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So long ... till Melbourne!

Hanna Dąbkowska

It is summer already and today we are only 50 days from the beginning of the 26th IUCr Congress in Melbourne. I often visit the Congress website and smile back at Michael Parker, the Chair of the Organizing Committee, and Brendan Kennedy, the Program Chair. They both look relaxed and in a very good mood, but it is well understood how much work and stress lies behind the organization of such an event. Unlike all the other IUCr Congresses, the Melbourne teams had only two years to prepare the venue, usually prepared in three. It is a very big difference and the effort is very much appreciated.

This is my eighth and last Letter. I am grateful to those of you who have commented on my Letters and encouraged me to continue. In these Letters I have tried to highlight what has been happening in different parts of our community.

Staying positive is not easy in these challenging times – but now I realize that it never was. Natural cataclysms and man-made wars and conflicts add to the stress we all have to deal with. Fortunately, with COVID-19 now in the back mirror, we can concentrate on implementing the vision for the future. This is what the IUCr Commissions will be suggesting during their discussions with the IUCr Executive Committee (EC) in Melbourne. This is what the IUCr General Assembly (GA) will be discussing as well.

To understand what is happening around us, the EC will also be listening to the reports of IUCr Representatives to other organizations (ISC, CODATA, COSPAR, IOCG, IUPAC, ICTNS, ISO). All these organizations face similar challenges to those faced by the IUCr – we all have to promote new, emerging science and embrace different ways to approach research, learning and teaching. We have to encourage the inevitable change of generations and the important fact that many more people from around the world are making their input There is a lot of unknown in the future: How should ethical problems be addressed? Will artificial intelligence help in solving today's questions? Are we creating a better world for the future of humanity? Are we moving too fast? Too slow? For sure crystallography is in the background of many innovations. Are we only solving the imposed problems or are we being really creative like our Award winners, proposing new questions (and answers) for science? How are we dealing with new (and old ...) challenges? How can we stop “for-profit” journals taking a bite from our income or some pseudo-scientific groups announcing “crystallographic” meetings in suspiciously attractive places? No President or EC or even GA can answer these questions. But we all have to be aware of them and think about them.

Fortunately, the IUCr is blessed with an active, international community of leaders in many corners of science, a loyal staff and an excellent reputation. Our schools, conferences, workshops and OpenLabs teach new generations of structural scientists, providing a good background and understanding of crystallography for future leaders in such diverse areas as solid-state physics, materials science, chemistry, structural biology and pharmaceutical research. We are well positioned to be successful in the near future and in the next 75 years of this organization.

Of course to achieve it all, the IUCr needs a lot of support from all of us volunteers: teachers, lecturers, organizers, leaders. Aside from our “day jobs”, we work to prepare meetings, schools, congresses. We dedicate our time assessing applications, refereeing papers, attending meetings around the world.

Being a scientific union we try to be as non-political as possible but at the same time we have to declare our position in addressing injustice in the world and promoting a better and safer environment for our meetings and well beyond. We have no direct influence over devastating forest fires or tornadoes around the world but we can actively help to develop vaccines and cures for known and not so well known diseases. We are essential in the search for new, technologically important materials, assessing resources and in investigating the behavior

of materials in extreme conditions – opening the door for limitless future explorations. We understand our own strengths, but more action is needed. We need to project our values to other communities, so the name Crystallography means something. It meant a lot 75 years ago, it meant progress. Now it is time to decide – are we sticking to this name or are we changing it to something more appealing to the new generation – like Structural Science perhaps?

To be able to proceed and promote our research we need to actively support IUCr Journals. This means publishing our best results in these journals and confirming that they are available in our universities and company libraries. I stressed many times that unlike our main competitors, all the surplus income generated by our journals goes to supporting future crystallographers to attend schools and meetings.

I apologize for not visiting as many conferences and meetings as some of my predecessors. This was partially because of the lingering COVID threat at the beginning of my term. Despite many invitations I did not manage to attend any African meetings in person, but I am extremely happy to be the President connecting the African Crystallographic Association (AfCA) to the IUCr. And I am immensely grateful to the many of you who worked so hard to achieve it. I am very sorry that Professor Claude Lecomte, Chair of the Steering Committee for the IUCr Crystallography in Africa initiative, is not able to join us in Melbourne. I hope he will come and celebrate the African success with us at the next Congress in Calgary.

And here I would like to end my Letters. I want to thank you all for trusting me with this fascinating job and I am also very grateful to a long line of people who helped me over these two years and who helped this Union to flourish.

I am looking forward to seeing many of you in Melbourne, please stay safe.

Continuing support for Ukrainian scientists

Marek Konarzewski

Dear Professor Dabkowska, I would like to express our sincere thanks for your continued cooperation with our Academy. We are particularly grateful for your support of our programs for Ukrainian researchers fleeing war zones.

The Polish Academy of Sciences has taken a number of steps to support scientists from Ukraine. As early as 1 March 2022, we launched a short-term program to enable scientists who had left Ukraine to conduct research in the institutes of the Polish Academy of Sciences. In total, we hosted 192 Ukrainian fellows for up to 10 months. The total expenditure for this purpose amounted to 5.8 M PLN. Nearly 84% of PAS fellows were women scientists, which makes our programs one of the most notable endeavors also in this respect.

Throughout the year, we organized 9 training opportunities in English and Ukrainian addressed to Ukrainian scientists. In total, nearly 600 participants attended these workshops.

All of the above would not be possible without intensive cooperation between the academies and international scientific organizations in Europe and beyond. We thank you for all your support and assure you that in 2023 our Academy will continue to pay our membership dues as we always did in the past.

Yours sincerely, Marek Konarzewski

Editorial

Mike Glazer

As we are now in summer here in Europe, we are turning our thoughts to the IUCr Congress to be held in August in Melbourne, Australia, where it will be winter. Our international congresses take place every three years and always attract a large number of participants. The IUCr Congress is a great place to be as this is where you can hear about the vast range of topics covered by Crystallography, meet others, and often form valuable collaborations. Despite its time of year, the Melbourne arrangements look great, and I look forward to attending. I intend on the way to spend three days in Singapore, one of my favourite stopovers, before flying on to Melbourne, first of all for the IUCr Finance Committee. By the time this issue of the Newsletter appears, the Congress will probably be in full swing.

Our subject, Crystallography, one of the oldest of scientific disciplines, continues to throw up surprises. For most of the time, it was accepted that what defines a crystal is connected with the concept of periodicity, namely that groups of atoms repeat in an ideal crystal in much the same way as one can tile a floor with single shapes (or monotiles). This concept of periodicity led crystallographers long ago to believe that the symmetries of these shapes must be confined to 2, 3, 4, and 6 fold rotations (the so-called Crystallographic Restriction Theorem). Then, along comes Dan Shechtman, who spoilt all our cherished views when he found that crystals do exist with 5 or 10-fold symmetries, a discovery that earned him the Nobel Prize in 2011. This discovery, which is now accepted, but admittedly after some resistance, raised the question of how you can tile a floor without leaving gaps using local 5-fold symmetries. The famous Penrose tiling (https://en.wikipedia.org/wiki/Penrose_tiling) is an example where this problem is solved by using two shapes. The result is what is called an aperiodic array, i.e., one that never repeats, but becomes periodic in a higher-dimensional space.

Mathematicians are quite happy with that, even though we may find it challenging to get our heads around higher-dimensional space! Now since then, mathematicians have been wondering if it is possible to have a tiling still consisting of a single shape that is infinitely aperiodic. Such a shape has been labelled the “Einstein” shape. But then, to everyone’s surprise, just last year, a retired print technician, David Smith, discovered such a shape based on divisions of a hexagonal periodic array. This shape has now been called the “Hat”. Symmetry enthusiasts have become so excited by this discovery that they have convened a special conference in Oxford in July called the “Hatfest”, celebrating the discovery of an aperiodic monotile. The conference will include some of the world’s leading authorities on symmetry. I hope in the next issue of the Newsletter, to have a report on the meeting.

Why is this important for us humble crystallographers? Well, the existence of aperiodic crystals found by Shechtman meant that we have had to revise our long-held understanding of crystals. So, is it possible that genuine aperiodic crystals may exist out there with symmetry using monotiles? That an amateur can make such a discovery shows that we don’t have to be experts in Crystallography to make important contributions to mathematics and science. It even made the national press! By the way, you can experiment with the “Hat” yourself at <https://cs.uwaterloo.ca/~csk/hat/app.html>.

In this issue of the Newsletter, we have a number of contributions. Mohan Bhadbhade (ref) considers the importance of molecular shapes and how they stack together in a crystal. Piero Macchi raises an interesting question in a letter about who actually “owns” crystallography – well worth a read. Do send in any thoughts yourself.

David Brown, well known for his work on bond valence theory, has provided an article explaining the concept and how it relates to the so-called First Rule of bonding due to Linus Pauling (ref). Also, as has become something of a tradition now, the Hargittai’s have submitted another nice article (ref), this time on the wonderful earth science museum based within Moscow State University. Do take a look at their introductory comments on the terrible situation right now between Russia and Ukraine.

Also, take a look at the “Golden Oldies” where 10 significant past publications in Crystallography have been highlighted (ref).

As usual, I have the sad task of reporting on the deaths of several colleagues, well known to many of us. Uri Shmueli (ref) was a good friend of mine. We first met at a European Meeting, and we spent the day together, walking and chatting. He told me the story of his childhood during the Second World War in his home city of Kraków, Poland, and how he experienced concentration camps such as KZ Mauthausen (see his memoir at <https://doi.org/10.1107/S2053273323005405/es5051sup1.pdf>). I recall saying to him that he should return to Poland to see how it had changed, but his bad experiences from that time were such that he was afraid of doing that. However, several years later, when we had the European Crystallography Meeting in Kraków, there I saw him in a restaurant, beaming from ear to ear. He had taken my advice and had been visiting all his old haunts, including where he used to live. He found everyone to be kind and welcoming, and he was generally having a great time.

We also have an obituary on Jimpei Harada (Japan), well known for his work on diffuse scattering from materials undergoing phase transitions. Because of a common interest in the structures of perovskites, I first came to know him when he was working on electron diffraction with the great Goro Honjo in Japan. The formidable André Authier, one-time President of the IUCr, was one of the world's leading greatest experts in the dynamical theory of diffraction. Much decorated, he was especially proud of his achievement in receiving the Légion d'Honneur. His book on the History of Crystallography (Early Days of X-ray Crystallography - Hardback - André Authier - Oxford University Press (oup.com)) is a significant contribution and I strongly recommend it to you.

Others who have left us and are in this issue are Aldo Craievich (Argentina/ Brazil), Carles Miravittles (Spain), and David Watson (United Kingdom), all well-known in our community.

Who owns crystallography?

Piero Macchi

This, to me surprising, question was asked during the ECA lunch webinar #20 by the lecturer, Dr Claire Murray from Diamond Light Source. The lecture was thought-provoking, and this was the first provocation. However, the true shocks were the answers. Many people wrote that it belongs to “everybody” (the answer expected by the lecturer). Few, including myself, wrote “nobody”. Some started kidding, with answers like “Mike Glazer”! I have a long-term strong admiration for Mike, as a scientist and intrepid aviator, and I found myself thinking that if he really owned it, crystallography would probably be in a much better state.

Others wrote “Laurence Bragg”. Not so sure if that was also a joke, in keeping with the common misconception of considering crystallography synonymous with X-ray diffraction and therefore recognizing Bragg as the father of crystallography, whereas he certainly was not. There is an additional misconception, which is that the science produced by someone belongs to that person.

Let us come back to “everybody” and “nobody”, though. While Claire answered me that this is basically the same, I strongly disagree. Saying that everybody owns crystallography means that none has a golden share. Saying that nobody owns it means that none has a share.

So the question is: can anyone own (a) science?

No!

The United Nations Educational, Scientific and Cultural Organization (UNESCO) has included in the list of Intangible Cultural Heritage a number of arts and techniques, but has not included any science and will not include it even though the list is growing at a rapid pace.

Why?

Because there is an enormous difference between paternity/maternity and ownership. To me, saying that someone owns science is almost like saying that someone owns a human being. Nonetheless, every human being has a mother/father. When a mother or a father says “my son/daughter” does not imply his/her possession (and when this unfortunately occurs, it is a crime). To avoid the ambiguity, though, it would not help saying that the son/daughter is owned by everybody!

Similarly, to avoid the ambiguity in the pronouns (I, we, our group did this research...) or in the adjectives (my, our science...) it does not help saying that the science is owned by everybody.

While this could be merely semantic, the next step in Claire's presentation was that "taxpayers" could be science owners because of their financial contribution. Now it becomes clear that it is not just semantics. Apart from the fact that "everybody" and "taxpayers" are not synonymous.... the implication of taxpayers owning science is extremely dangerous.

Let us see it from a different perspective. Taxpayers in some (developed) countries contribute with their taxes to the national health system. Does it mean that they own the national health? No, at most, they collectively own hospitals, medicines, and instruments, but not the health.

The same holds true for culture. Thanks to taxpayers, we build schools, libraries, research centers and universities; we buy books, instruments, chemicals, and software. This does not mean that taxpayers own the culture, the ideas exposed in those books, the knowledge produced with those items, in other words, the science. If that were so, research would no longer be free, the worst sin that scientists could commit (see Bertold Brecht, *Lebens des Galilei*).

This is the reason why I think that messages like that launched in the ECA webinar, and often proposed by politicians and decision-makers, strongly and negatively affect scientific research, in crystallography as well as in any other science. I am surprised that many colleagues do not realize this threat, and I sincerely hope that they would reconsider their answers (or better that they would consider the title question to be not acceptable at all).

Science progresses because research is free, and research is free because nobody owns science.

I thank A. Guagliardi, N. Masciocchi, V. Meille, and A. Sironi for helpful discussion.

Golden Oldies and their continued role in education

Chiara Massera and John R. Helliwell

Acta Crystallographica Section E: Crystallographic Communications has recently launched a special virtual issue on Modern approaches and tools for teaching crystallography (edited by G. Diaz de Delgado and S. Perkin), introducing a new category of articles aiming at education matters, including "experiences of teaching in a pandemic and accessing diffraction equipment remotely, as well as practical advice on all aspects of crystal structure determination" (read the Foreword here).

Whereas Acta E's education articles focus particularly on chemical crystallography, our paper, which highlights ten seminal crystallographic articles, is obviously much broader, being across the science disciplines and also including the philosophy of science (Massera & Helliwell, 2023).

We should explain first why we wrote this Golden Oldies article. Quoting from it: "One of us (CM) had the idea and invited JRH to join in. We had already discovered our similar approaches to our science, of using multiple methods to move beyond the precision of one method alone (crystallography) and reach accuracy when we both taught at the European Crystallography School 6 ('ECS6 Budapest'). Yet our areas of science were distinctly different, smaller and bigger molecules, respectively, and thereby nicely complementary for this article. The choices of these publications are inevitably our personal ones. We first opted for those authored only by individuals who are no longer with us. This is a neat mechanism to minimize the risk of losing our friends. Secondly, a maximum of ten articles is going to be woefully inadequate, so we foresee a series of future articles from colleagues who will make their own top ten selections. As our overall aim is education, with a historical focus, we draw attention to the article by Jenny Glusker (1998) 'The teaching of crystallography: A historical survey'; her selection of references provides an independent suite of examples". For each of our choices, we created a new title that emphasizes how the paper's importance worked out from a present-day perspective and added a brief biographical sketch of the authors. We dedicated our paper to the memory of Olga Kennard for her contributions to disseminating quality data in structural science.

It became clear to us from the reactions of the editor, Graciela Diaz de Delgado of the Universidad de Los Andes Mérida in Venezuela, and the referees that they rather liked our article. That said, we did have to respond to some obviously learned comments from all three! Also, as one of us is on Twitter (@HelliwellJohn), the tweets about our article coming online attracted a lot of likes (>100) and views (>9000). Then there was an enthusiastic note about it on LinkedIn. At this point, thanks are due to the IUCr Newsletter Editor, Mike Glazer, for inviting us to write a short note to highlight our paper.

The ten articles we selected, following a historical timeline, are as follows: Ewald (1969, but which is really 1912 to 1914) Reciprocal space and Ewald's sphere W. L. Bragg (1913) The first X-ray crystal structures Lonsdale (1929) The determination of the planar structure of benzene Banerjee (1933) The first description of a direct method of phasing Megaw (1934) The nature of ice and the importance of collecting crystals in their mother liquor Bernal & Crowfoot (1934) The initiation of protein X-ray crystallography Hughes (1941) The first least-squares refinement of a crystal structure against its X-ray diffraction data Bijvoet et al. (1951) Determination of the absolute configuration of optically active compounds by means of X-rays Okaya & Pepinsky (1956) Solution of the phase problem by altering the X-ray wavelength Coppens (1977) Charge density analysis to elucidate the nature of chemical bonding It proved a very interesting commission to write this article. Overall, we sought to describe where in the philosophy of science each article fitted. A paradigm shift, maybe? We assigned this accolade to W. L. Bragg and his 1913 paper on the alkali halide crystal structures (Fig. 1).

Figure 1. The three-dimensional structure of the alkali halides (Fig. 10 in Bragg, 1913).

Mainly we thought our chosen articles were examples of incremental science, although rather large increments and maybe even leaps forward. They were articles that were examples of science pull, even well ahead of their time, as well as technology push. We tried to convey the scientific context in which all this crystallographic research was conducted, and we also noticed the importance of community agreed standards, i.e. consensus, such as the IUCr checkCIF and the PDB Validation Report procedures. These had been developed by extensively discussing topics and challenges together in the IUCr Journals and the IUCr Commissions, as well as the PDB's Expert Advisory Groups.

Suffice to say we hope that you enjoy our article.

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AlphaFold and the future of structural biology

Randy J. Read, Edward N. Baker, Charles S. Bond, Elspeth F. Garman and Mark J. van Raaij

The landscape of structural biology changed dramatically in 2020 with the emergence of the second version of the AlphaFold protein structure-prediction program (Jumper et al., 2021). Since then, structural biologists, and the many other scientists whose research is informed by knowledge of macromolecular structure, have scrambled to adapt. Much of the hype in both the scientific literature and popular media has indeed been justified: the current version of AlphaFold is astonishingly powerful, and it would be foolish not to make full use of it. Unfortunately, recent anecdotal reports suggest that some scientists reviewing grants and papers believe that AlphaFold is so powerful that it has made experimental structural biology redundant. There is clearly still a need for education about the strengths and weaknesses of current machine-learning methods for protein structure prediction, and the essential role that remains for experiment.

The advance in AlphaFold was unveiled at CASP14, the 14th edition of the Critical Assessment of protein Structure Prediction. For the first time in the history of CASP, the best models of protein targets were judged as being competitive with experimental structures in their backbone accuracy, almost independent of the difficulty of the modelling problem (Kryshtafovych et al., 2021). Since then, other powerful machine-learning algorithms for structure prediction have emerged, including the first (Baek et al., 2021) and second (Baek et al., 2023) versions of RoseTTAFold, ESMfold (Lin et al., 2023) and OpenFold (Ahdritz et al., 2022), an open-source reimplementation of AlphaFold including training code.

Within half a year of CASP14, the AlphaFold algorithm was made freely available through Google Colab notebooks, including a community-developed version (Mirdita et al., 2022). Pre-calculated structures of a large collection of proteins from important genomes were made available through the AlphaFold Database at the European Bioinformatics Institute (Tunyasuvunakool et al., 2021), which has since been expanded to include about 200 million proteins representing most of the UniProt database (Varadi et al., 2022).

Structural biologists quickly embraced the advantages that these models bring (Perrakis & Sixma, 2021), including insights into improved construct design, the generation of compelling hypotheses about interacting proteins or domains, and the acceleration of structure solution by molecular replacement (Millán et al., 2021) for crystallography or docking for electron cryo-microscopy (cryo-EM). A particularly notable example was integrative modelling of the nuclear pore complex by combining AlphaFold (Jumper et al., 2021) and RoseTTAFold (Baek et al., 2021) models with cryo-electron tomography and complementary data (Mosalaganti et al., 2022).

Most structural biologists are aware that the models are not actually as accurate as experimental structures. The backbone accuracy measured in CASP does not ensure the accuracy of all coordinates including side chains. An objective evaluation of how well different models explain experimental diffraction data showed that experimental structures from alternative crystal forms (in spite of different crystal-packing interactions) are generally better than AlphaFold models (Terwilliger et al., 2023). It has also been reported that AlphaFold models perform less well than experimental structures as targets for the computational docking algorithms used in drug design (Karelina et al., 2023).

It is also important to remember that multi-domain targets in CASP are subdivided into 'evaluation units' when predictors fail to predict their relative orientations (Kinch et al., 2021). Many AlphaFold models, including those submitted to CASP14, indeed have large errors in the relative orientations of domains.

The authors of AlphaFold acknowledge its limitations, and one of the great strengths of AlphaFold is its ability to assess its own accuracy: the predicted aligned error (PAE) matrix presents clear warnings when relative domain orientations are uncertain, and the predicted value of the local distance difference test or LDDT (Mariani et al., 2013) statistic (pLDDT) correlates rather well with the actual local model accuracy (Jumper et al., 2021).

The most serious limitations of AlphaFold and other machine-learning algorithms for structure prediction arise from the fact that they are based on learning patterns and know almost nothing about physics and chemistry.

They can generate a single structure that is most consistent with the patterns they know about, but not a collection of alternative conformations that are influenced in their relative stability by factors such as pH, temperature or the binding of ions, other ligands or other proteins. For the foreseeable future, we will certainly need experiments to assess these effects. In addition, variants with amino-acid substitutions will satisfy the same patterns, even though such substitutions may destabilize the protein or change its conformation. Nonetheless, other algorithms exist that can use the AlphaFold model to predict the effects of variants on stability as accurately as with an experimental structure (Akdel et al., 2022).

One of the most powerful aspects of experimental structural biology is the discovery of the unexpected, including the discovery of obligate cofactors and specific metal ions in structures, as well as structurally important post-translational modifications, including various kinds of spontaneous chemical cross-linking such as is observed in fluorescent proteins. Crystallography and cryo-EM will also give an answer to the question of stoichiometry of a homomer (or heteromer), while AlphaFold, despite valuable developments in multimer prediction (Evans et al., 2022), still requires hypothetical stoichiometries to be tested.

Papers describing macromolecular structure-prediction algorithms and their use are welcome in the relevant IUCr journals: Structural Biology (Acta Crystallographica Section D), Structural Biology Communications (Acta Crystallographica Section F) and IUCrJ. For new structures, authors should bear in mind that the use of predicted structures as molecular-replacement models has already become standard practice, and papers describing the resulting structures must make new contributions to our biological understanding.

The field of structural biology and the nature of its challenges has, for the second time this century, undergone a major change. The resolution revolution in cryo-EM has allowed previously intractable systems to be studied at resolutions permitting 'de novo' model building, but it has not made X-ray crystallography or NMR spectroscopy redundant (Kühlbrandt, 2014). In the same way, the major leap in structure prediction that AlphaFold has spawned does not mean that experimental techniques have suddenly become meaningless.

As other commentators have said (Perrakis & Sixma, 2021; Kleywegt & Velankar, 2022), this change is accelerating progress and bringing us more power to address deeper questions, and we should embrace the new possibilities.

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Mapping structural correlations in real space

Ray Osborn

The very first issue of *Acta Crystallographica* contained an article by Kathleen Lonsdale on single crystal diffuse scattering (Lonsdale, 1948). Admittedly, her focus was on thermal diffuse scattering, but it illustrates the fact that the value of understanding the scattering between the Bragg peaks was recognized from the earliest days of X-ray diffraction. Since then the power of diffuse scattering, whether of X-rays or neutrons, in probing disorder within crystalline materials has been demonstrated by measurements on a wide range of materials from metallic alloys to molecular solids. An excellent introduction to the subject is provided by one of Lonsdale's last students, Richard Welberry (Welberry, 2022). Nevertheless, in spite of this long history, I think it is fair to say that diffuse scattering is not as widely used as might be expected, given the importance of local structural correlations in the functionality of so many materials. In the past, this was due to two major challenges, the challenge of measuring scattering that was several orders-of-magnitude weaker than Bragg peaks over large three-dimensional volumes of reciprocal space and the challenge of modeling the results. With advances in the power of both X-ray and neutron sources as well as the more widespread availability of large area detectors, high-quality diffuse scattering data is now much easier to collect, but the second challenge is still a deterrent to non-specialists, in spite of the existence of a number of software tools for atomistic modeling (Proffen & Neder, 1997; Paddison, 2019).

The relatively recent development of three-dimensional pair-distribution function analysis (3D- Δ PDF) may encourage some scientists to give diffuse scattering another look. Patterson maps, i.e. 3D maps of interatomic vector probabilities produced by the Fourier transformation of $S(Q)$, have long been used by crystallographers as a tool in solving crystal structures. What Thomas Weber and colleagues at ETZ Zürich realized is that if it were possible to eliminate scattering from the long-range ordered structure before performing the transform, the resulting maps would only contain interatomic vectors whose probabilities differ from the average (Weber & Simonov, 2012). These are difference Patterson maps, hence the Δ in 3D- Δ PDF. This is accomplished by removing the Bragg peaks at integer (hkl) values and replacing them with interpolations of the surrounding diffuse scattering, a procedure known as 'punch-and-fill.' 3D- Δ PDF maps filter out the average structure entirely, allowing us to focus on the changes in site occupations and atomic relaxations caused by local disorder. This is not possible with polycrystalline PDF data, in which there is no way to separate Bragg and diffuse contributions without sophisticated modeling. In 3D- Δ PDF maps, the smoothly varying distributions of intensity in Q -space are transformed into discrete spots in real space, with both positive and negative intensities reflecting increases or decreases in their respective vector probabilities compared with the average crystal structure (see Fig. 1).

The beauty of this method is that 3D- Δ PDF maps are relatively easy to interpret even without any modeling. The article by Schmidt et al. (2023) in this issue demonstrates this with an analysis that combines new neutron and X-ray data from yttria-stabilized zirconia (YSZ). The diffuse scattering in YSZ is extremely strong because of a high concentration of oxygen vacancies. This, coupled with the commercial availability of large single crystals produced as artificial diamonds, has encouraged several diffuse scattering investigations using both neutrons and X-rays over the past forty years. These have used increasingly sophisticated instrumentation as it became available, from the initial raster scans of a single Q -plane using a neutron triple-axis spectrometer that I once participated in (Osborn et al., 1986) to more complete reciprocal space volumes collected with neutron and X-ray area detectors (Welberry et al., 1995; Goff et al., 1999). However, the results have been somewhat qualitative even after employing a variety of modeling methods. In the new study by Schmidt et al. (2023), shifts in interatomic vectors are determined directly from the 3D- Δ PDF maps, producing more definitive values of the relaxations of both anions and cations around vacancies. The authors also performed atomistic simulations to reproduce the PDF peak intensities but these only served to confirm their original interpretations. Intriguingly, the size of the relaxations that they observe are significantly greater than those derived from Bragg peak analysis, but the consistency between the neutron and X-ray data suggests the numbers are reliable.

The observed relaxations of nearest neighbors around a vacancy do not yield many surprises. More controversial is whether the vacancies tend to form pairs along the unit-cell diagonals, with or without cation

interstitials. By contrasting the neutron PDFs, which are sensitive to oxygen pairs, with X-ray PDFs, which are less so, Schmidt et al. (2023) concluded that there was an increased probability of $\langle \frac{1}{2} \frac{1}{2} \frac{1}{2} \rangle$ vacancy pairs, but not between cation interstitials. They also found no evidence of longer-range correlations, which would have provided evidence of extended vacancy complexes. This is somewhat surprising as, with 18 mol% Y_2O_3 , there are quite sharp diffuse peaks in Q-space, indicating that correlations extend to 15 Å or more (Osborn et al., 1986; Goff et al., 1999).

One of the strengths of 3D- Δ PDF maps is that they allow correlations to be determined over a much greater range of length scales than polycrystalline PDFs. In our own work on sodium-intercalated V_2O_5 , we were able to measure the growth of structural correlations in the sodium substructure with decreasing temperature from 10 Å to 200 Å (Krogstad et al., 2020). The new X-ray measurements were performed with a laboratory source, so synchrotron studies to look for very weak PDF signals at longer distances might be worth considering.

In the latest edition of his book, Welberry points out that 3D- Δ PDF vector probabilities 'are simply related to the Warren–Cowley short-range order parameters that have frequently been used to parametrize diffuse scattering models' (Welberry, 2022). In other words, 3D- Δ PDF maps can, if properly interpreted, provide as much, if not more, information than can be derived by atomistic modeling in reciprocal space. Some modeling might still be necessary in multi-component systems, in which there is ambiguity about the origin of each PDF peak, but the problem is considerably simplified by the dimensionality reduction produced by transforming $S(Q)$ to a discrete set of vector probabilities. This presupposes that the original data is of high enough quality and completeness that the transforms are numerically robust and that care is taken not to introduce spurious Fourier artifacts in the 'punch-and-fill' process. Exploring methods of improving the reliability of 3D- Δ PDF maps could help to stimulate the surprisingly undeveloped field of three-dimensional spectral analysis. Nevertheless, there are an increasing number of 3D- Δ PDF results appearing in the literature each year, and this new work illustrates why it is becoming so popular and promises soon to become a commonly used tool in characterizing disordered materials.

Acknowledgements

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Figure 1 (a) Diffuse scattering in Q-space from equal concentrations of two different atomic species with differing ionic radius occupying random sites on a square lattice. (b) 3D- Δ PDF map in real space showing

peaks with both positive (red) and negative (blue) intensities representing the change in the probabilities of their respective interatomic vectors compared to the average structure. The 3D- Δ PDF transforms reveal both the size of the local relaxations and the length scale over which those relaxations are correlated (P. Upreti, private communication).

How much do molecular shapes matter?

Mohan Bhadbhade

Polymorphism, a phenomenon where the same chemical entity yields different crystal modifications has been known since the discovery of the phenomenon in benzamine (Wohler & Liebig, 1832). In recent years, polymorphism has become an intensively researched area because of its direct impact on the behaviour of industrial organic materials, particularly pharmaceutical solids, and to some extent dyes, pesticides and explosives (Brittain, 2016; Bernstein, 2020). In the case of pharmaceutical solids, the impetus came from real situations when problems faced with the large-scale crystallizations of drug compounds produced polymorphs with properties affecting the efficacy of the drug (solubility and bioavailability) (Bauer et al., 2001).

Polymorphism is just part of the story of molecules crystallizing in unwanted, uncontrollable forms. Another layer to this area is the study of the growth of crystals containing crystallization solvents (or water) in the crystal structure; a phenomenon with many terms: solvates, solvatomorphs, pseudo-polymorphs, inclusion compounds and clathrates. Research efforts in this area seem to be ever growing, in part because of the promise of improving solubility and the shelf life or avenues to grow molecular cocrystals incorporating other bioactive components. Therefore, it is not surprising that this research area has become an indispensable part of R&D programs of several large multi-national pharmaceutical companies and has also seen engagement from chemists and chemical engineers worldwide. Of course, this research has both a strong commercial angle in the form of protecting new formulations through patents and a research angle deepening our understanding of crystal nucleation and growth and the intermolecular interactions that hold these crystals together. There have been several books, reviews and monographs on these topics (see Griesser, 2006; Cruz-Cabeza et al., 2015; Healy, 2017) and the research interest in this field is likely to continue growing, as shown by one very recent example in which the journal *Pharmaceutics* will publish a special issue in 2023 entitled *Polymorphism and Pseudopolymorphism of Pharmaceutical Substances*.

Therefore, the article *Exploring the thermal behaviour of the solvated structures of nifedipine* by Jones et al. (2023) is a timely and important contribution to this research area. Their research has thoroughly investigated solvates of nifedipine (NIF), a dihydropyridine drug [Fig. 1(a)] developed as a L-type calcium channel antagonist (Tang et al., 2016). The authors, after a wide screening of solvents, reported crystal structures of seven solvates studied using differential scanning calorimetry and thermogravimetric analysis and by variable-temperature X-ray powder diffraction to understand their desolvation behaviour, stability and structural changes during these processes. The structure of nifedipine without any solvent (the stable α form) was reported by Trigg et al. (1980) and there have been several publications on other polymorphs and solvates of this drug (Caira et al., 2003; Klimakow et al., 2010; Gunn et al., 2012). However, the paper by Jones et al. (2023) supplies a much broader landscape on the behaviour of solvated forms of this drug. Studies such as these are valuable in many ways, providing experimentally observed conformations of the drug molecule in different crystalline environments, enriching our understanding of the roles played by solvents in crystal growth and providing an insight into crystal engineering principles by analysing intermolecular interactions in different crystal forms.

It is intriguing that all seven solvates (including those with significantly different motifs, such as the THF solvate) desolvate to the thermodynamically stable α form. This implies that there would be a conserved stable framework of NIF molecules to which all solvated forms return once the solvent molecules leave the crystal lattice! It is worth exploring what (if any) commonalities may exist in the patterns of molecular packing.

The NIF molecule resembles a T shape [Fig. 1(b)] and interlocks itself with its centrosymmetric counterpart forming a dimeric pair which form layers [Fig. 1(d)], as seen in the original unsolvated crystal structure of NIF (α

form). Could this centrosymmetric dimer making C—H $\cdots$ O and C—H $\cdots$ π contacts [Fig. 1(c)] be a synthon (Desiraju, 1995) in the family of structures of this molecule?

The category 1 system of NIF packing can be seen in the zoomed-out views in Fig. 2. The NIF (in blue) adopts similar structures incorporating 1,4-dioxane, morpholine, DMSO and DMA (orange, orange, green and orange, respectively).

Despite containing different solvents, the host molecular association bears a close relationship with that seen in the α -NIF structure.

What is interesting is the packing of the molecules in the second category, which yield different structures (Fig. 3). As discussed in detail by the authors, solvents interact with the NIF molecule quite differently compared to the first category; also, the conformation of the NIF molecule is cis–cis in Figs. 3(b) and 3(c). But the pattern of host molecular packing, although with more modulations, is seen to exist in all three solvates. An intriguing case is that of pyridine solvate which has added complexity of crystallizing in a chiral space group.

In this case, the two molecules of the asymmetric unit (light blue and dark blue) form this dimeric embrace, whereas in the other solvates it is the association of centrosymmetrically related molecules.

Therefore, it is conceivable to trace the possible mechanistic pathways for desolvation that converge to the stable α form with the least molecular movement. This case study of conserved packing patterns is of interest for crystal engineering purposes and reminds us of the geometrical approaches discussed years ago by Kitaigorodsky (1961). Do angled frameworks of molecules exhibit these isostructuralities during their molecular packing in forming crystals? Many solvates formed from L-shaped host molecules (Alshahateet et al., 2015; Bishop et al., 2018) were also noted to form a centrosymmetric dimeric association. Host molecule organization governed by relatively weaker interactions creates a well conserved layered framework allowing intercalations of several solvents that form stronger hydrogen bonds with the host.

Jones et al. (2023) also state an interesting use of the seeding technique to produce a β form of NIF using crystals of a similar molecule, felodipine, that produces a cis–cis conformation for the NIF molecule (felodipine is not a symmetric molecule, but it does show this packing feature). Could this form a co-crystal, and would such studies lead us to the complementary ‘fitting’ in producing multicomponent molecular crystals? It is very likely that in future we will see fascinating multi-component crystals; as creatively combined fishes with birds and fishes with horses by the legendary artist Escher (Fig. 4).

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Figure 1 (a) Molecular structure of NIF, (b) T-shaped molecule, (c) packing in the stable form of NIF and (d) centrosymmetric dimer (in 1,4-dioxane solvate).

Figure 2 View of molecular packing in structurally similar solvates of (a) 1,4-dioxane, (b) morpholine, (c) DMSO and (d) DMA.

Figure 3 NIF with solvates (a) THF, (b) pyridine and (c) MeOH. For clarity, all views are down arbitrary orientations.

Figure 4 M. C. Escher (1898–1972) tessellations: (a) fish and bird (<https://artdocents.wordpress.com/tag/mc-escher/>), and (b) fish and horse (<https://www.pinterest.com/pin/397794579557584028/>).

Continuous development in macromolecular crystallography with CCP4

Martín Martínez-Ripoll and Armando Albert

People engaged in X-ray crystallography since the early 1970s have been spectators and beneficiaries of the contributions of many colleagues who dedicated a significant part of their professional careers to the development of computational methodology for X-ray crystallography. Indeed, from the earliest standalone programs for processing experimental measurements extracted from Weissenberg diagrams, to the handling of the resolution and refinement programs and the earliest graphic representation programs, crystallographers will always be grateful to this community effort. But over the years, small-molecule crystallographers benefited from the great advances made in the development of integrated systems, such as the XRAY76 System, which for the first time offered a full collection of tools for full resolution of small-molecule structures from single-crystal X-ray diffraction data.

The field of macromolecular crystallography also underwent a development equivalent to that of small molecules, although somewhat later. The establishment of the Collaborative Computational Project No. 4 (known as CCP4) in 1979 represented a spectacular qualitative advance in the field. CCP4 is a public resource for producing and supporting a world-leading, integrated suite of programs that allows researchers to determine and analyze macromolecular structures by X-ray crystallography. Indeed, the CCP4 project has evolved in line with structural biology advancements, becoming an essential resource for researchers and scientists worldwide (Fig. 1).

Nowadays, the CCP4 initiative is not merely a collection of programs, it includes a graphical interface that guides less experienced users through the resolution pathway to the structural analysis and provides traceability of jobs. In addition, CCP4 supports various educational projects around the globe. These initiatives extend beyond self-promotion and include an open mailing list that anyone can join to share conference and workshop announcements, questions and discussions, that sometimes turn into debates, and information about job offers.

The article by Agirre et al. in this issue (Agirre et al., 2023), provides a thorough review of the CCP4 suite of programs. It constitutes a long-awaited initiative intended to review the current state of the CCP4 project and future developments. In addition, it offers an up-to-date literature citation for the suite, which has had multiple references in the past, and for each of the individual programs. The review aligns with the idea that the complexity of macromolecular crystallography should be accessible to both non-expert and advanced users and should offer computing tools regardless of the difficulty of the project.

The article also provides a critical analysis of the challenges and opportunities that the field of macromolecular crystallography faces now and in the future.

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Figure 1. The evolution of CCP4 from 1996 to the present day.

Pauling's rules revisited

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Almost a century ago, Linus Pauling (1929) proposed a set of rules governing the structural chemistry of inorganic crystals. The rules were a tentative step toward creating a valence theory for inorganic compounds. Unfortunately, the new quantum mechanics that promised to answer all of chemistry's questions appeared at the same time, and Pauling's rules were soon forgotten. They are worth a second look because they point to a simple but rich theory of valence that describes the chemistry of both organic and inorganic compounds using only the simple concepts of valence, atoms and bonds.

Curiously, for all its success, quantum mechanics has never provided definitions for either bonds or valence, or even for atoms once they are incorporated into a molecule. The reason for this failure is simple. Quantum mechanics calculates the energy and other physical properties using the electric field that connects electrons to nuclei, but any calculation using a force field is a mathematical integration that requires a set of initial conditions, such as the spatial coordinates of the nuclei. This restricts each calculation to a single spatial arrangement of atoms. Valence theories are more flexible because they do not use atomic coordinates. Instead, they define the location of an atom by its place within the network of bonds that links the atom to its neighbours. Chemical properties such as molecular structure and reactivity are determined by how the network distributes the valences of the atoms among its various bonds. By not having to specify atomic coordinates, valence theories are simpler and more intuitive, but at the cost of being unable to calculate energies. It follows that quantum and valence approaches provide complementary descriptions of the same compound. Quantum theory describes the physics of electrons bound to nuclei, valence theory describes the chemistry of atoms linked by bonds. In the past, when the atom was still just a hypothesis, valence theory brought order to organic chemistry where it is still widely used, but finding a comparable theory of inorganic chemistry has proved elusive.

Pauling presented his rules in an early attempt to formulate an inorganic valence theory. His first two rules are visionary because they express the idea that structural chemistry is largely determined by the sizes and valences of the atoms, concepts that serve as surrogates for the quantum picture of the core and the valence shell, respectively. Hidden unnoticed within these rules lie the clues to a unified theory of valence, one that provides an enriched description of the structure and properties of both organic and inorganic compounds.

Pauling's first rule states that the coordination number of a cation depends on the ratio of the cation to anion radii, but all attempts to define the radius of an atom or ion have failed because atoms do not behave like hard spheres. What has hitherto been overlooked is that the proper measure of atomic size in chemistry is not the radius of the atom, which is undefinable, but the coordination number that the atom adopts in different chemical contexts. The elemental property that best characterizes the size of an atom is the average of its observed coordination numbers.

Pauling's second rule defines the bond strength of a cation as its valence divided by its coordination number. The rule states that the valence of an anion is approximately equal to the sum of the bond strengths it receives from its cation neighbours. This rule introduces four important ideas. (1) Even though the ionic model uses an electric force field to link cations to anions, Pauling assumes that this field can be transformed into a network of localized bonds. A formal derivation shows that while such a transformation is possible, it is not reversible because the atomic coordinates are lost in the process. (2) The most important chemical property of an atom is neither its valence nor its coordination number, but its bond strength which indicates its preferred bond partners. (3) Two atoms contribute equal valences to form a bond. (4) The bond strength, being a ratio, is not restricted to integral values. The traditional association of valence with an electron has no physical basis. Valence and electrons can never be measured at the same time: the valence of an atom can only be measured when it is part of a compound, but an individual electron can only be observed when it is an isolated particle.

A unified theory of valence is possible if non-integral valences are allowed. It describes the chemical structures of both organic and inorganic compounds by a network of localized bonds that obey a number of simple rules. Elements are characterized by their observed properties of valences and average coordination number, but their most important property is their bonding strength, equal to the ratio of their valence to average coordination number. Bonds are found to form only between atoms whose bonding strengths differ by less than a factor of two, though atoms with lone pairs, such as anions, can form stronger bonds by making their lone pairs stereoactive, thus accounting for the different chemistries of anions and cations. The ionicity of a bond is the difference between the electronegativities of its bonded atoms, where the electronegativity can be shown to be equal to the bonding strength of the element in its highest valence state. Organic molecules are formed by atoms with bonding strengths close to 1.0, allowing them to form bonds of low ionicity in many different ways. Hydrogen and fluorine necessarily terminate the bond network to form discrete molecules.

The resulting unified valence theory (Brown 2023) is quantitative and can predict which atoms will form bonds, as well as the bond lengths, geometries and chemical properties of the resulting compound. The structure and chemistry of hydrogen bonds, and likely also of halogen bonds, are predicted from atomic valences and sizes. The theory describes solubilities and the species present in aqueous solutions at various pHs. Where practical considerations often limit quantum mechanical calculations to isolated clusters of atoms, valence theory incorporates a knowledge of the chemical environment and its influence on the internal structure of a molecule. Even though valence theory cannot determine physical properties, its simplicity makes it an ideal way to introduce students to chemistry, and for those who later graduate to quantum mechanics, it provides a way of selecting a structure for a more comprehensive quantum investigation.

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Women in Crystallography project

Annalisa Guerri

For the third time since its launch in Oviedo at ECM31, and with a more international scope, the "Women in Crystallography" project is in the limelight again - this time in a different continent, with a very special host: our colleagues from down under in Melbourne. We thank all the crystallographers for the hospitality, and we hope we will be able to keep up with the tradition of making this T-shirt fundraising event a fabulous success. The T-shirts will be available at the IUCr booth, as well as at the desks of Dectris and STOE, which are supporting and sponsoring this initiative.

The money collected will be used to support more and more female crystallographers to attend congresses and schools around the World.

Take a picture wearing your T-shirt and post it on Twitter with the hashtags:

#Womenincrystallography

#IUCr2023

See you in Melbourne!

History of the “Women in Crystallography” logo

The “Women in Crystallography” project was launched in 2018 during the ECM31 in Oviedo (Spain) thanks to the first organized microsymposium on Women in Crystallography (MS45). The Chairs of the microsymposium (Julia Contreras García and Annalisa Guerri) were asked to provide a logo and a motto for the MS to be shown at the beginning of the session.

The logo originated from the worldwide famous “Photo 51”, the X-ray fiber diffraction by DNA taken by Raymond Gosling, a graduate student working under the supervision of Rosalind Franklin. This pattern is an iconic symbol for crystallographers and represents female scientists in crystallography.

After a short email exchange, the following picture and wording below came to light for the introduction of the MS45:

“N'oubliez jamais qu'il suffira d'une crise politique, économique ou religieuse pour que les droits des femmes soient remis en question. Ces droits ne sont jamais acquis. Vous devrez rester vigilantes votre vie durant.”

“Never forget that a political, economic, or religious crisis is enough to cast doubt on women's rights. These rights will never be vested. You have to stay vigilant your whole life.”

Simone de Beauvoir

Starting from this idea, Laura Roches Fernández and Julia Contreras García elaborated the logo and gave birth to the one used to print the T-shirts. After a first draft, the logo was refined at the university of Oviedo as it appears below.

The idea was also inspired by another project born in 2015: the “women under high pressure” movement with the aim to improve the participation of women, especially young scientists, at events around the World and to create a balanced attendance among participants and also among the speakers.

Recent news from the European Crystallographic Association

Arie van der Lee

After the very successful European Crystallographic Meeting in Versailles (ECM33), France, in August 2022, activities moved along at a slower pace but were not completely absent. ECA's Executive Committee met in Padova, Italy, from 17 to 19 February 2023, where we were hosted by the ECM34 chair Gilberto Artioli, and visited Padova's brand new Congress Center, where the 34th European Crystallographic Meeting will take place in 2024. Progress in the organization of future ECA events (ECM35, Lviv; ECS8, Berlin, July 2023; ECS9, Nancy, June 2024) was discussed also with the different organizers. A bid for the organization of a European Crystallography School in North Macedonia in 2025 will probably be submitted so that it can be discussed and voted on during this year's annual Council meeting, which will be held virtually in September 2023. The Executive Committee met in Padova from 17th to 19th February 2023. Some officers were not present physically.

From left to right: Andy Maloney, Klaudia Hradil, Arie van der Lee, Marijana Daković, Antonia Neels, Angela Altomare (IUCr representative), Consiglia Tedesco. Photo taken by Gilberto Artioli in front of the building of the Dipartimento di Geoscienze of the University of Padova

ECA's Executive Committee also considered the way ECA's prizes are attributed and how to increase the attractiveness of the prizes. We had discussions with the Council, the young crystallographers in Versailles, and colleagues of the boards of the American Crystallographic Association (ACA) and the European Neutron

Scattering Association (ENSA). Following these discussions, new guidelines will be drafted and presented at the forthcoming Council Meeting. We will also announce the birth of one or two new prizes.

The Erwin Félix Lewy Bertaut Prize was awarded to Dr. Matilde Saura-Múzquiz this year, currently at Universidad Complutense de Madrid, Department of Materials Physics, Spain. ECA and ENSA jointly award the Bertaut Prize in memory of the scientific achievements of the late Erwin Félix Lewy Bertaut, representing cornerstones in both crystallography and neutron scattering. The laureate is expected to be a young scientist (up to 8 years after finishing their Ph.D. thesis) having a clear affiliation with the ECA/ENSA region in recognition of notable experimental, methodological or theoretical contributions to the investigation of matter using crystallographic or neutron scattering methods.

Matilde Saura-Múzquiz has impressive early career contributions in the field of the crystallography of functional materials, in particular those related to the studies of magnetic and non-magnetic complex oxide structure (scheelites, fergusonites, perovskites, pyrochlores, ...) and those on nanoparticle morphology, nuclear and magnetic texture and magnetic performance of sintered materials, while combining neutron and X-ray diffraction methods. The Bertaut Prize ceremony has taken place this year in Garching, Germany, during the European Conference on Neutron Scattering 2023

Work is in progress to establish a gender balance and equity statement by ECA, which should be taken into consideration for ECA's own events, such as ECMs and ECSs, but also as a condition to receive financial support for non-ECA events. ECA's General Interest Group GIG3 is making a proposal that will be edited by the Executive Committee before discussion at the Council Meeting in September 2023.

The successful series of ECA lunchtime webinars is at the time of writing (May 2023) at its 21st edition. ECA's young crystallographers organize this series, and it will continue to be held after the summer. Another series of webinars, Distinguished Lectures on Quantum Crystallography and Complementary Fields, initiated by ECA's Special Interest Group 2 (Quantum Crystallography) and the IUCr Commission on Quantum Crystallography continued as well: 7 webinars took place since April 2022, usually with two lectures during the same webinar.

ECA continues to support the development of crystallography in Africa. The African Crystallographic Association (AfCA) was established in 2021. With respect to National Membership, AfCA and ECA have decided that ECA's African National Members may remain ECA National Members as long as they wish. ECA was represented by its secretary Andy Maloney at the 3rd African Conference on Crystallography in Nairobi, Kenya, from 17 to 21 January 2023. ECA's National Member Officer Delia Haynes was, of course, also present in Nairobi in her role as AfCA's Executive Committee president.

ECA members are also involved in the AFRAMED/Remote labs project led by its past president Claude Lecomte who has initiated this exciting development aiming to train African crystallographers in the techniques of single-crystal diffraction in laboratories equipped with single-crystal diffractometers elsewhere and to give them the opportunity to run their own experiments by remote access to the diffractometer in the distant laboratory. This project was launched in Nancy, France, on August 31st, 2022.

Meeting report on 24th Heart of Europe Bio-Crystallography meeting

Milton T. Stubbs

The 24th Heart of Europe Bio-Crystallography meeting (HEC24; <https://www.xray.cz/hec24>) took place in September 2022 on the shores of the beautiful Lake Lipno in the South Bohemian village of Dolní Vltavice (Czech Republic). Organized in collaboration with the Czech and Slovak Crystallographic Association by Ivana Kutá Smatanová and her team from the University of South Bohemia in České Budějovice, HEC24 received financial support from seven companies, the European Crystallographic Association (ECA) (which awarded twelve bursaries for young scientists), as well as IUCr Journals who provided two copies of "State of the Art of Macromolecular Crystallization" as prizes for students' presentations.

This first post-COVID-19 meeting was attended by 109 structural biologists from 22 research groups in central Europe (Austria, the Czech Republic, Germany and Poland), and opened with the introduction of new HEC

group Przemek Grudnik (Jagiellonian University, Krakow). Over the next three days, 26 PhD students and four young postdocs presented current topics of their research. The quality of the talks was excellent, making it hard for the HEC Prize committee to reach its decision. After much deliberation, Elżbieta Wątor (Jagiellonian University, Kraków) was awarded the prize for her presentation “Half way to hypusine. Molecular basis of (deoxy)hypusination”. 10 flash talks, introduced for the first time at HEC23, were also presented, and Jakub Hrubý (CTU Prague) was awarded for his presentation “Effects of the Zn²⁺ to Cd²⁺ Exchange on the Structure and Activity of S1 Nuclease”. The HEC lecture, presented each year by a prominent scientist outside the HEC community, was delivered by Kay Diederichs (University of Konstanz). His talk “A better understanding of X-ray data quality indicators” was truly inspirational, reminding participants young and old (!) of the importance of statistics.

Interspersal of the programme with short company sponsored presentations served to introduce new technologies to the participants, and the hearty Bohemian food and drink fostered a warm atmosphere for both formal and informal discussion. The afternoon boat ride provided time for relaxed discussions over a Czech beer or two, and the last night disco was thoroughly appreciated.

Ivana and her team are to be thanked for the excellent organisation of HEC 24, which ended with an (almost) impromptu live sing-along of the HEC song that was penned for HEC23 during lockdown. The next Heart of Europe Bio-Crystallography meeting (HEC25), organized by Michael Lammers of the University of Greifswald, will also be lakeside, taking place on the shores of Lake Kummerow in Salem, Mecklenburg-Vorpommern (Germany) from 21st to 23rd September 2023 (biochemie.uni-greifswald.de/aktuelles/hec25-bio-crystallography-meeting).

Milton T. Stubbs

Participants at the 24th Heart of Europe bio-Crystallography meeting in Dolni Vitavice, Czech Republic.

This year's HEC prizes were awarded to Elżbieta Wątor (second from left) of the Jagiellonian University, Kraków for her talk “Half way to hypusine. Molecular basis of (deoxy)hypusination” and Jakub Hrubý (second from right) from the CTU Prague for his flash talk “Effects of the Zn²⁺ to Cd²⁺ Exchange on the Structure and Activity of S1 Nuclease”. Each were awarded a copy of the “State of the Art of Macromolecular Crystallization”, edited by Howard Einspahr and kindly sponsored by IUCr Journals. The award was presented by Ivana Kutá Smatanová (left) and Manfred Weiss (right).

19th BCA/CCG Intensive Teaching School in X-ray Structure Analysis

Natalie Pridmore, Local Organiser

The 19th BCA/CCG Intensive Teaching School in X-ray Structure Analysis was back in person, for the first time since 2019, and held at Trevelyan College, Durham from the 25th March – 2nd April 2023. The school was once again heavily oversubscribed, due to the school's national and international reputation for providing a good basis in crystallography and this year we welcomed almost 80 students from the UK, Ireland, Germany, Hungary, Malta, Croatia, Poland, Spain, Italy and Australia. The variety of nationalities, academic backgrounds and crystallographic experience created a great environment for both learning and meeting new people, with many students and staff commenting on the positive and friendly atmosphere.

As a result of feedback from students and staff over the years the format of the biennial course has evolved. It currently consists of a mixture of lectures and tutorials designed to help students improve their understanding of the lecture material. As the name suggests, the course is intensive with a full timetable across the 7 days providing the students with the opportunity to gain a good theoretical understanding of various aspects of crystallography from a single crystal perspective. Beginning with an introductory lecture shortly after arrival on Saturday evening, the lectures given by Professor Richard Cooper; Dr Lukas Palatinus; Dr Claire Hobday; Dr Helena Shepherd; Dr Andrew Bond and Dr Mark Senn covered Maths; Symmetry; Data collection; Fourier/Patterson; Electron Diffraction; Direct Methods; Charge Flipping and Superspace; Parameterisation; Least Squares; Refinement; Twinning and Derivation of Results. An introduction to databases was also given

by Dr Chris Kingsbury and the use of Synchrotron and Neutron facilities were highlighted by Dr Mark Warren and Dr Amber Thompson.

Attendees were assigned to a tutor group, consisting of one tutor and up to eight students, and worked together throughout the week to tackle a series of problems related to the lecture material. This year we welcomed new tutors, Dr Natalie Johnson; Dr Carsten Lenczyk; and Dr Natalie Pridmore (as a floating tutor) and welcomed back Dr Samantha Chong, Dr Matic Lozinsek and Dr Jeremiah Tidey, who were tutoring in person for the first time, and Dr Andrew Cairns; Dr Iain Oswald; Dr Amber Thompson; Dr Mark Warren and Dr Hamish Yeung. The lectures and tutorials were once again held in the Sir James Knott Hall which enabled us to switch easily between formal lectures and tutorial work, with minimal disruption. The accommodation and meals were provided in Collingwood College which is less than a 5-minute walk away but provided a pleasant chance for some fresh air and brief exercise during the day.

As is traditional at the school, apart from the Math's lecture on the first day, the evening activities are designed to be more relaxed and provide an opportunity for the students to mix with each other through a combination of educational and fun activities. On the Sunday evening, a successful bar quiz, organised by Richard Cooper, was enjoyed by all those in attendance (including the bar staff). While Monday evening's session was a chance for the students to get to know some of the lecturers and tutors better with a panel question session, which included a discussion of the favourite or most difficult structure they have solved and their favourite space group.

This year's student presentations, on the Friday evening, were organised by Dr Jeremiah Tidey and Dr Mark Warren. Each of the tutor groups put together a five-minute presentation on a crystallographic topic, drawn from a hat earlier in the week, and performed it in a style that was also chosen at random. This year, this included Crystal Growth and Selection in the style of Shakespearean Theatre, asking the age-old question to measure or not to measure; Disorder as a Public Service Announcement/Breaking News, which warned of the dangers of using squeeze routinely, and The Lab Diffractometer in the style of a Pantomime (oh yes they did!). As with previous years the scientific quality, thematic accuracy and entertainment value of each presentation was assessed by our elite panel of judges, the lecturers, who were very impressed by all the entries.

The conference dinner, held in Trevelyan College, on the Saturday evening provided the chance to thank all the people who had contributed to the success of this year's school including the local staff, organisers, lecturers, tutors and students. The hard work and positive attitude from the staff and students alike helped to create a very friendly school. After this year's school Dr Hazel Sparkes, who did not attend this year's school but was instrumental in its organisation, is stepping back from her role as local organiser and Dr Claire Wilson is stepping down from preparing the notes for the course. We would like to thank them both for their contributions for over a decade, their organisation, enthusiasm and drive have enabled the course to run and helped maintain its high standards. We are delighted that Dr Natalie Pridmore and Dr Andrew Cairns have agreed to take over as local organiser and to prepare the notes, respectively.

Following on from the school an optional hands-on Olex2 workshop was held on the Sunday, run by Dr Oleg Dolomanov, Dr Florian Kleemiss, Florian Meurer and Dr Toby Blundell. This was well received by the over 45 registered participants, who had the opportunity to use Olex2 to apply concepts that they had learnt on the course to both test structures and their own data.

I would like to finish by saying thank you to all the sponsors of this year's school: IUCr, ECA, CCG, ICG, Bruker, Rigaku, Almac and CCDC. Without the financial support from these organisations, we would not have been able to help as many students attend the school, or run it so successfully, and we are very grateful for their continued support.

Third International SAXS excites 2023 Symposium

Andreas Keilbach

In April 2023, Anton Paar and the Institute of Inorganic Chemistry at Graz University of Technology successfully hosted the third edition of the SAXS excites Symposium series. More than 80 participants from over 18 countries gathered in the Austrian city of Graz – home to many key figures in the field of small-angle scattering, such as Otto Kratky, Günther Porod and Otto Glatter.

The event connected to that history and brought together an array of users from the field of SAXS, with the aim of encouraging multidisciplinary cooperation and an open exchange of experience between renowned scientists, young scientists and industry. In this unique setting, researchers with different scientific backgrounds – ranging from biology to materials science – got together, learned about their individual progress and challenges in the application of small-angle scattering, and sparked new ideas for their own experiments.

The symposium featured 21 high-level presentations from keynote speakers such as Jan Ilavsky (Argonne National Lab) on the new age of (U)SAXS applications in metallurgy, Denise Erb (Helmholtz-Zentrum Dresden-Rossendorf) on GI-SAXS observations of spontaneous nanopattern formation on crystal surfaces under extreme conditions, Stefan Salentinig (University of Fribourg) on SAXS-guided engineering of antimicrobial nanomaterials, and Cy Jeffries (EMBL Hamburg) on the significance of small-angle X-ray scattering with regard to biological materials for structure determination in the age of AlphaFold.

A poster session offered an opportunity to discuss the latest scientific findings in more detail and initiate possible future collaboration projects between the participants.

It wasn't all work though! A short Anton Paar company tour ended with a visit to the Anton Paar Sudhaus brewery, where head brewmaster Gebhard Sauseng explained the details of the brewing process. And no brewhouse tour would be complete without the option to also sample and taste the beers fresh from the tap. From there, it was only a few steps to the conference dinner.

With this third SAXS excites Symposium, Graz University of Technology and Anton Paar – together with all the participants – again placed impressive emphasis on SAXS in a city that has a long, strong connection to the field.

"The scope and quality of the scientific presentations were impressive." "The discussed topics allow me to look beyond the horizon of my own research." "The organization of the conference was very professional." "The scientific meeting as well as the company tour and conference dinner were awesome!" For more information please [click here](#).

Contact: Andreas Keilbach.

Hot Topics in Contemporary Crystallography 5 (HTCC5)

Aleksandar Višnjevac

Dubrovnik, Croatia, April 16th to 21st, 2023

George Bernard Shaw wrote, after his visit to Dubrovnik in 1929: „These who look for paradise on earth should come and see Dubrovnik". Since then, the unique beauty of this medieval city hasn't changed, but it has, to the delight of many crystallographers from across and beyond Europe, become home to the series of advanced crystallography workshops organized by Croatian Association of Crystallographers, and called Hot Topics in Contemporary Crystallography. The fifth edition (HTCC5) of this series took place from 16th to 21st April 2023 in the enchantingly picturesque village of Mlini, a mere 9 km from the old city gates of Dubrovnik. The venue was the luxury Sheraton Dubrovnik Riviera hotel and conference centre, which in mid-April, is smoothly embedded into this drowsy place. The venue is ideally suited for many reasons, one of them being the Dubrovnik International Airport situated a "stone's throw" away (but far enough to avoid disturbance from the roaring engines of many landing and taking-off iron birds).

HTCC5 was entirely dedicated to macromolecular crystallography (as it was its predecessor, HTCC4, held at the same location back in 2019). During the four working days, four topics were thoroughly tackled: crystallization (HT1), processing (HT2), databases (HT3) and visualization (HT4). This was achieved through a balanced number of lectures (15), tutorials (14) and demo-sessions (2). An absolute delight for the students and HTCC5's *fil rouge* of a kind, was the "Bring your own sample" activity, with three formal sessions and many informal gatherings, permitting students to bring their ill-crystallizing samples, analyse them by means of DLS (Xtal Concepts) and improve the crystallization conditions using micro seeding techniques with a help of an onsite installed Douglas Instruments crystallization robot.

I couldn't be prouder of the list of lecturers whom we gathered at HTCC5. Crystallization was masterfully presented, through an entire day, by (in alphabetic order) Areej Abuhammad, Terese Bergfors, Martin Caffrey and Elspeth Garman. The students practiced 'crystal fishing' with the aid of a video microscope that projected onto the main screen, allowing everyone else to see exactly what was happening, and to applaud when the 'fisher' was successful. Processing was introduced by two delightful introductory lectures by Edward Lowe and continued through a whole day with a series of alternating lectures and tutorials delivered by people who actually create and develop CCP4 - one of the most popular packages for it, Eugene Krissinel and Rob Nicholls. We had contributors from both PDBe and the CCDC (David Armstrong, Rupesh Chikhale and Fabio Montisci) who demonstrated the hottest features of these databases with a particular emphasis to the zones where small molecule structures and macromolecular ones intertwine (docking). Hands-on sessions introduced students to the practical use of PDB-KB, CCDC Crossminer and Gold. The visualization topic was a short and sweet one. Master minded by Zoran Štefanić, this topic acquainted students with the techniques of visualizing allosteric pathways in oligomeric enzymes by a variety of most popular programs. The cherry on the top was the interactive and competitive web-based game in which students were tasked to explore symmetry in two dimensions and compete with the others in a search for the right "crystal" packing. The score-board was regularly updated and displayed on the screen, which created a cheerful and positively competitive atmosphere.

The workshop, which was largely supported by the Croatian Science Foundation through project calixDNA (PI: Aleksandar Višnjevac), and generously sponsored by Bruker, Douglas Instruments, Formulatrix, Mitegen, Anton Paar, Oxford Cryosystems, Dectris and Rigaku) gathered 52 registered participants from 16 countries (Algeria, Austria, Croatia, Czech Republic, France, Germany, Italy, Ireland, Jordan, Poland, Serbia, Sweden, Slovenia, Turkey, UK, and Ukraine) with 28 students and 11 lecturers. 13 students received bursaries to cover, partially or entirely, their registration fees, accommodation and travel expenses. The bursary scheme was generously funded by the International Union of Crystallography, Croatian Association of Crystallographers and European Crystallographic Association.

Martin Caffrey's live demo on LCP crystallization

Rob Nicholls and Eugene Krissinel running tutorial at the Processing HT

Students presented 19 posters and 15 short discussion triggering presentations (DTPs). The best presentations were rewarded with a monetary 100 € award which was generously provided by Dectris (best DTP) and the Croatian Association of Crystallographers (best poster). The best poster prize was awarded to Daniel Mokos (University of Graz, Austria), for his poster entitled "Crystal structure and proposed mechanism of A622 homologues from the nicotine biosynthesis pathway", while Marika Majerova (Masaryk University, Czech Republic) was awarded for the best DTP for her presentation entitled "An extant enzyme with dual dehalogenase–luciferase function".

More on HTCC5 is available at htcc5.org, on the Facebook page "Croatian Association of Crystallographers", Instagram profile "Croatian Crystallographers" and on the Twitter profile @hrvukris. We are very much looking forward to the HTCC6 and we are inviting you to keep an eye on our social networks so you don't miss it.

Areej Abuhammad presenting award for the best DTP to Marika Mayerova

8th International School on Biological Crystallization

Juan Manuel García-Ruiz

(Granada, Spain, May 21st – 26th 2023)

Introduction

The Laboratory of Crystallographic Studies (CSIC-UGR) has successfully organised the 8th International School on Biological Crystallization (ISBC2023, <http://www.isbcgranada.org/>) under the auspices of the International Union of Crystallography (IUCr) through the Commission of Crystal Growth & Characterisation of Materials, Biological Macromolecules and Teaching, with the support of the International Doctoral Summer School Programme of the School of Science, Technology and Engineering (University of Granada), the Spanish Royal Society of Chemistry (RSEQ) and the Spanish Specialized Group of Crystallography and Crystal Growth (GE3C). The School was held at Hotel Abades Nevada Palace at close distance from the Centre of the beautiful City of Granada, an ideal place to promote close scientific and social interactions between attendees.

The ISBC2023 attracted the interest of postgraduate/postdoctoral students as well as research scientists from industry and academia that deal routinely with crystallization processes but seek fundamental knowledge on the crystallization phenomena and the behaviour of crystallizing solutions. Many participants, from 19 different countries around the world, all came to Granada to learn from top quality international speakers, to hear case study presentations, to watch practical hands-on demonstrations and to present their research results in the purposely dedicated poster sessions.

ISBC2023 delivered five days of lectures and practical demonstrations related to the crystallization of biological macromolecules, including large crystals for neutron diffraction and tiny crystals for XFEL or EM. One day was fully devoted to case studies on the crystallization of membrane proteins, viruses, large macromolecular complexes, and sample preparation for cryoEM.

As in previous editions, the Demonstrations Fair was very successful with many positive feedbacks from the participants. A round-table discussion on “Teaching Crystallography” was also highly appreciated among tutors, academics, students and industrial representatives.

Programme Committees

International Programme Committee Ivana K. Smatanova (Czech Republic) Pavlina Rezacova (Czech Republic)

Bernhard Rupp (USA)

Terese Berdforg (Sweden) Giuseppe Falini (Italy) Janet Newman (Australia) Joseph Ng (US)

Abel Moreno (Mexico) Hartmut Luecke (Norway) Jose A. Gavira (Spain)

Juan Manuel García-Ruiz (Spain)

Local Organising Committee

José Antonio Gavira & Juan Manuel García-Ruiz, Directors of the School Alfonso García Caballero

Luis Antonio González Ramírez Cristóbal Verdugo Escamilla

M^a Angeles Hernández Hernández Sergio Martínez Rodríguez Concepción Jiménez López

Valeria Risso

Gender Balance Advisor

Dr. M^a Angeles Hernández Hernández

Grants evaluation committee Juan Manuel García-Ruiz José Antonio Gavira

Ivana Kuta Smatanova

Pavlina Rezacova Joe D. Ng

Attendance

The turnout of the School was excellent having a total of 113 participants from 19 different countries, most of which were students (50 students, 41 %), speakers (30 speakers, 24 %) and academics (21 academics, 17 %), being the rest composed of industrial representatives (1) and exhibitors (7) (Figure 1). The participants were supported by a team of 4 people from the organisation. We achieved our goal of gender balance, having 60 female participants (53%) and 53 male (47%).

Figure 1. Left: Distribution of the type of participants in ISBC2023 by country of origin; Right: Distribution of participants in ISBC2023 by type.

The multicultural nature of the School is also evident in the breakdown of nationalities of the academics and speakers (Figure 2).

Figure 2. Left: Countries of origin of academics attending ISBC2023; Right: Countries of origin of speakers attending ISBC2023.

A considerable effort was also made to provide financial support to as many students as possible. All of the 39 applicants were awarded with a bursary to attend the School (¡Error! No se encuentra el origen de la referencia.), including all the students coming from outside Spain (24 students, 62 % of all granted students).

Figure 3. This graph shows the number of students receiving a grant to attend ISBC2019 by country of origin.

Programme of ISBC2023

ISBC2023 covered five days of lectures and practical demonstrations carried by 30 selected experts in the field of crystallization of biological macromolecules.

Main topics of ISBC2023

Nucleation: Classical and non-classical approaches.

Crystal growth kinetics and mechanisms.

Properties of macromolecular solutions (DLS/SAXS).

Screening: The search for crystallization conditions

Crystallization techniques: Batch, Vapour and Counter Diffusion, MMS, How do they work?

Crystallization and diffusion transport: gels, microfluidics and microgravity.

Crystallization of large crystals for Neutron diffraction.

In vivo crystallization of tiny crystals for XFEL.

Serial Crystallography.

Polymorphism in protein crystals.

Membrane protein crystallization: Lipid cubic phase, bicelles and detergents.

Crystallization of Macromolecular Complexes.

Electron microscopy for structural studies

Sample manipulation, preparation and characterization by electron microscopy.

List of Speakers in ISBC2023

Bernhard Rupp, k. k. Hofkristallamt, US.

Janet Newman, UNSW Sydney, Australia.

Martin Caffrey, Trinity College Dublin, Ireland.
Petra Fromme, Arizona State University, US.
Juan Manuel Garcia-Ruiz, IACT, CSIC-UGR, Spain.
Jeroen Mesters, University of Lüneburg, Germany.
Marc Pusey, iXpressGenes, Huntsville, US.
Naoko Mizuno, NHLBI/NIH, Bethesda, US.
José A. Gavira, IACT, CSIC-UGR, Spain.
Hudel Luecke, University of Oslo, Norway.
Brent Nannenga, Arizona State University, US.
Sergio Martínez, UGR, Spain.
Ivana K. Smatanova, University of South Bohemia, Czech Republic.
Claude Sauter, IBMC, CNRS, France.
Christian Betzel, University of Hamburg, Germany.
Fermin Otálora, IACT, CSIC-UGR, Spain.
Guillermo Calero, University of Pittsburgh, US.
Christian Biertümpfel, NHLBI/NIH, Bethesda, US.
Edward H. Snell, Hauptman-Woodward Institute, Buffalo, US.
May Marsh, Swiss Light Source at Paul Scherrer Institut, Swiss.
Jose Manuel Martin-Garcia, IQFR, CSIC, Spain.
Joseph Ng, University of Alabama, US.
Eva Cunha, University of Oslo, Norway.
Monica Budayova-Spano, Université Grenoble Alpes, France.
Crissy Tarver, Stanford University, US.
Pavína Řezáčová, University of Prague, Czech Republic.
Lars Redecke, University of Lüneburg, Germany.
Tom Peat, UNSW Sydney, Australia.
Filipa Castro, Universidade do Porto, Portugal.
Isaac Rodríguez, CNRS, Toulouse, France.

The first day, Monday, started with an introduction to the School and was fully dedicated to explaining the whole process of crystallization “From solution to protein crystals”, from the purification and preparation of protein solutions to the basic concepts of crystallization, nucleation, phase diagrams, crystal growth kinetics and the different crystallization techniques (Figure 4).

Figure 4. Prof. B. Rupp is showing how to protein crystals growth.

Tuesday was devoted to special hot topics, including femtosecond Crystallography, microseeding, microfluidics, how to grow crystals for neutron diffraction, the crystallization of membrane proteins and large macromolecular complexes (Figure 5).

Figure 5. “Femtosecond Crystallography, a New Era in Structural Biology” a talk given by Prof. Petra Fromme.

On Wednesday there were sessions on especially relevant topics such optimization of crystal growth for neutron diffraction, SAXS, EM, etc. (Figure 6).

Figure 6. Prof. Lars Redecke impress the audience with his lecture "Overview of protein crystallization in living cells".

Thursday was dedicated to the very popular 'Demonstration Fair', at which specialists offered 23 short (20-40 minutes) practical sessions periodically at scheduled times. Participants were free to choose what sessions they wanted to attend and in the order they wished, so that they selected their own learning programme "a la carte". The Demonstrations' Fair proved to be an excellent teaching tool as it provided students with plenty of opportunities to interact on a personal basis with the teachers and to watch closely how to perform crystallization experiments (Figure 7).

Figure 7. Upper picture shows in first plane Prof. Rupp with Dr. Crissy Tarver behind preparing her second round followed at her right by Prof. Petra Fromme who is showing how to crystallized the membrane protein PSI in situ. In the bottom picture Dr. Janet Newman caught the attention of many students describing relevant tips & tricks to perform vapour-diffusion (hanging and sitting drops) experiments.

The last day of the School started with a very appealing lecture given by Prof. B. Rupp title "The Chemistry of Mushroom Magic (Why you should not lick toads)" followed by the round-table discussions on "Teaching Crystallography" driven by Prof. JuanMa Garcia-Ruiz how present the successful story of the "Crystallization Competition" with the help and presentations of Dr. Ivana Kuta Smatanova and Dr. Janet Newman (Figure 8). There were also 5 minutes talks given by the poster winners

Figure 8. Round-table discussion on "Teaching Crystallography" driven by Prof. Garcia-Ruiz with the help of Dr. Ivana Kuta Smatanova (left) and Dr. Janet Newman (middle).

Poster Sessions

The students made a great contribution to the success of the School with 41 posters. There were poster sessions (Figure 9) on Monday, Tuesday and Wednesday coffee breaks, proving to be a very valuable time in order to discuss the scientific work. The six poster winners (Table 1), who were selected by an international panel of lecturers composed of Bernhard Rupp, Crissy Tarver, Christian Biertümpfel, Lata Govada, May Marsh and Joe Ng, gave a 5 minutes presentation on Friday morning.

Table 1. Poster prize winners in ISBC2023 and group picture.

Student | Affiliation | Prize

Filipa Engrola | UCIBIO (Portugal) | IUCr

Uxía Pérez de José | CSIC-IQFR (Spain) | IUCr

Yevgeniya Karibjanova | Génie Chimique Toulouse (France) | IUCr

Markéta Šoltysová | IOCB (Czech Republic) | AUSE/LEC

Ángela Fernández García | CSIC-IQFR (Spain) | AUSE/LEC

Aumonier Sylvain | Paul Scherrer Institut (Switzerland) | B. Rupp

Figure 9. One of the lively poster sessions during ISBC2023.

Social events

In addition to the scientific course, there was a parallel social programme which consisted of a welcome cocktail on Sunday, a night guided walk of Albaicín & Sacromonte on Wednesday (Figure 10) and a Flamenco dinner party on Thursday in the traditional district of Albayzin (Figure 11), which is worldwide renowned for its flamenco music.

Figure 10. A picture of the attendants during their night guided walk of Albaicín & Sacromonte.

Figure 11. A picture of the Flamenco Party on Thursday evening.

Evaluation and Conclusions

Overall, the School was deemed to be very successful as judged by the majority of positive comments written by the participants. The attendees were asked about three major items: the quality of the scientific programme, the demonstrations Fair, and the organisation (Figure 12). These are some of the comments:

"I really enjoyed my time, learned a lot, met some really enthusiastic students and thankfully didn't have much of a hangover from the sangria on Thursday night." (Martin Caffrey, speaker).

"It was my great pleasure to be a part of your School... you did super job and I am looking forward to the 9th run:)... (Ivana Smatanova, speaker).

"Was a pleasure and honour to be a part of ISBC 2023. The meeting, the talks, the posters were all of such high standard. This year got to experience 'the Rain in Spain on the plains' for the first time &😊"#\$% Thank you once again for everything". (Lata Govada, academic).

"It was wonderful to see everyone again in 3D after such a long time! Thank you Gavi, JuanMa and team for organizing such a wonderful workshop again. I know it is a lot of work, but everyone one of us including students and instructors, appreciate everyone's effort, energy and enthusiasm." (Joseph Ng, speaker).

"Yes, indeed- thanks to all of the organisers for putting together a wonderful course for the students and participants." (Tom Peat, speaker).

"It really was a pleasure to be a part of ISBC 2023! I enjoyed the science, time in Spain, and time with friends. Thank you and your team for everything." (Crissy L Tarver, academic).

"MUCHAS GRACIAS to you and to all the school organisers. It was a great pleasure to take part in ISBC2023 and to have the opportunity to meet the biological crystal grower community again after such a long time for such a high quality event in Granada." (Monica Spano, speaker).

"Thank you very much for hosting us for such a great meeting! I enjoy the energy of teachers and students, active discussions, and exchanges of ideas. I am glad

that everybody is well after 4 years. Take care and see you again!" (Naoko Mizuno, speaker).

"Thank you so much for organizing such a great event! I am really grateful for the opportunity to contribute and meet you all in person! Muito obrigada :) (Filipa Castro, speaker).

"Thanks very much for organizing this wonderful meeting/workshop. As always, everything was superb. The talks very exciting; the students, very talented and had great posters. Thanks also to everyone for this effort." (Guillermo Calero, speaker).

"Thank you to you and your team for organizing the workshop again, and making it run so smoothly. It brings together many old friends and helps creates new ones. It also showcases the amazing beauty of Spain. I love Granada and I love the country. I will say it once more – Thank you." (Edward H. Snell, speaker).

There was a general feeling among the participants that the School had been very valuable partly because of the quality of the programme and partly due to the contribution of some of the best lecturers for the wide range of topics covered.

All in all, the ISBC2023 was an enriching experience for all of those involved triggering several fruitful scientific discussions. The positive approach, the openness and active participation of each of the participants made it a wonderful experience worthwhile to be repeated in the future.

Finally, we would like to express our gratitude to all of the participants; to the teachers for their full commitment and to the students and colleagues from academic and industrial background for believing in these Crystallization Schools. We also wish to express our heartfelt thanks to the Members of the Organizing Committee for their substantial contributions to the Schools. We are very grateful to all the people who have worked very hard in preparing the Schools to make it successful. Last but not least, we would also like to express our special gratitude to the Sponsors and Exhibitors for their great support.

Figure 12. Top: Opinion of the delegates about the quality of the scientific programme; Middle: Opinion of the delegates about the quality of the presentations; Bottom: Opinion of the participants about the quality of the demonstrations fair.

Figure 13. Top: Opinion of the delegates about their expectations for the School; Middle: Opinion of the delegates about the location and venue; Bottom: Opinion of the participants about the duration of the course.

58th Course of the International School of Crystallography – Structural Drug Design 2023: Biology, Chemistry and Computers

Annalisa Guerri

2 - 10 June 2023

The Course, the 58th of the International School of Crystallography, was held at the Ettore Majorana Foundation and Centre for Scientific Culture. The Centre is situated in the old pre-mediaeval city of Erice (Italy) where four restored monasteries provide an ideal setting for scientific and professional exchanges. The event was initially scheduled for 2020 but postponed because of the Covid 19 pandemic. The number of participants was limited to 83, in addition 28 lecturers and workshop presenters, and the organizers of the conference. The participants included 65 (58,5%) men and 46 (41,5%) women, from 23 countries. Particularly, among the speakers there are 65% of male and 35% of female lecturers while among the students there were 60% of male participants and 40 % of female attendees.

Participants were largely from university (PhD students, postdoctoral and young researchers), with some industry participants.

The schedule for a typical day included a morning session, with four 45-minute lectures, followed by a lunch break. The afternoon session included different workshops/tutorials.

The aim of the organizers was to provide the students with an overview of the current structural and biophysical techniques and informatic tools used in the field and their applications in different areas. The program was subdivided by topic, each day covering a particular theme: Introduction to the general techniques (crystallography, CryoEM, Machine Learning), biophysics and binding (computing and measuring binding affinity, conformational and allosteric landscapes), Informatics (Machine learning, docking, FEP, Molecular dynamics), small molecule chemistry (compound design, compound optimization, crystal structure prediction), biologics (rational design, and developability) and case studies describing the many steps in the process of drug discovery, from initial library screening to back-up studies. After each lecture, some time was set aside for discussion.

Nine workshops were offered to the participants in the afternoons, providing hands-on experience on a diverse set of techniques necessary in Drug discovery from ligand fitting into electron density maps, to cryoEM data processing, to in silico drug discovery and optimization using different software to biologics design. Each workshop was repeated at least twice, to give the participants more opportunity to attend.

Two poster sessions were held in the evening, giving the young participants a chance to showcase their work and discuss with the lecturers and more senior participants. Sixty-six posters were presented in total, half in each session. Each poster session was preceded by a poster preview session (at lunchtime), to increase the time for poster viewing and informal discussions.

During the last afternoon, two talks, one describing the trials and tribulations of starting a new company and one offering a vision for where structural biology and drug discovery could be in 10 years, provided ground for a final discussion.

The lecturers and workshop organizers were a mix of individuals from pharmaceutical companies and academia, all with a very high level of expertise and that represented the different branches of science required to meet the diverse challenges of drug design.

Awards and participant feedback

66 abstracts were submitted for poster presentation, among these, ten were selected for a short oral presentation (12 minutes + 3 minutes question time).

During the closing ceremony, several awards were presented. For the posters, the first place was assigned to Zuzanna Kozicka (University of Basel, CH); the second place was assigned to Francesca Vallese (Columbia University, New York, NY, US) and the third ones was conferred to Dennis Peter Stegmann (Swiss Light Source, Villigen PSI, CH).

The Lodovico Prize (acknowledging the most active student inside and outside the lecture hall) was given to Kristýna Adámková (Institute of Biotechnology of the Czech Academy of Sciences, Prague, Czech Republic).

At the end of the Course, participants were asked to participate in a survey to judge and comment on the quality of the Course. Their responses indicates that a similar meeting should be held at least in 3-4 years' time and that the course have been successful in most of its objectives (score 85/100).

Special event

During the course a “special event” was organized to further promote participants socialization and interactions outside the lecture and workshop halls (Icebreaker). Eight groups were formed (each including a lecturer as well) and given the objective of identify one aspect of the Course they most enjoyed, and then present the outcome in a 5-minute presentation at the end of the last day. The presentations were very creative and extremely entertaining and provided a nice intro to the Course final remarks.

Photo1: Winner of the Lodovico Prize (center) Kristýna Adámková (The Czech Academy of Sciences, & University of Chemistry and Technology Prague, Czech Republic) with Director of the Course (left), Giovanna Scapin (NanolmagingServices, US) and ExecSecretary (right), Annalisa Guerri (University of Florence, Italy).

Photo2: The three winners of the poster prizes, from left to right: Dennis Peter Stegmann Swiss Light Source, CH (third prize), Francesca Vallese, Columbia University, NY, US (second prize), Zuzanna Kozicka University Hospital Bonn, DE (first prize), Annalisa Guerri and Giovanna Scapin.

Photo3: Group Photo

29th Slovenian–Croatian/Croatian–Slovenian Crystallographic Meeting

Author not stated in source

The 29th Slovenian–Croatian/Croatian–Slovenian Crystallographic Meeting (SCCM 2023) was held on 14–18 June 2023 in Topolšica, Slovenia. There were 60 registered participants from Austria, France, Germany, Morocco, Ukraine, the United Kingdom, Croatia and Slovenia.

Four plenary lectures were presented: Crystal engineering of organic and metal-organic multicomponent halogen-bonded solids by Dominik Cinčić, Univ. of Zagreb, Croatia; Order from disorder: towards molecular architecture of the muscle Z-disk assembly by Kristina Djinović-Carugo, EMBL Grenoble; High-pressure phase transitions in molecular crystals by Simon Parsons, University of Edinburgh, United Kingdom; and DFT modelling of materials and crystal structures using periodic-boundary conditions by Anton Kokalj, Jožef Stefan Institute, Slovenia.

Besides that, 45 short oral presentations were given, which addressed contemporary topics in crystallography: structure determination of organic, inorganic and coordination compounds, crystal architecture, engineering and design, phase transitions, structure–property relationships, synergy of diffraction and complementary techniques etc. One of the advantages of the Slovenian-Croatian meetings is that all participants present their work as short oral contributions, which is especially important for young scientists who therefore have the possibility to deliver their results in friendly but professional atmosphere. At this year's meeting, the young scientists were offered the possibility to enter the best presentation award competition – it turned out that there were 28 competitors in three different categories (MSc students / PhD students / postdoctoral researchers who

defended their theses not more than five years ago). While all presentations were excellent, the jury unanimously awarded the following presentations:

MSc student Lea Čolakić (University of Zagreb, Croatia), Picky halogen bonding in isocyanate-based Werner complexes; PhD student Erik Uran (Jožef Stefan Institute, Slovenia), Salts, adducts and cocrystals formed in reactions of SO₂ with organic amines, and postdoc researcher Ivica Cvrtila (Ruđer Bošković Institute, Croatia), Chiral crystallization of hippuric acid from carvone.

Another special award for an outstanding presentation on contemporary topics in chemical crystallography and advances in small-molecule crystallographic information sponsored by the CCDC was awarded to Klemen Motaln (Jožef Stefan Institute, Slovenia), The elusive crystal structure of XeOF₂.

The representatives of CCDC also held a hands-on workshop focusing on Mercury and its new features, such as CSD Particles.

The meeting was co-organized by the Faculty of Chemistry and Chemical Technology, University of Ljubljana, and the Croatian Crystallographic Association under the auspices of the University of Ljubljana and promoted by the Slovenian Chemical Society. There was no registration fee; therefore, we thank the sponsors and advertisers: CCDC, Renacon, Rigaku, Aparatura, Mettler-Toledo, Vigor, Mitegen, Technobis, Dectris, Optik Instruments, Aparatura, Lek-Sandoz, Krka and Scan.

More information about the meeting can be found on the webpage of the meeting: SCCM 2023 – 29th Slovenian-Croatian Crystallographic Meeting 2023 (uni-lj.si)

Photo: best presentation award winners; from left Ilaria Gimondi (CCDC), Ivica Cvrtila, Erik Uran, Lea Čolakić, Klemen Motaln and chairs of the meeting, Prof. Anton Meden and Prof. Marijana Đaković. (Photo taken by Mirela Dragomir).

CCDC news and updates

Author not stated in source

Blog - Boosting Research Efficiency in Industry with FAIR Data

In this blog (based on the webinar 'Boosting Research Efficiency in Industry with FAIR Data') we discuss the FAIR data principles and their potential. Topics include how these principles are applied at the CCDC and how the chemical industry can benefit from them. Read more.

New CSD-Particle Online Training Courses

We have six online training courses to help you learn the basics of how to use the CSD software. The latest course added to the collection is "Surface Analysis with CSD-Particle", presented in a "watch, try, test" format, allowing you to receive a completion certificate for your efforts.

Alongside these free courses, if you want to learn more about CSD-Particle, we have two new self-guided workshops: "Surface Analysis with CSD-Particle Tools in Mercury" and "Investigation of New Plastic and Elastic Properties Tools in Mercury." In these workshops, you can explore the chemical and topological properties of particle surfaces and slip planes in crystals using a step-by-step workshop guide.

New How-To Videos

Discover how Mercury makes it easy to explore symmetry in crystal structures and how Mogul can be used as a structure validation tool during crystal structure refinement. Watch the videos to learn more.

Upcoming Events

In 2023 we are attending and sponsoring many events worldwide and delivering free virtual workshops and webinars. Visit our events page here for the full list.

7–12 July 2023: Meet us at the 73rd ACA Annual Meeting

The CCDC is exhibiting, presenting, chairing talks, and running the CSD leaderboard. Don't miss this opportunity to meet our team. Find out more

20th July - Webinar: CSD Python API for Ensemble Docking

The CSD Python API is an advanced toolkit for carrying out in-depth searching and chemical analyses of the chemical data in the Cambridge Structural Database (CSD). It provides customizable capabilities for users to develop their own automated workflows and analyses, and to perform large-scale standard analyses for knowledge sharing. Register here

13–17 August 2023: ACS Fall - Harnessing the Power of Data

Join the CCDC talk on Algorithm Development and Data Analysis in Chemical Space (CINF), presented by Jeff Jeff Lengyel, Materials Scientist. Find out more.

If you would like to suggest topics for our workshops and webinars email us at hello@ccdc.cam.ac.uk.

Follow us on Social Media

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A HALL OF FAME OF CRYSTALLOGRAPHERS AND RELATED SCIENTISTS

Istvan Hargittai and Magdolna Hargittai

This hall of fame, the Earth Science Museum at Lomonosov Moscow State University, is part of our universal scientific and cultural values. In the current tragic situation in 2023, we are moved to dedicate this account to those brave men and women who are being persecuted in Russia for protesting and condemning the ruthless and unjustified war by their country against Ukraine.

Floors 24–28 of the famous high-rise building of Lomonosov Moscow State University house an Earth Science Museum. It was established around 1950, at the time of the inauguration of this building, where much of the university relocated from downtown Moscow. The building has a magnificent location on the Vorobyovi Hills, which was called Lenin Hills at the time. After the collapse of the Soviet Union, its name was changed back to its pre-Soviet name, Vorobyovy Hills, but the official address of the university remained 1 Lenin Hills.

The tower of Lomonosov Moscow State University. The Earth Science Museum is in the top rectangular portion of the tower, floors 24–28

The top round portion of the tower houses the Rotunda, which is a festive hall. The top rectangular portion consists of 5 floors, and that is the museum. The museum also functions as an extended study room for students of various subjects, such as crystallography, geography, geology, anthropology, biology, environmental science, soil science, etc.

When the university was moving from downtown to the new location, considerable funds were devoted to an almost luxurious interior, which has, over the decades, considerably degraded as a result of the use and neglect. Still, the museum has kept much of its old glitter. A substantial part of its elegance comes from the large number – at least seventy-five – of busts of scientists. They were all created at the time of the museum's establishment by many of the best sculptors in the Soviet Union at the time.

Classroom exercise in Hall 8, 2016.

The 5 floors of the museum comprise 24 exhibition halls totaling an area of 25 hundred square meters (27 thousand square feet). On descending from Floor 28, the numbering of the halls increases. Each floor has a specific topic. Our recent book about science in Moscow [1] presents this museum floor by floor, hall by hall, and bust by bust, and there are many of them, including a few commemorating international scientists. In this contribution, we single out a few busts. For them, we indicate the names of the sculptors. The date of erection

of the busts was uniformly around 1950. All photographs in this paper were taken by the authors unless indicated otherwise.

In this account, 6 of the memorials are presented. Charles Darwin is mentioned for his general importance. The other 5 were crystallographers or closely related mineralogists and geologists. The careers of two of the scientists, Evgraf F. Fedorov and Vladimir I. Vernadsky, are presented in some detail.

In Hall 7, focusing on the methods of geological research. Here is a Charles Darwin (1809–1882) statue sculpted by the internationally renowned artist Sergey T. Konenkov

Bust of Nikolai I. Koksharov (1818–1893) by M. A. Gritsuk. Koksharov described the morphology of many minerals, and his bust stands in Hall 11, focusing on the occurrence of non-metallic ores.

From left to right: Suess plaque at 4 Duncan Terrace, N1, London [2]; bust (1928) in Schwarzenberg Square in Vienna; and bust by B. D. Korolev in Hall 5, Earth Science Museum

Eduard Suess (1831–1914) was an Austrian geologist of international fame, and a professor at the University of Vienna. He was born in London, and the Geological Society of London has commemorated his birthplace with a commemorative plaque. His family moved from London first to Prague, then to Vienna, where he completed his studies. He researched the geography of the Alps and was a pioneer in considering the issues of ecology in scientific discussions.

Bust of Evgraf F. Fedorov by A. V. Grubbe in Hall 8 and his photograph from about 1900 (Evgraf Fedorov Mondadori.jpg - Wikimedia Commons, public domain, accessed 03/04/23

Evgraf F. Fedorov (1853–1919) was a crystallographer and mathematician. He was born in Oranburg, Russia, lived most of his life in St. Petersburg, and died in Petrograd (but it was the same city). The name of St. Petersburg was changed in 1914 to Petrograd as an expression of nationalism. In 1924, it was changed to Leningrad, and today it is once again St. Petersburg, following a 1991 referendum. Fedorov's father was a high-ranking engineer-general who died when Fedorov was 14 years old. His mother brought up her 4 children. Fedorov studied in military schools and began military service. In 1874 he left it and started attending medical school lectures without being officially enrolled because of his lack of the proper high school (secondary school) diploma. After one year, he switched to the institute of technology to study chemistry. After one year, he changed again and embarked on a tour of Western Europe. He worked in typography, and upon his return to Russia, he published newspapers.

Fedorov became interested in crystallography, and in 1880, he enrolled at the Mining Institute, from which he graduated in 1883. He participated in geological expeditions in the Ural Mountains, and for a while, he and his family moved to the region in these mountains to ease their financial situation. His scientific contributions helped his advancement. He was appointed to professorships in St. Petersburg and in Moscow. In 1901, at Vladimir Vernadsky's recommendation, he was awarded the degree of doctor of mineralogy and geognosy, the latter being the science of the origin and distribution of minerals in the earth's crust – by now, an obsolete term which has given way to a broadened meaning of geology. During the 1905 revolution, he was elected to be the director of the Mining Institute. No such elections have taken place before or since. His appointment was terminated in 1910 and he continued at the institute as a professor of crystallography and petrography. His highest recognition was his election to the Academy of Sciences in 1919. However, in the same year he died of pneumonia caused at least in part by lacking food and heating in revolutionary Petrograd.

Fedorov's significant scientific production centered around crystallography. His most famous contribution is the derivation of the 230 three-dimensional space groups of symmetry. At about the same time, the English William Barlow (1845–1934) and the German Arthur Schoenflies (1853–1928) also derived the 230 space groups. The simultaneity of this discovery by the three authors, operating independently of each other, does not diminish the importance of their individual contributions. Of the three, Barlow's achievement is rather peculiar as his approach was largely intuitive. He considered oriented motifs: he hung pairs of gloves on a rack, thereby making space group models. We know from Marjorie Senechal about his empirical approach: "He bought gloves by the gross, so the story goes, mystifying the sales lady by answering 'I don't care' to her first question, "What size, sir?" [4].

Fedorov's five polyhedra, which can fill space in parallel positions. After Marjorie Senechal [5]; reproduced with permission.

Fedorov's lesser-known studies included a systematic investigation of space-filling parallelohedra. He determined all five that can fill the space in parallel orientation without gaps or overlaps: the cube, the hexagonal prism, the rhombic dodecahedron, an elongated rhombic dodecahedron with eight rhombic and four hexagonal faces, and the truncated octahedron. They are shown here after Marjorie Senechal [5].

Interior of the museum, Hall 9, with the busts of Aleksandr E. Fersman (by A. V. Babichev) and Vladimir I. Vernadsky (by E. M. Vilensky), highlighted.

Vladimir I. Vernadsky (1863–1945) was an internationally renowned geochemist, crystallographer, geologist, and contributor to many other fields of science. He was also a science historian and an organizer of scientific institutions. His father was a descendant of a Zaporozhye Cossacks, and his mother came from a Russian noble family. Vernadsky was born in St. Petersburg, studied in a Kharkov gymnasium from 1873, and completed his high school education back in St. Petersburg in 1880. During 1881–1885 he studied at the Physics and Mathematics Faculty of St. Petersburg University. He participated in soil science expeditions and was a student of the soil scientist Vasily V. Dokuchaev. Dmitry I. Mendeleev was among Vernadsky's professors.

Vernadsky was actively engaged in mineralogy during and after his university studies. He traveled to Italy, France, and Germany as part of his education. From 1890, he held professorial appointments in crystallography and mineralogy at the Imperial Moscow University. Many future well-known mineralogists were among his students. He became full professor in 1902. In 1911, he resigned along with many of his colleagues, to protest the ministerial policy of considerably curtailing university autonomy.

Detail of the front of the Ukrainian banknote 1000 Hryvnia with Vernadsky's portrait and his words: "Я вірю у величне майбутнє України" (I believe in the great future of Ukraine).

Vernadsky moved from Moscow to St. Petersburg and worked in the Geological Museum. For years he drew ever closer to the Academy of Sciences. Following the revolutions, he was among the founders of the Ukrainian Academy of Sciences and served as its first president. He did not stay long in Ukraine and returned to St. Petersburg. The next few years were turbulent in his life, as they were for the entire country, which in the meantime had become the Soviet Union. At one point, he was arrested and jailed but soon freed because of protests by various leading scientists.

Vernadsky was involved in creating institutions dealing with the new science of radioactive materials. He participated in expeditions to uncover sources of radioactive minerals. In 1922–1926 he often lectured in Paris and published a text on geochemistry in the French language. He became engaged in studies of improved utilization of natural resources and in drafting plans for the electrification of the Soviet Union, called GOELRO. He was active in building up the network of scientific institutions in Moscow after they had been moved there in 1934 from St. Petersburg. He and his closest colleagues, Aleksander E. Fersman among them, quietly survived the years of Stalinist repressions during the second half of the 1930s [1].

Vernadsky was not blind to the lawlessness of the tyranny and condemned its supporters among scientists. We mention one example. Vasily R. Vilyams (1863–1939) was among the founders of soil science in Russia. Under the Soviet system, however, he concocted unscientific plans causing harm to agriculture in the Soviet Union (also in Eastern Europe after World War II when Vilyams had long been dead, but his teachings had survived) [6]. Scientists who disagreed with Vilyams may have faced tragic consequences, even execution. A few years after Vilyams's passing, Vernadsky wrote that Vilyams left behind a bad and distorted school and that he used inaccurate data, which often contradicted reality. Vernadsky noted that Vilyams having joined the communist party did not make him a better scientist and predicted that he would soon be forgotten. Vernadsky's assessment of Vilyams's activities was correct, but not his prediction that Vilyams would be soon forgotten [6]. To this date, there is a conspicuous cult of Vilyams in Russia, complete with his large statue in Moscow and other measures to commemorate him and his teachings, including a bust in the Earth Science Museum. To be fair, however, we note that Vernadsky also has a cult, deservedly, with memorials in numerous places both in

Russia and Ukraine. There is a magnificent Vernadsky Geological Museum at 11 Mikhovaya Street in downtown Moscow.

Aleksandr E. Fersman (1883–1945) was a mineralogist, crystallographer, and geochemist. The author Aleksey Tolstoy called him “the Poet of stones” [7]. Fersman completed his studies at Moscow University and was among Vernadsky’s disciples. From 1917 to the end of his life, he was the director of what is today the Fersman Mineralogical Museum at 18 Leninsky Avenue in Moscow. During World War II, he was responsible for the evacuation of the most valuable minerals from the museum and for their safe return in 1944.

The Earth Science Museum is, in principle, open to the public, and there is no entrance fee. In practice, it is not easy to be admitted, and already entering the tower of the university is possible by permission only, and entering the museum is only by appointment. Unfortunately, we cannot offer any information on how one goes about getting the necessary paperwork for such a visit (we mean under peaceful conditions; under the current war, it is meaningless to contemplate such a visit). Again, supposing peaceful conditions, if one succeeds in getting through the red tape, such a visit offers a unique and unforgettable experience both for experts of earth sciences and crystallographers and for laypersons as well. Our last visit was in 2019, and the visit during which we photographed all the busts in the museum took place in 2016. On both occasions, our visits were arranged through personal connections rather than through official channels. The associates of the museum are most helpful in assisting the visitor; they are exceptionally knowledgeable and display obvious pride in presenting the riches of their institution.

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SIG4 Publication Award for 2023

Tatiana E. Gorelik, chair of SIG4

Electron crystallography (3D ED/MicroED) has experienced significant growth in recent decades as a powerful method for structure determination. Many crystal structures that were previously challenging to determine using classical crystallographic techniques can now be elucidated with the aid of electron diffraction. Recognizing the importance of this field, the flagship journal of the International Union for Crystallography (IUCr, <https://www.iucr.org/>) – IUCrJ (<https://journals.iucr.org/m/>) has introduced a dedicated section on electron crystallography.

To further support method development and encourage innovative applications of this technique, the Special Interest Group for Electron Crystallography (SIG4, <https://ecaelectronsig.wordpress.com/>) of the European Crystallographic Association (ECA, <https://ecanews.org/>) has established a distinguished publication award in the field of electron crystallography. The award committee consists of internationally renowned scientists,

including established electron diffraction experts and newcomers to the electron crystallography field. The involvement of diverse committee members ensures an unbiased evaluation of the submitted nominations.

After carefully evaluating the nominated publications, the committee unanimously decided to present the SIG4 Distinguished Publication Award for 2022 to the paper titled "Direct Location of Organic Molecules in Framework Materials by Three-Dimensional Electron Diffraction" by Meng Ge, Taimin Yang, Hongyi Xu, Xiaodong Zou, and Zhehao Huang, published in the *Journal of the American Chemical Society* (Ge et al., 2022, 144, 15165–15174, <https://doi.org/10.1021/jacs.2c05122>).

The presented research is driven by the application of electron crystallography to framework materials. It clearly delivers a number of important structures which illustrate the power of the technique. The authors provide ample detail regarding the structure solution process, refinement, and a careful analysis of the factors influencing the outcome. This work illustrates to a wider, more applied audience that some of the promise of electron diffraction is now possible, i.e. the location of hydrogen atoms, and provides a basis by which others may follow. This paper 'moves the dial' in terms of demonstrating the power of electron crystallography while giving an empowering feeling that others can achieve the same kind of results. The chemistry that this paper presents, made possible by electron crystallography, is both exciting and indicative of the promising future of this technique. Consequently, this publication surpasses being perceived as "just another demonstration of the power of electron crystallography" and stands as much more than that.

Meng Ge, the first author of the awarded publication.

We extend our heartfelt congratulations to the authors of this publication and wish them continued success in their future endeavours. Furthermore, we eagerly anticipate the publication of other exciting research in the field of electron crystallography in the years to come.

Uri Shmueli (1928–2023)

Carolyn P. Brock

Uri was born on 13 May 1928 in Kraków, Poland. His parents, Moshe Szmulewicz and Nina Seidenfrau Szmulewicz, both of whom were Hebrew teachers and Zionists, named their only child Uriel. He did not become Uri Shmueli until 1954.

In his memoirs dated 2013 ([insert link](#)) Uri described his childhood as happy. There were skiing vacations in the winter and two months in a family camp each summer. But Jews in Poland were also subject to increasing harassment. Walking to school could be dangerous.

Starting in September 1939 life for the Szmulewicz family became difficult (see the memoir). When it became illegal for him to attend school, Uri's mother taught him Hebrew, Bible and German, and arranged lessons for him in Polish, history, Latin, mathematics, geography, natural history, and English. The lessons continued after the family moved to the nearby town Wieliczka, where much of his mother's family lived. At 13 Uri had his Bar Mitzvah, necessarily in a private house because the synagogues had been closed. Later he found he was unwelcome for prayers in two different minyans because at home his family spoke Hebrew, the holy language, and because he knew no Yiddish.

The family was separated in August 1942. Uri and his father were sent to a work camp in Płaszów, where they were still allowed to wear their own clothes; somewhat later they were relocated for a time to the Kraków ghetto. Because their factory made electrical cables and Bakelite sockets, they were protected as essential workers. Uri made friends in the camp and, because of his skills, became an informal apprentice to his department's mechanic. He remembered that there were supervising Poles at the camp who were kind to him. One sneaked him a book about the theory of sets.

In January 1944 Płaszów was converted into a concentration camp. That August Uri and his father were among the 4500 put on a train for KZ Mauthausen, where they were separated. Uri ended up at the subcamp KZ Linz III, located on an island in the river Traun, where conditions became steadily worse as the end of the war

approached. In May 1945 Uri finally became free, eight days before his 18th birthday. Shortly thereafter he learned that his father had perished. Of his whole extended family, only a few cousins had survived.

From August 1945 – November 1947 Uri was in Italy, first in a youth camp near Bari and later in Rome. He managed to learn enough on his own to pass, in Italian, the exams for an external, scientific, high school degree.

Uri had many gifts; one of them being for languages. He learned Hebrew and Polish as a child, and had good training in German, English, and Latin. In KZ Linz III he learned Russian because it was the language spoken by most of the prisoners in his Block. While in Italy he learned Italian and Yiddish, which during his childhood his parents had retained as their private language.

Using false papers Uri entered Palestine in November 1947. He settled in Tel Aviv, where he first worked as salesman of oil products but then apprenticed as a grinder of optical lenses. He was, to his regret, found unfit for military service. In Tel Aviv he met Miriam Ajzenfeld, and they were married in 1954. She encouraged him to continue his studies and then worked to support them both while he did.

At 28 Uri started university at the Technion. He described the first year as being incredibly difficult because of all he had forgotten while grinding lenses, but he succeeded, earning a B.Sc. in physics in 1960, and an M.Sc. in 1961. From there he went to the Weizmann Institute for graduate studies in polymer crystallography. By late 1961 Uri and Miriam were secure enough to start a family. Their son Rami was born in 1962, and their daughter Yael in 1967.

After completing his Ph.D. in 1966 Uri joined the teaching staff of Tel Aviv University. There he set up the Laboratory of Chemical Crystallography. That lab was later taken over by one of his students, the late Professor Israel Goldberg, who became Uri's longtime collaborator and very good friend. The Cambridge Structural Database includes 35 structures from Uri's work in that lab.

Uri published papers about the crystal packing and thermal motion in donor-acceptor compounds and on the effects of molecular vibrations on NMR spectra. His 1974 paper Libration of 9, 10-Anthraquinone at 5 Temperatures with Peter Kroon in Vol. A of Acta Cryst. was pioneering in its analysis of thermal motion in a crystal studied at multiple temperatures. He was one of the eight authors of the 1996 publication in Acta A titled Atomic Displacement Parameter Nomenclature - Report of a Subcommittee on Atomic Displacement Parameter Nomenclature. That 12-page report has been cited a surprising 284 times.

Towards end of the 1970s Uri became interested in structure-factor statistics, which remained his focus until and beyond retirement. His last paper was published in J. Appl. Cryst. in 2016. Altogether there were more than 80 publications that have been cited nearly 1700 times.

In 1982 Uri started his long service as editor of Vol. B (Reciprocal Space) of International Tables. (Vol. B is the successor of Vol. II of the "red" series). He edited the 1993, 2006 and 2010 editions, and wrote more than a few of the included articles. The staff in Chester very much appreciated his diligent and careful work, and they remember him very fondly as a friend and as a pleasure to work with. He was always polite and kind, and always very tactful.

Uri retired in 1996. The next few years were marred by the passing of his wife Miriam in 1997 after a long illness. Later, however, Uri enjoyed the long, productive, and happy retirement that he so deserved. He wrote a book (Theories and Techniques of Crystal Structure Determination, Oxford University Press, 2007), and continued editing Vol. B of International Tables.

In his later years Uri also reconnected with Magda Leuchter, whom he had first known in 1947 while in Rome. They shared 25 years together and enjoyed their combined four children and eleven grandchildren.

In 2001 and 2003 Uri returned to Poland after an absence of more than 60 years. The first trip was to deliver a plenary lecture at the European Crystallographic Meeting; the second was to show his family the places where he had grown up. Later Uri became involved in projects to remember the Jewry of Wieliczka (see <https://www.youtube.com/watch?v=C4bzb2wut0I>, especially minutes 9:30 – 16:30).

No remembrance of Uri can be complete without mention of his remarkable personal qualities. I first met him in 1981 in Tel Aviv and was immediately struck by his humanity. He was gentle and kind, but also tough. I remember him as surprisingly hopeful and optimistic about mankind. At Tel Aviv University he was recognized year after year as a beloved instructor whose door was always open. His memoir shows that he made friends easily with all kinds of people, learning their language if necessary. People were drawn to Uri. While he described himself as secular, he shone with a kind of inner light that was appropriate for somebody who had been given the name of an archangel.

I am very grateful for Yael Shmueli-Friedland's help with this remembrance.

Aldo Félix Craievich (1939-2023)

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Keywords: Obituary; Aldo Félix Craievich

On April 24, 2023, we received the very sad news of the passing of Prof. Dr. Aldo Félix Craievich at the age of 84. He was a brilliant Argentine-Brazilian crystallographer who not only had the remarkable vision to create the first synchrotron in the Southern Hemisphere but also played a leading role in the construction of the Brazilian Synchrotron Light Laboratory (LNLS) in Campinas, São Paulo, Brazil, serving as its first deputy director and head of the scientific department. He coordinated the projects of the LNLS beamlines and the construction of the first seven of them, but also, he put in a lot of effort to create the user community of LNLS. He organized and gave by himself numerous courses and conferences on synchrotron light techniques throughout Latin America, becoming a mentor and great teacher for many crystallographers in the region.

Aldo was born in 1939 in the city of Zavalla, in the Province of Santa Fe, Argentina, and lived in this country until age 34, except for when he resided in France to conduct the research work for his Ph.D. thesis. He graduated in Physics in 1964 at the Balseiro Institute of the National University of Cuyo (San Carlos de Bariloche, in the Argentine Patagonia), where he received a highly advanced education that profoundly impacted his future career as a researcher. In 1965, he joined the Institute of Mathematics, Astronomy, and Physics (IMAF, currently FaMAF) of the National University of Córdoba (UNC, Córdoba City), where he was tasked with creating a laboratory of X-ray techniques. To gain a deeper understanding of these techniques and complete his training in experimental physics, he decided to undertake a Ph.D. In mid-1966, he moved to the Laboratoire de Physique des Solides (LPS, Laboratory of Solid-State Physics) in Orsay, France, which at that time was part of the University of Paris and later became part of the newly established University Paris-Sud or University Paris XI (nowadays University Paris-Saclay). Thanks to the support of the authorities at IMAF and of another Argentine who had worked there, Alberto Bonfiglioli, Aldo was able to join the research group of the renowned crystallographer André Guinier, widely known for his contributions to small-angle X-ray scattering (SAXS) among others. Aldo presented his Ph.D. thesis at the Balseiro Institute in early 1969 and from that moment on, he resumed the establishment of the X-ray laboratory at IMAF, installing X-ray diffraction and SAXS instruments. In the case of the latter, this was the second one in the country, following the facility implemented by Bonfiglioli at the Constituyentes Atomic Center of the National Atomic Energy Commission (CAC-CNEA) in Buenos Aires. Unfortunately, both SAXS facilities were discontinued some years later when both researchers left their institutions, and Argentina did not have similar instruments for decades. This situation only started to change a few years ago, largely thanks to Aldo's work in teaching and promoting X-ray techniques and Crystallography.

Aldo worked at IMAF for a few years and published the first papers using the equipment from the laboratory he established. However, in 1973, he accepted an invitation from Prof. Yvonne Mascarenhas to work at the Institute of Physics and Chemistry of São Carlos (IFQSC, now IFSC) in São Carlos, São Paulo State, Brazil.

There, he set up the first SAXS instrument in Brazil, making again a valuable contribution to the region. He initially planned to stay at IFQSC for only one year, but because of the serious political situation in Argentina, he extended his stay, and years later, when the Argentine democracy was restored, he led the very important project to create a synchrotron facility. As a result, Aldo resided in Brazil for the rest of his life. In relation to this, it is worth mentioning that Aldo never forgot his home country: he was always grateful for the education he received and returned many times to visit family, colleagues, teachers, and friends. Furthermore, he made significant contributions to the progress of science in Argentina.

At IFQSC, Aldo continued his previous work on glassy materials using SAXS experiments but after a few years, he decided to align his research work with the institute's trend of studying biological systems and started by exploring organic molecular crystals. To deepen his knowledge in this area, he embarked on a postdoctoral stay at the LPS in 1976, returning to IFQSC the following year to initiate this new line of research, which also relied on SAXS experiments.

In 1980, Aldo decided to leave São Carlos to undertake a new challenge in Rio de Janeiro: the creation of an X-ray laboratory at the Brazilian Center for Research in Physics (CBPF), an institution that had a reputation for excellence in theoretical research. Since he had to wait approximately a year for the purchase of the instruments, he decided to do another stay in Orsay, but this time at the recently established Laboratoire pour l'Utilisation du Rayonnement Electromagnétique (LURE, Laboratory for the Use of Electromagnetic Radiation). At that time, synchrotron radiation sources were still in their early development stages, and the LURE laboratory, being one of the first facilities open to users, played a crucial role in expanding the use of techniques based on this radiation. During Aldo's stay at LURE from 1981 to 1982, which was aimed primarily at conducting in-situ SAXS experiments on glassy materials and exploring Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy, the idea of creating the first synchrotron radiation source in Brazil emerged. This initiative gained strength when Aldo organized a visit to LURE by the president of the National Council for Scientific and Technological Development (CNPq) of Brazil in early 1982. Shortly after, the Synchrotron Radiation Project (PRS) of CNPq was established. This was developed from 1982 to 1985, with Aldo serving as the director of its executive committee from 1983. This role led him to promote the project and the importance of synchrotron radiation techniques in Brazil and other countries in Latin America. Additionally, Aldo coordinated a CNPq scholarship program for human resource development in these techniques. Finally, in 1985, it was decided to create the Brazilian Synchrotron Light Laboratory (LNLS) in Campinas, São Paulo State, and in 1986, CNPq designated Cylon Gonçalves da Silva, a professor at the Institute of Physics of the University of Campinas, as the director of LNLS, while Aldo served as the deputy director.

The construction of LNLS took 10 years and had unique characteristics. Particularly noteworthy is the fact that most of the components needed for the first source, called UVX, and the beamlines were manufactured either at LNLS itself or by Brazilian industry. Undoubtedly, this project can be considered one of the most important milestones in science and technology in Latin America. While the UVX source construction project was led by Antonio Ricardo D. Rodrigues, Aldo took charge of leading the projects for the beamlines and the construction of the first seven, which were made available to users in July 1997. Additionally, Aldo recognized the vital importance of building a user community, the true "owners" of an open facility like LNLS, and to achieve this, he taught courses and lectures not only in Brazil but also in many other Latin American countries, including Argentina, Chile, Colombia, Cuba, Mexico, Peru, Uruguay, and Venezuela. In 1989, long before the laboratory was opened to users, he organized the First LNLS User Meeting, an activity that has continued every year and still takes place with increasing interest.

Photo taken during the VIII Annual Meeting of the Argentinian Association of Crystallography, in Santa Fe City, in 2012. Prof. Dr. Aldo Félix Craievich was recognized as a guest of honor of the National University of the Littoral.

It is worth noting that Aldo believed that, in order to successfully fulfil his important role at LNLS, he needed to stay updated with advances in synchrotron radiation instrumentation and techniques. Therefore, every year he returned to the LURE synchrotron as a user for at least one or two weeks. He continued conducting experimental work, particularly in the study of nanomaterials and glassy materials using SAXS technique, and publishing the results of his high-level scientific research work.

Towards the end of 1997, after many years of intense work and with LNLS operating successfully, Aldo decided to leave the institution and dedicate himself fully to research and university teaching. Therefore, in January 1998, he joined the Institute of Physics at the University of São Paulo (IF-USP) in São Paulo city, where he obtained a position as a full-time professor. However, he never distanced himself from LNLS. He not only remained a frequent user but also continued to work on building the user community. Aldo continued to deliver courses and lectures and promoted scientific collaborations with groups sharing similar research interests. It was during this time that I had the honour of collaborating closely with Aldo, sharing 20 years of scientific challenges, teaching activities, crystallography outreach, and friendship.

In 2009, upon reaching the age of 70, Aldo was forced to retire, as mandated by Brazilian law. However, he continued as a senior professor at IF-USP until the end of his days. He never stopped to travel the world to teach and learn, always with great enthusiasm. He followed with great interest the creation of LNLS's second source, Sirius, whose characteristics were discussed with users in the same year of Aldo's retirement. Construction began in 2013, and the first users were welcomed in 2020. Much earlier than its operational start-up, it was understood that Sirius would be one of the most advanced synchrotron sources in the world, a fourth-generation source, and that the user community needed to prepare itself to match such advancements. Aldo accompanied us in this process and encouraged us to continue growing as researchers. The COVID-19 pandemic and subsequent health issues prevented him from further travels, but he remained engaged in all LNLS activities and the numerous scientific societies that interested him, including the International Union of Crystallography (IUCr), the Brazilian Crystallographic Association (ABCr), the Argentine Crystallographic Association (AACr), the Latin American Crystallographic Association (LACA), the Brazilian Society for Materials Research (SBPMat), the Argentine Association of Materials (SAM), the Argentine Physical Association (AFA), among others. Regarding the IUCr, it is worth mentioning that Aldo served as co-editor of the Journal of Synchrotron Radiation from 2009 to 2020.

Aldo received numerous awards and distinctions throughout his career. In 1980, he became a full member of the São Paulo Academy of Sciences (Brazil) and, since 2015, also of the Brazilian Academy of Sciences. He received recognition from the LNLS (staff and users), ABCr, AACr, SBPMat, the National University of the Littoral, and the Balseiro Institute. Additionally, he received the Mercosur Science and Technology Prize twice (2004 and 2010), jointly with colleagues from Argentina and Brazil, in the "integration" category, awarded by UNESCO and the Network of Science and Technology of Mercosur (RECyT).

Working with Aldo was a fascinating experience, not only for me but also for many other colleagues. Whenever there was something we didn't understand, Aldo would take a pencil and start reasoning deeply, not letting go of the subject until the issue was resolved. He always encouraged us to comprehend the phenomena we were studying in great detail, believing that any question could be solved with enough effort. By sharing scientific activities with him, we discovered that we had so much more to offer as scientists if we didn't settle for superficial answers or quick solutions. Another aspect I want to highlight is that Aldo was incredibly generous and open with his knowledge, a quality that unfortunately is not always found and one we truly appreciated. Furthermore, Aldo was a person of great culture, and when he shared anecdotes of his experiences, he always left us with valuable lessons.

The first LNLS source, UVX, ceased operation in 2019 after 22 years. However, Sirius is now fully operational, and the construction of new beamlines shows a bright future ahead. In addition, after 40 years since the initiation of the PRS-CNPq project, the large Latin American user community, which was created through Aldo's generous teaching efforts, is now embarking on new challenges in the development of Sirius. The renovated synchrotron facility at LNLS and its well-established user community are the main legacies of Prof. Dr. Aldo Félix Craievich, who had the vision to recognize the tremendous importance of creating the first multi-user synchrotron radiation laboratory in the Southern Hemisphere and dedicated most of his scientific life to turning that vision into a reality. At the same time, he promoted the fundamentals of Crystallography and many of its techniques. In recent years, his SAXS courses in Argentina led to the establishment of two advanced instruments dedicated to this technique, both of them being opened to the scientific community. Following Aldo's example, the leading researchers of these SAXS facilities continue to disseminate the fundamentals and

applications of the technique he learned from Guinier. We will deeply miss Aldo, our dear friend, teacher, and mentor.

Carles Miravittles

Xavier Obradors, Elies Molins, Jordi Rius and Anna May-Masnou

Carles Miravittles | ICMAB, CSIC

We are deeply saddened to announce the death of our dear friend and colleague, Prof. Carles Miravittles, founder of ICMAB in 1986 and director of the center for 21 years, from 1986 to 2008. Carles passed away on April 16th, 2023, at the age of 80.

The legacy and memory left by Carles Miravittles, who was born in Barcelona on September 9th, 1942, is extraordinary, both for his human and professional qualities. He was a key figure in the creation of the Institute of Materials Science of Barcelona of the Spanish National Research Council (ICMAB - CSIC) and in the promotion of research in Catalonia.

Enric Banda, Carles Solà and Carles Miravittles

Carles, a visionary man

Carles was a person who loved Science, undoubtedly influenced by the figure of his father, Lluís Miravittles Millé (Professor of Applied Geology at the University of Barcelona, UB). He received his Ph.D. in Pharmacy under the supervision of Manuel Font-Altaba (Prof. of Crystallography of the UB) and performed several stays in the Dpt. of Chimie-Physique et Crystallography of the University of Leuven (Belgium), where he came in contact with Dr. Gabriel Germain, who, together with Prof. Michael Woolfson and Dr. Peter Main, was one of the leading scientists in direct-methods which were emerging as a powerful technique for solving crystal structures. In 1974, he was appointed as 'Scientific Researcher' at the Institute of Earth Sciences 'Jaume Almera' (now GeoSciences Barcelona) of the CSIC and contributed decisively to popularizing this methodology in Catalonia. During this time, his research interest focused on structural Crystallography and X-ray diffraction, mainly on organic compounds with pharmacological interest. In 1980, he organized the European Crystallographic Meeting (ECM-6) in Barcelona (Spain). He became Full Professor of the CSIC in 1986 and, in the same year, was nominated Director of the Institute of Materials Science of Barcelona (ICMAB).

Apart from his interest in scientific research, in the second half of the 1980s, he combined a very successful vision and a great capacity for work to create and promote the ICMAB in the first-world division of Materials Science research. He was able to mobilize this emerging discipline, anticipating it within the CSIC, achieving the creation of four new Materials Science Institutes in Spain and later promoting the existence of a "National Materials Science Plan". He was also very active in promoting the international collaboration of ICMAB with many research centers and institutions, mainly all around Europe. The debt we owe him goes far beyond the ICMAB community and extends to this field's scientific community.

Inauguration of the ICMAB building in 1991

On the other hand, Carles Miravittles' wisdom in promoting a new CSIC research center in the Bellaterra Campus of the Autonomous University of Barcelona (UAB) was the seed that later turned this campus into one of the largest research concentrations in southern Europe. Carles' ability to attract diverse talent and to convince political and institutional leaders to launch large-scale operations was flattering. And this is the legacy he has left to all of us at ICMAB: the passion for excellence, internationalization, and scientific ambition that has led us to be recognized twice as Severo Ochoa Excellent Centre in the area of advanced functional materials.

Jaume Casabó, Carles Miravittles and Andreu Mas-Colell

Carles Miravittles not only contributed to building the basic skeleton of the ICMAB, he was also determinant in other areas of management of the CSIC and his beloved Catalonia. First, as CSIC Delegate in Catalonia (from 1987 to 1992), where he was able to promote institutional relationships with the Generalitat de Catalunya. Later, by encouraging the CSIC to create a new research center in Nanoscience and Nanotechnology that

eventually became the current Catalan Institute of Nanoscience and Nanotechnology (ICN2). He also managed to collaborate with companies with the capacity to carry out research on the campus, creating the MATGAS Economic Interest Group, with the participation of the company Carbueros Metálicos (now, part of Air Products), the CSIC and the UAB. Once released from the direction of ICMAB, he agreed to become the director of the 'Eduardo Torroja' Institute in Madrid (2008- 2009) to modernize and reorganize the center. Finally, Carles Miravittles returned to ICMAB, and until a few days ago, he was still regularly coming to the Institute.

In addition to the positions and dedication to CSIC, Carles Miravittles was president of the Spanish Committee of Crystallography and, since 1993, a full member of the Royal Academy of Arts and Sciences of Barcelona, of which he was also vice-secretary. He was a member of the Chemistry Section of the European Academy, president of the Expominer Fair, and an academician of the Royal Academy of Pharmacy of Catalonia since 2016. In 1992 he received the Narcís Monturiol Medal in scientific merit from the Generalitat de Catalunya, for his dedication to the study of new materials and for contributions to the fields of crystallography.

Crystallography research group at ICMAB in 2012: (bottom, left to right): Oriol Vallcorba, Joan Esquiús, Xavier Campos; (top, left to right): Anna Crespi, Noelia García, Joana Martínez, Elies Molins, Muling Zeng, Ignasi Mata, Carles Miravittles, Anna Laromaine, Jordi Rius, Anna Roig, Cosmin Cotet, Marta Vendrell, Xavier Torrelles.

Carles Miravittles' human qualities and bonhomie were hallmarks that accompanied him throughout his life and were recognized by everyone. He distinguished himself by being very positive, kind to everyone, whether they shared his opinion or not, and always keeping a certain degree of irony and sarcasm about the research and administration management structures, both state and autonomous. In any case, his mastery of human relations at all levels and of political structures made him an undisputed leader among research managers.

To preserve his memory, the conference room of the ICMAB has been named after him.

ICMABers, when Carles Miravittles was director of the center

Xavier Obradors, Elies Molins, Jordi Rius, Anna May

They say about Carles...

"Carles is the person who has most influenced my scientific and professional career. He first encouraged me to move to ICMAB in 1989 when I was a young Full Professor at the Faculty of Physics of the University of Barcelona. His support and that of the president of the International Scientific Committee, Prof. Manuel Cardona, were decisive in creating a powerful research team in Magnetism and Superconductivity. Later, in 2002, he proposed me to be the deputy director of ICMAB and, finally, the 2008 director. I always thanked him for his trust in me and for the unconditional support, help and expertise I received from him when I took on the tasks of directing the center". Xavier Obradors, director of the ICMAB between 2008 and 2023.

"Carles Miravittles brought the Institute into being; we already know that he made a very wise choice of researchers from the beginning and guided the expansion of the Institute throughout the 21 years that he was its director. His dynamism, intelligence, and creativity allowed ICMAB to grow both in size and quality. His mark was indelible, and those of us who have been able to interact with him know what a great loss his passing means. In the broadest sense, he had a significant influence on research in Catalonia and Spain. He will be greatly missed". David Amabilino, current director of ICMAB.

"Carles was a nice person. He was generous, honest, respectful, funny and creative (his head was buzzing with ideas) but at the same time, like a good scientist, he was rational, that is, sensitive to arguments. I guess that's why we never argued once in over 40 years. He also had a remarkable global and future vision. At the beginning of my research career I had him by my side and later on when I needed him he always helped me. He was also a person who knew how to listen and give advice, something that was very useful to him, later, during his more than twenty years as Director of the Institute of Materials Science in Barcelona. I will miss you." Jordi Rius, Research Professor of ICMAB.

"Carles Miravittles 'took me in' at ICMAB at a complicated time for me; it was 1992. This determined my professional career. From the beginning, we had a trusted relationship. Carles was an intuitive, social person;

he had a visionary point of view and a humor that was not always politically correct. He was a tireless and tremendously restless worker with the ambition and obsession to make ICMAB a modern research center of reference. He used to head his e-mails with a 'benvolgut amic i company'. Anna Roig, Research Professor at ICMAB.

"Of Carles I can say that he had an advanced vision, both scientifically and technically. He had the virtue of knowing how to surround himself with good or very good people in his field. He had an idea of the future (I am talking about the late 80s) of ICMAB of scientific and technical excellence, and obviously also in the field of computer science. For example, by making proposals ahead of his time, such as the idea of making a kind of Virtual Institute (he said without walls), where you could work remotely securely as if everyone was in the same institution. At that time, talking about Virtual Private Networks was a very advanced idea, which led ICMAB to have a world-class Computer Network in the following years, being a computing reference, both at the CSIC and at the UAB campus". Joan Figuerola, Head of Computer Science Department at ICMAB for many years.

"All those who were lucky enough to know Carles recognize his affable and conciliatory nature. Everyone was happy when they found him. He always had some anecdote to tell or some news that no one else knew. His smile was encouraging and his story charmed you. In the CSIC he has been considered as the director of the Institute that all researchers would have liked to have. Tireless worker, rooted in his land, empathetic and generous. No sports lover, except for dominoes. Spartan in tastes, although a good gourmet. He left us just two days after losing his wife. He started by doing complicated crystallography calculations when there were no computers, and became an excellent promoter and manager of research and science, always looking for excellent researchers. We will remember him for his eternal affability, firm commitment to a job well done and knowing how to enjoy the little things. We will never be able to appreciate the great influence he had on the people with whom he came in contact. Sometimes exceptional people make this world a little better. Despite the moments of sadness, we will always be proud of having known him." Elies Molins, Head of the Advanced Structural and Functional Crystallography Department of ICMAB and Co-president of the FMTS-WFSW.

Marta Vendrell, Joan Figuerola and Carles Miravittles in December 2022 for the ICMAB Christmas party

Kirara Service for High-Quality Protein Crystal Growth in Microgravity

Author not stated in source

Kirara #5 Call for Samples (Article for IUCr Newsletter)

Greetings from space!

We are happy to share that Kirara#4 recently returned from its mission to the International Space Station (ISS) and that we are already planning and preparing for the upcoming mission. Read more about the samples flown so far by the Kirara service.

Kirara #5 is already under preparation! And so we are calling for samples for the upcoming missions, and these are not strictly limited to proteins, as shown through the examples of previous missions.

In case you missed it, Space Commerce Matters, together with ICE Cubes and the Japan Manned Space Systems Corporation (JAMSS) organized a webinar focused on "Crystal Growing in Microgravity". The keynote speaker, Dr. Anne Wilson from Butler University (USA), presented her project on a meta-analysis of Crystals Grown in Microgravity. The recorded webinar can be viewed [here](#).

What is Kirara? A low-cost crystallization service in space, providing the opportunity to take advantage of the unique microgravity environment on-board the International Space Station (ISS) for crystal growth in support of many applications, such as drug discovery. The service uses an original small incubator unit developed by JAMSS and accommodated inside the ICE Cubes Facility on the ISS.

Why Space? The microgravity environment on-board the ISS has been proven beneficial to enable and study complex molecule 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

to those produced on Earth. The unique microgravity laboratory and environment of the ISS can therefore be used to support, for example, the investigations for the development of novel drugs that could treat viral outbreaks or antibiotic-resistant bacteria.

Why Kirara? Because it offers a unique end-to-end service where microgravity and crystallization experts determine the ideal crystallization conditions for the user. Several options are available to users to analyze their crystals once returned to Earth. These include support to crystal testing with the same experts also helping in the set up and performance of post-flight analysis (e.g. X-ray diffraction of the crystals), as requested. All the deliverables and intellectual property rights obtained belong to the customers.

Previous missions: The Kirara crystallization service had four successful missions so far. During the first mission in December 2019, seven pharmaceutical companies and research centers 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 redemsvir-based medicament for treating COVID-19, from InnoStudio Inc. and CycloLab Cyclodextrin C&D laboratory Ltd. 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. Recently, Kirara #4 hosted samples for drug R&D (Covid-19 related research) and academic research (life sciences and agriculture), as well as educational and inspirational projects.

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



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