked new ideas for their own research.

The symposium featured 23 high-level presentations from keynote speakers such as Claudia Weidenthaler from the Max-Planck-Institut für Kohlenforschung on in situ studies of energy materials, Monica Dapiaggi from the University of Milan on coupling laboratory and synchrotron NA-XRD data, Scott Misture from Alfred University on in situ powder XRD and high-resolution XRD studies of oxides, David Walker from the University of Warwick on non-ambient XRD analysis in the laboratory, Rémy Guillet Nicolas from CNRS LCS – ENSICAEN on small-pore zeolites, Volker Kahlenberg on non-ambient powder XRD studies in mineralogy and geology, Vishnu Shanker from NIT Warangal on graphite-based carbon nitrides, and Stefan Weber from Abbvie Germany on the use of non-ambient XRD for biological drug development.

A poster session offered an opportunity to discuss the latest scientific findings in more detail and initiate possible future collaboration projects between the participants. Last but not least, participants were given a deeper insight into non-ambient XRD in a special workshop that also included hands-on sessions with different types of non-ambient XRD attachments.

It wasn’t all work though!

A guided city tour in Graz – a UNESCO World Heritage Site – and company tour at Anton Paar ended with a visit of the Anton Paar Sudhaus brewery, where head brewmaster Gebhard Sauseng explained the details of the brewing process. Of course, no brewhouse tour would be complete without the option to also sample the beers fresh from the tap. From there, it was only a few steps to the conference dinner.

With this first XRD excites: Non-Ambient XRD & Beyond Symposium, Graz University of Technology and Anton Paar – together with all the participants – placed impressive emphasis on non-ambient X-ray diffraction in a city that has a long history and deep connection to the field.

For more information please click here:

https://www.anton-paar.com/corp-en/xrd-excites/?utm_source=IUCr_Newsletter_pr&utm_medium=media&utm_campaign=hq_education-research&utm_content=C-00066872

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