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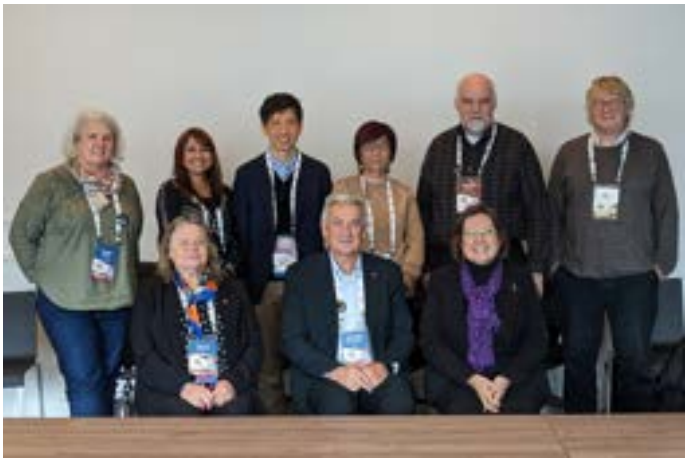
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LETTER FROM THE PRESIDENT

President's Letter



The IUCr Executive Committee 2023–2026. Front row (l-r): Hanna Dabkowska, Santiago García-Granda, Graciela Díaz de Delgado. Back row (l-r): Susan Bourne, Maria Cristina Nonato, Atsushi Nakagawa, Angela Altomare, Thomas Proffen, Trevor Forsyth. Manfred Weiss was not present when the photo was taken.

Santiago García-Granda

The 75th anniversary of the IUCr marks a turning point in our organisation, where we still have a close memory of our origins and the people who have built the International Union of Crystallography, from both our personal experience and the references of many colleagues. This August, we had our 26th General Assembly and the triennial Congress of our Union in Melbourne, where we enjoyed our history as told by some of its protagonists. Many of our referents are no longer with us; very recently two of our former presidents passed away, Professor André Authier earlier this year and even more recently Professor Henk Schenk. Many other crystallographers of our community left us in these 75 years of history, and all of them deserve our recognition and our loving memory.

Although we stand on the shoulders of giants, we are facing a very different world from that encountered by our first General Assembly (GA) in 1948. That is why it is so important that we invigorate and adapt our organisation to face the future with confidence and renewed enthusiasm. The process that began in Melbourne to define our Purpose, Vision and Values in an open and participatory way is essential; we must find the keys that will allow us to face, with the new generations, women and men, the new challenges to continue developing and leading structural science in a very different world. The results of the consultation and discussion will help the new Executive Committee (EC) make the right decisions to ensure the scientific and social leadership of crystallography and structural science for the remainder of the 21st century.

The IUCr must keep going on and reinforce the initiatives started almost 10 years ago, on the occasion of IYCr2014, focusing on the following elements:

Education, to provide new generations of crystallographers and structural scientists;

Research, by fostering scientific collaboration and leadership in structural science through the Commissions and our journals and books;

New generations, creating a young division to attract the early-career scientist to have a strong voice in and from the IUCr;

Society, by reinforcing the impact of crystallography on society so as to obtain the support of stakeholders and put crystallography and structural science on the agenda of the decision-makers;

Organisation, favouring the links between the Regional Associates, boosting their influence within the IUCr, and reinforcing our team in the Chester Office;

Promotion, keeping the momentum and favouring gender equality at all levels and activities;

Attraction, extending the family with child-friendly crystallographic conferences.

After IYCr2014, the IUCr has been more active in demonstrating, fostering and coordinating the impact of crystallography and structural science on humanity, thus providing networking between scientists worldwide and having an active role in the International Science Council. The experience with the successful hybrid 25th IUCr Congress in Prague offers new opportunities to adapt the IUCr to new environments.

Our organisation has grown in its geographical presence with the latest addition of AfCA, the African Crystallographic Association, at the Melbourne GA, completing the five Regional Associates that make up the IUCr. These regional branches of the Union will contribute to bringing science to new emerging countries where structural science is less developed and will allow for a more diverse voice to be heard from crystallographers all over the world, without exception. The collaborative projects being developed with governments, companies and non-governmental organisations will give an extraordinary boost to the development of science in all regions of the world. The Light Sources for Africa, the Americas, Asia and the Middle East Project (*LAAAMP*) is one of them.



AfCA President Professor Delia Haynes charts the development of the Association at the IUCr 75th Anniversary session at IUCr2023. (Online platform build and capture: ICMS Australasia.)

This *Newsletter* is a great tool to bring our community together, being a meeting point for philosophical discussions, not only on scientific issues but also on issues that affect our societies and the planet, contributing effectively to the discovery of our disciplines by the global society and giving us the possibility to disseminate our activities worldwide. Many thanks to the Editor, Mike Glazer, and all contributors.

We must be able to maintain the bonds of scientific collaboration above conflicts and align ourselves with the progress of global society in terms of peace, justice and equity, diversity and sustainability. We have to ensure that future generations have the resources and conditions to sustain life on the planet, and this is not only to maintain the human species but also to maintain the planet's biodiversity and the wildlife.

It was very good to be back in Australia 36 years after the well-remembered 14th IUCr Congress in Perth in 1987. The scientific programme was excellent; the setting, the facilities, the organisation and the human atmosphere were perfect, managing to regain a sense of normality after our extraordinary experience in Prague. The participation of young scientists with excellent lectures put us in the best possible scenario for the future. The lecture of our Ewald laureate, Professor Wayne Hendrickson, led us through many years of the development of anomalous dispersion and its extraordinary influence on the development of macromolecular crystallography. The consolidation of new methodologies such as AlphaFold has revolutionised our approach, and the emerging development of artificial intelligence opens new and unimaginable future challenges for structural science. All of this was complemented by an ambitious programme for the social integration of our discoveries and the attraction of scientific vocations from the earliest ages, which will help ease the imbalances in science and technology. Many thanks to SCANZ (Society of Crystallographers of Australia and New Zealand) and to its President, Professor Charlie Bond, for inviting us to Melbourne. Thank you very much indeed to the organisers of the 26th Congress and General Assembly, to Professors Michael Parker, Brendan Kennedy and Megan Maher, and also many thanks to all the Melbourne team. You made us feel at home. Thanks to the sponsors and to the participants, and thanks to all of you who made this Congress and the IUCr possible.



Dr Hanna Dabkowska (left) presents Professor Wayne Hendrickson with the 13th Ewald Prize during the IUCr2023 Opening Ceremony. (Photo credit: 26th IUCr Congress, SDP Media.)

I am very happy that my election as the 27th President of the IUCr was in Melbourne, in Australia, and at the heart of this magnificent conference and superb scientific framework, especially because of the contributions from young crystallographers. After this conference, we will start a new term after celebrating our first 75 years of history together. Some of the colleagues I met in 2014 in Montreal when I joined the EC, and later, are leaving the EC after Melbourne or have done so already; many thanks to all of them. In particular, thanks to the members who left immediately after the last GA: Sven Lidin, Jennifer Martin, Masaki Takata and Bo Iversen. Many thanks to past Presidents Marvin Hackert and Hanna Dabkowska, who will continue as Immediate Past President of the new EC, as well as to Graciela Díaz de Delgado, our new Vice-President, and I welcome the four new committee members: Trevor Forsyth, Atsushi Nakagawa, Susan Bourne and Maria Cristina Nonato. I would like to finally mention our wise

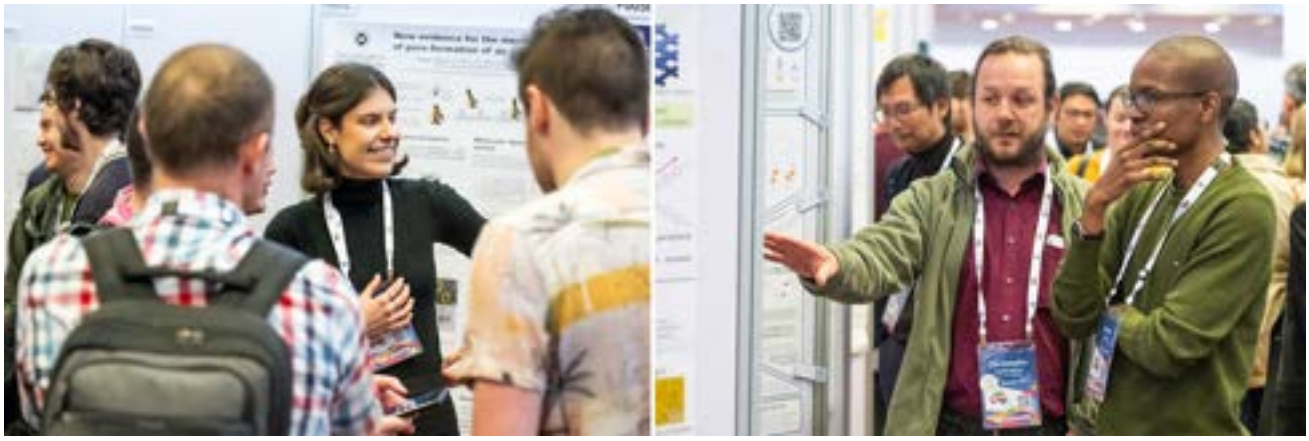
convener, Professor Malcolm Cooper, and the members of the Finance Committee.

Last but not least, thanks must go to our IUCr team in Chester, who always work hard, especially in a Congress year, and to all our sponsors, who give the necessary support to make our meetings and many of our projects feasible.

We have initiated a process to redefine our Purpose, Vision and Values. Let's do it in the next triennium. The new EC is ready to face the challenges of the Union until our meeting at the Calgary Congress in 2026.

We all must support our team in Chester; we must be aware of their needs and ensure a suitable working environment and exciting projects that will enable their professional development and make the office attractive to new recruits, thus allowing for an orderly generational handover. The change of domicile from Switzerland to the UK, which is currently under investigation, would, if possible, improve the efficiency of our administrative processes considerably, with the consequent improvement of our activity in Chester.

One of our tasks will be to create a Young Division of Crystallographers and Structural Scientists as the generational renovation is of great importance for the Union, and their input vital.



Young crystallographers discuss their research during the IUCr2023 poster sessions. (Photo credit: 26th IUCr Congress, SDP Media.)

A critical aim will be to improve our finances and revitalise our journals; this is one of our major issues. Everybody, the Chester production and marketing team, together with the Editor-in-Chief of IUCr journals and his team, should work towards making our journals more competitive. But not only them; our scientific Commissions must also play a key role in the development of our editorial work and so must our regional and national committees and each crystallographer by publishing his/her results in an IUCr journal.

The IUCr is in continuous evolution, and in this triennium, with the help of the new EC and the Chester Office, and with your support, our task is to maintain, revitalise and renew our activities, redefining our Purpose, Vision and Values, as well as to maintain the highest scientific and social impact with IUCr Congresses in Calgary in 2026 and Berlin in 2029, as was accomplished in Melbourne.

We will work to maintain our excellent partnership with our associated companies in order to achieve the best possible integration of projects of mutual interest, generating constant interactions to establish a fluid relationship of trust necessary to tackle new initiatives.

We stand at the service of all IUCr members and humbly ask for your full commitment with your Union.

All of us are necessary to keep the IUCr strong, particularly the Regional Associates, the IUCr Commissions and Committees, editors, co-editors, referees and authors of our journals, and all individual crystallographers, women and men, collaborating in the best scientific and human environment. It's important for us that you feel comfortable in our Union and be proud to belong to the IUCr.

Many thanks to all for keeping the IUCr at the forefront of structural science.

EDITORIAL

Editorial



Mike Glazer

Many of us have now returned to our home countries after attending the IUCr Congress in Melbourne. I hope that everyone found it both enjoyable and, even more importantly, scientifically fruitful. Having attended every IUCr Congress since 1966 (apart from the Prague meeting, which I watched remotely), I can look back and think about the value of these big international meetings that we hold every three years. Obviously, they provide an opportunity to learn about new science by listening to the talks and looking at the posters. But it also enables us to meet with each other, sometimes seeing old friends but also making new acquaintances. And often, this leads to new scientific collaborations. This is why the Congresses matter. At the Melbourne conference, in particular, a considerable effort was made to advertise our subject to the general public through a superb talk by Jenny Martin: “How I fell in love with Crystallography and why you should too!” In addition, schoolchildren were invited to learn about crystallography through talks specifically aimed at them with the chance to see and play with several crystal models. Part of this involved everyone helping to construct the largest crystal model ever made (see above). You can read some more about the Congress in an article in this issue by Chris Sumby. I hope to have further details in the next issue of the *Newsletter*.



Another important aspect of IUCr Congresses is the chance to celebrate the IUCr Prizes, awarded for outstanding contributions to the field. At the Melbourne Congress, I was pleased to present the Second W. H. and W. L. Bragg Prize to Arkadiy Simonov (left; ETH Zürich, Switzerland), who gave an excellent lecture on his development of the three-dimensional difference pair distribution function (3D-ΔPDF) approach and its transformative effect on the field of materials. Photo courtesy of Samar Hasnain.

In the last issue, I mentioned the then-upcoming Oxford Hatfest. I am pleased that Marjorie Senechal has written us a report of that meeting where you can see just how much excitement was generated by the discovery of a single shape that could be stacked together, leaving no gaps but also not having periodic symmetry (at least in our three-dimensional world!). While obviously a rather exotic bit of the mathematics of symmetry, one question I would raise is this: are there any actual crystals out there that have this kind of aperiodic structure? Start searching: a possible Nobel Prize may await you!

For crystallographers, it is essential that they learn about the concept of symmetry and how it applies to crystals. The MathCryst Commission of the IUCr performs a valuable service in this regard through holding regular schools in different parts of the world. These are led mainly by Mois Aroyo and Massimo Nespolo together with other instructors. The latest school was held in Nancy and is described here.

Now, while it is the case that the concept of symmetry lies at the heart of our understanding of crystals and their structures, it should be emphasised that this is a concept that only really applies to a so-called infinite *ideal* crystal. Such a crystal does not exist, as in reality there are all sorts of defects and disorder always present, plus the crystal surfaces. Nonetheless, an understanding of symmetry is an essential starting point for describing crystal structures and their physical properties. If symmetry were all there were to a crystal, then I think it is fair to say that none of us would exist. Sometimes it is said that “symmetry is death.” This makes sense because true symmetry is by definition, unchanging and frozen, and therefore has nothing to say about any progress or development. It is the breaks in symmetry that are responsible for the world we live in. Every new discovery can be thought of as symmetry breaking. But to understand the breaks, one needs first to understand symmetry itself. I often illustrate this idea by playing some awful music to my students. I start with a set of repeating notes, *i.e.* highly symmetric and periodic, showing that such “music” soon becomes boring (see upper line in the figure).



However, if, along the way, we introduce two or three different notes (lower line), this immediately captures our attention. Admittedly this is still not great music but it does serve to illustrate the effect of symmetry breaking. So, symmetry on its own is boring! I often upset the “crystal healing community” by pointing out that crystals are the “deadest” things in the universe! Now, having said that, symmetry does mean that crystals are very pretty and in this vein Istvan and Magdolna Hargittai have written an entertaining article entitled “Crystals humanized”.

Another way by which the beauty of crystallography is brought into the public square is through the holding of crystal growing competitions. Here, schoolchildren are given the necessary chemical agents and learn how to grow crystals from solution. The best crystals are then judged for quality and size. In this issue, we have reports from Canada and the USA of the latest crystal growing competitions.

As ever, as Editor I have the sad task of reporting the deaths of fellow crystallographers. Bruce Forsyth (RAL) and John White (ANU, Canberra) were well known for their work in neutron scattering. S. K. Sikka (BARC) was an eminent high-pressure physicist. Michael James and Raimond Ravelli were well known structural biologists working in Edmonton and Grenoble, respectively. And then very recently we heard of the death of Henk Schenk, President of the IUCr from 1999 to 2002. I hope we shall have an obituary for him in the next issue of the *Newsletter*. I well remember his lectures on the crystallography of chocolate!

IUCR CONGRESS

The long road to Melbourne, Australia – the 2023 IUCr Congress



The Melbourne skyline by night, overlooking the Yarra River, with part of the Melbourne Convention and Exhibition Centre on the bank to the right. (Photo credit: Chris Sumby.)

Christopher Sumby

Six years after successfully bidding for the IUCr Congress, the Society of Crystallographers in Australia and New Zealand recently hosted the 26th Congress in Melbourne, Australia. The meeting was held in the Melbourne Convention and Exhibition Centre over seven and a half days between 22 and 29 August 2023, attracting nearly 1800 participants (including 402 early-career researchers) from 66 countries. The path to Melbourne was a long one in many ways, in part for the organisers who had to deal with several uncertainties during the organisation, and for many of the participants who had to make their way to Melbourne from places as far away and as diverse as Albania and Venezuela.

Australia was the host to the IUCr Congress for the second time. The first instance was the 1987 IUCr Congress held in Perth in Western Australia, a meeting that left a significant legacy in Australia regarding crystallography. For the 2023 event, the organisers did a fantastic job of promoting Australia and the meeting *via* Twitter, the *IUCr Newsletter* and E-Zines, promising the opportunity to experience a meeting that showcased Melbourne's culture and Australia's unique landscapes, and highlighted the vibrant local scientific community that has made remarkable contributions to crystallography. In addition to showcasing Australian and New Zealand science, the meeting was also to serve as a meeting point for the world's crystallographic community, who hadn't been able to meet in person as one since 2017 (noting the mostly virtual 25th IUCr Congress in Prague in 2021), and to allow attendees from various countries to gather to exchange knowledge, foster collaboration and celebrate the recent breakthroughs in the field of crystallography.



The final moments before six years of hard work get under way. (Photo credit: 26th IUCr Congress, SDP Media.)

Two days of Pre-Congress Workshops kicked off on Monday 21 August 2023, with workshops covering topics ranging from “Next-generation atomistic-level structural modelling…” to “CCP4/CCP-EM” and “Using the CSD to go from data to discoveries”. These comprehensive sessions brought together experts and newcomers alike to delve into the latest developments, technologies and methodologies in crystallography.

The Congress officially started on Tuesday afternoon with an inspiring opening session, headlined by the award of the 13th Ewald Prize to Professor Wayne Hendrickson who spoke on the refinement of crystal structures at ultralow resolution using approaches such as *AlphaFold* modelling. Delegates were welcomed to Melbourne by the Congress Chair, Professor Michael Parker, and indigenous performers from Australia and New Zealand. The opening session not only marked the commencement of the Congress but also celebrated the spirit of scientific exploration and collaboration that are hallmarks of the global crystallography community. The opening lecture was followed by the Congress Welcome Reception, which was held in the IUCr 2023 Exhibition Hall. Delegates were able to catch up with friends and colleagues; enjoy a drink, free-flowing oysters and cheese; and have the opportunity to “network” with some of Australia’s native animals.



Experiencing the fauna of Australia at the Congress Welcome Session. (Photo credit: 26th IUCr Congress, SDP Media.)

The Congress got under way in earnest on Wednesday with up to 12 parallel sessions available throughout the meeting. In addition to the presentations of various awards and a medal, including the Ewald, Bragg and Struchkov Prizes as well as the Gjønnes Medal, there were three plenary lectures and 35 keynote lectures throughout the Congress. In addition to the award of the Ewald Prize to Professor Hendrickson, the Bragg and Struchkov Prizes were awarded to Professor Arkadiy Simonov [development of the three-dimensional difference pair distribution function (3D-ΔPDF) approach] and Dr Robert Fayzullin (high-resolution X-ray diffraction crystal structure determination), respectively, and the Gjønnes Medal to Professor Jian-Min Zuo (contributions to the development and application of quantitative electron diffraction).

Although the Congress was in-person, most of the plenary and keynote lectures were recorded and made available online, making the Congress accessible to members of the world community who could not travel to Melbourne. These included the plenary lectures, with the first two given by Professor Hideo Hosono and Dr Junko Yano on Friday and Saturday nights, respectively. Throughout the meeting, there were 120 microsymposia representing all the Commissions of the IUCr. This provided all participants with an abundance of talks covering a wide spectrum of topics, ranging from fundamental crystallography principles to groundbreaking discoveries.

For the first four full days of the Congress, coffee breaks and lunches were held in the large IUCr Exhibition Hall amongst exhibition booths for the 42 sponsors and exhibitors of the meeting. These ranged from Rigaku Oxford Diffraction, having a networked MicroED instrument that participants could use to collect data on a pre-loaded sample, through to the Cambridge Crystallographic Data Centre (CCDC) running their CSD Leaderboard. The food was plentiful and easily accessed at the fully catered lunches, and a healthy mix of fruit was provided throughout the meeting. The large poster sessions were spread throughout the Exhibition and adjacent to the rooms used for the concurrent sessions.

In addition to the scientific program, three sessions of the General Assembly of the IUCr were held to transact the business of the IUCr as the organisation reached its 75th anniversary. Among a range of decisions made was the official recognition of the African Crystallographic Association (AfCA) as the fifth

Regional Associate of the IUCr, the awarding of the 28th IUCr Congress to the German Crystallographic Association (Berlin, Germany, following the 27th Congress in Calgary, Canada), and the election of a new IUCr Executive Committee under the leadership of Professor Santiago García-Granda (University of Oviedo, Spain) as IUCr President.

Another highlight of the meeting was the excellent outreach opportunities associated with the Congress, including the Crystal-A-Con day on Friday 25 and Saturday 26 August. This event was spearheaded by Professor Stuart Batten and Dr Helen Maynard-Casely, and aimed to engage the broader community in the wonders of crystallography. Over 480 Bragg Your Pattern delegates were in attendance over both days. The event consisted of seven awesome activities (based around the seven crystal systems) to inspire the next generation of scientists and ignite a passion for crystallography in young minds, along with an exhibition of patterned artwork, crystallographic-themed fashion and some gigantic crystal structure models. The activities ranged from helping to build a giant diamond structure (cubic) through to meeting real-life crystallographers (triclinic). Some amazing local volunteers helped, with support from the CCDC, Protein Data Bank and the Australian Nuclear Science and Technology Organisation. On Saturday, Professor Jenny Martin gave a public lecture entitled “How I Fell in Love with Crystallography and why you should too,” which touched upon the history and practice of crystallography, crystallography-themed cakes and the discipline’s enormous impact on science and the world around us.



The completed diamond structure. (Photo credit: Chris Sumby.)

A particular personal highlight of the Crystal-A-Con activities was the building of a large model of diamond to break the record for the largest chemical model. Over many days preceding the event, the team (mostly at the Australian Synchrotron and including the control room staff) built components of the model, which were then pieced together and extended during the IUCr Exhibition and Crystal-A-Con event. After some stressful hours late on Saturday, when the team thought they were going to be ejected before the model was completed, the final layers were added, and a few defects were removed with minutes to spare. The final numbers, courtesy of Professor Batten, were 62,356 atoms + 121,547 bonds

= 183,903 parts or 341 kg, with dimensions over the 24 layers being a bottom edge of 3.69 m, top edge of 2.31 m and height of 1.11 m.

To celebrate the 75th anniversary of the IUCr, a dedicated microsymposium, the IUCr 75th Anniversary, was held on the afternoon of the second to last day of the Congress. This touched upon topics ranging from the role and importance of the IUCr in international science, to what the various committees and instruments of the organisation do, through to opportunities for the future of the society. These latter points focussed on making sure everyone feels welcome in crystallography and looking to future applications of the science and technique. Reflective of some these ideals, the 26th IUCr Congress had childcare available throughout the entirety of the meeting and had 16 registered children in attendance.

The IUCr Congress dinner, themed as a “Night at the Museum” Congress Celebration Party, was held at the Melbourne Museum on Monday night. The Congress dinner was included into all registrations to make it inclusive. Guests were welcome to explore many parts of the Museum, seeing the exhibits and sampling food from Melbourne, Victoria and Australia. Some fantastic images of people mixing under dinosaur skeletons and being photographed with performers dressed as giraffes, geishas and Egyptian cats marked this a night to remember for all who attended. The dinner certainly provided an iconic location and allowed the attendees to unwind, share experiences and celebrate the meeting.



An image from the Congress dinner at the Melbourne Museum. (Photo credit: 26th IUCr Congress, SDP Media.)

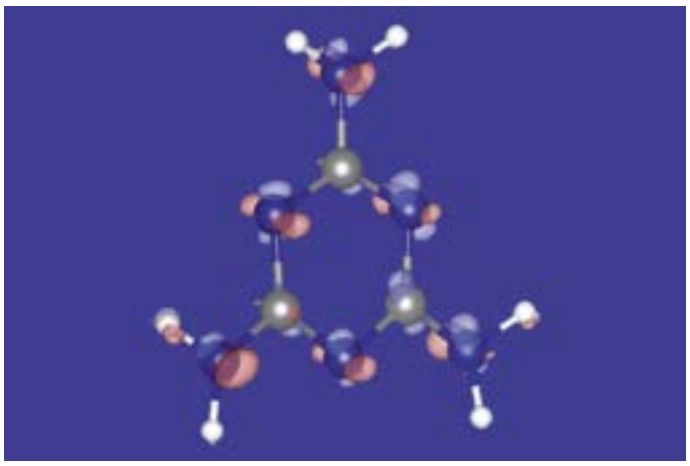
The next day after the dinner, delegates were back to hear from the third plenary speaker of the meeting, Professor Mark Spackman from the University of Western Australia, talking about “Molecules as Crystals”. This was the opening to another full day of scientific activity before the meeting close in the afternoon. The poster sessions, this time on the balcony areas outside the session rooms, were again in full swing on Monday and Tuesday as the second tranche of posters were on display; organised together in this way, it was apparent how many posters were being presented at the Congress. Late on Tuesday afternoon, the 26th IUCr Congress was closed by Professor Parker, bringing to an end a week (and a bit!) filled with scientific exploration and discussion. The closing session acknowledged the dedication and passion of the crystallography community, especially the Local Organising Committee and the International Program Committee, in bringing the meeting to fruition and looked ahead to future

Congresses and continued success for the IUCr.

Christopher Sumby is Head of the School of Physics, Chemistry and Earth Sciences and Professor of Chemistry at the University of Adelaide, SA, Australia, and the Asia-Pacific Regional Editor of the IUCr Newsletter.

COMMENTARY

In data we trust: X-ray diffraction experiments for charge density investigations



Regine Herbst-Irmer

Investigations into charge density focus on deviations from spherical valence density to describe the bonding situation in a specific structure. The Hansen & Coppens (1978) multipole model can be used to describe this asphericity, because this model partitions the electron density in the core, the spherical valence density and the aspherical valence density. This model needs more parameters compared to the independent atom model which uses just spherical atomic form factors. The deviations from spherity are very small compared to the electron density from the core. Therefore, excellent high-resolution data are necessary. The information about the valence density is mainly contained in the low-order data, while high-resolution data are needed to deconvolute aspherical atomic electron density from thermal vibrations. The data need to be of very good quality along the whole resolution range, and especially the low-order data need to be collected with high accuracy.

In recent decades, there have been numerous new developments in the fields of sources and detectors. In terms of detectors, technology has progressed from point detectors to CCD and nowadays energy-discriminating pixel detectors, which greatly reduced the data collection time and which foster spectral purity. The development in sources from sealed tubes to microsources, rotating anodes, MetalJet to synchrotrons radiation supplies more and more beam intensity. There is a strong tradition to examine which of these new developments really provide better data for charge density investigations, *e.g.* Martin & Pinkerton (1998), Coppens *et al.* (2005), Jørgensen *et al.* (2014), Wolf *et al.* (2015), Graw *et al.* (2023), Ruth *et al.* (2023). Higher resolution is not enough, excellent low-order data are also needed, and the question is which combination of hardware leads to reliable statements about the bonding situation in a particular compound.

This tradition continues with the paper of Vosegaard *et al.* (2023). The authors compare data collected at 100 K from new in-house diffractometers, a Rigaku Synergy-S (Mo and Ag source, HyPix100 detector) and a Stoe Stadivari (Mo source, EIGER2 1M CdTe detector) and an older Oxford Diffraction Supernova (Mo source, Atlas CCD detector) to an investigation with excellent synchrotron data collected at 25 K and λ = 0.248 Å at the BL02B1 beamline at SPring-8 (Vosegaard *et al.*, 2022). As the test structure, melamine was selected.

First, the authors investigate the data quality by comparing figures of merit such as R_{int} and I/σ. Of course, the SPring-8 data win concerning the highest possible resolution and lowest collection time. However, considering the variation of R_{int} and I/σ over the whole resolution range, the modern

diffractometer Synergy-S and Stadivari can keep up to *circa* 0.9 $Å^{-1}$, while the older Supernova delivers noisier data. This is probably due to the virtually noise-free pixel detectors compared to the older CCD technology. However, all data, even from the Supernova, could be used to a resolution up to at least 1.17 $Å^{-1}$.

The derived unit-cell parameters of the four datasets at 100 K differ only a little – with a small feature that the differences between the values derived from the Synergy Mo and Ag as well as those from the Supernova and the Stadivari are smaller than the differences between these two groups.

For the refinements (Volkov *et al*., 2006), an $I < 3\sigma$ intensity cutoff was used, leading to a very different amount of used data in the five datasets. Although the data to parameter ratio is larger than 10 in all refinements, I wonder if, especially for the Supernova dataset, overfitting could be excluded (Krause *et al*., 2017), which the authors had tested for the SPring-8 data but not for the new datasets. All five datasets deliver low R factors (≤ 3.4% for Supernova and < 1.7% for the other datasets) and min/max residuals (≤ ±0.25 e $Å^{-3}$ for Supernova and < ±0.15 for the other datasets), *DRK* plots with the value 1±5% across the whole resolution range (Zavodnik *et al.*, 1999; Zhurov *et al*., 2008), and Henn–Meindl plots (Meindl & Henn, 2008) with virtually no features.

U_{eq} values for the heavy atoms agree well, while the values for hydrogen atoms derived from Hirshfeld atom refinement (Capelli *et al*., 2014; Fugel *et al.*, 2018; Kleemiss *et al.*, 2021) from the Supernova data deviate significantly from those of the other three datasets.

The derived multipole parameters show the same trend for all five datasets, although the differences for the carbon atom parameters are significant. The derived monopole population even spread between 4 and 4.5 e, indicating slightly negatively charged carbon atoms. However, the Bader charges are more sensible with slightly positively charged carbon with a small spread of 0.2 e and negatively charged nitrogen atoms. In addition, the topological values ρ_{BCP} and $\nabla^2\rho_{BCP}$ are in good agreement except for the Supernova data, where the bond critical point of one weak π–π interaction could not be found.

Overall, it was found that even with conventional diffractometers and good quality crystals of small organic molecules reliable electron densities can be achieved with the multipole model. However, the better the data the more features can be seen: only for the excellent SPring-8 data set hydrogen κ values could be refined, while weak interactions could not be found with the weakest Supernova data.

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IUCR JOURNALS NEWS

Foreword to the special virtual issue on Modern approaches and tools for teaching crystallography



Graciela Díaz de Delgado, Sean Parkin

Since its early days, crystallography has proven to be a highly interdisciplinary and collaborative science. At the same time, it stands out as a field whose members are strongly committed to education. Crystallographers are well recognized for their dedication to teaching. The determination of the structure of even a simple molecule could become complicated by disorder, twinning, incommensurate modulation, low crystal quality, *etc.* In addition, analysis of geometrical parameters and intermolecular interactions, graphical representation, structure validation, and manuscript publication often require the help of an expert crystallographer to take the results to publication in a prestigious journal.

At the core of IUCr activities is the sponsorship of schools and workshops around the world on different aspects of crystallography, from basic and advanced concepts in symmetry, to structure determination of small and large molecules, powder and single-crystal diffraction techniques, to new experimental methods, among other topics. Many young crystallographers have benefited from attending prestigious crystallography schools and workshops such as the International School of Crystallography in Erice, the ACA Summer Course on Crystallography, the European Crystallography School, *etc*. These efforts, strongly supported by the IUCr, aim to compensate for the absence of formal courses in crystallography at the undergraduate and graduate degree levels, as noted by Kantardjieff, Kaysser-Pyzalla, and Spadon in the foreword of the special issue ‘Crystallography education and training for the 21st century’ in the *Journal of Applied Crystallography* (Kantardjieff *et al.*, 2010).

It is well recognized that the crystallographic community rapidly adapts to new technological advances, in many cases even driving them. This community is also always looking for new approaches and teaching tools, and makes extensive use of online resources, as became evident during the lockdown measures established globally to control the spread of Covid-19. As soon as it was possible, teaching, research, collaboration, meetings, schools, and workshops resumed, using different meeting platforms. Since online teaching requires a great deal of preparation, many crystallographers worked hard to develop online content for students and newcomers to the field, some produced step-by-step guides to the solution of difficult problems, and others dedicated time to contribute to the teaching of fundamental concepts.

The special issue (https://journals.iucr.org/special_issues/2023/teaching/index.html) features contributions by B. M. Foxman (Foxman, 2021) and by S.-L. Zheng and M. G. Campbell (Zheng & Campbell, 2021) on teaching space groups. Foxman’s approach consists of a tutorial, conceived and

written with the late Jerry Jasinski, that presents the crystal classes in five modules of more than 200 PowerPoint 'slides'. Humor (a distinctive trademark of Professor Foxman), historical context, hypothetical dialogues between 'Great Figures of Crystallography', and Q&A combine into an entertaining pedagogical presentation of space-group symmetry.

Zheng & Campbell (2021) then describe how they use Foxman's tutorial in a 'peer-tutoring' approach to teaching space-group diagrams. Through explaining to their peers the recently acquired understanding of symmetry and space-group diagrams, students are able to consolidate the concepts learned and become more engaged in learning crystallography.

The importance of a good understanding of space-group symmetry is evident in the paper by van Terwingen & Englert (2022). The structure of trimethylpyrazole, a very simple heterocycle, which crystallizes in the interesting space group *Pnma* is reported. The authors describe the structure in terms of Kitaigorodskii's and Wilson's ideas of crystal packing.

Bart Kahr (Kahr, 2023) presents us with a very interesting idea: the design of a periodic-like table of space groups. The table is constructed based on the symmorphic space groups arranged over two non-linear non-orthogonal axes. The corresponding non-symmorphic space groups are treated as 'isotopes'. As Kahr suggests, such a table would be of value to expert and novice crystallographers as well as researchers in solid-state sciences. The design is certainly open to improvements or to new design ideas.

Crystal-growth experiments provide excellent opportunities to discuss many fundamental concepts such as crystal packing, use of crystallographic databases, determination of physicochemical properties, stereoisomerism, among many others. Crystal-growing competitions have become one of the most important and engaging outreach activities of IUCr. Wouters & Van Meervelt (2022) present a simple procedure to grow large crystals of the artificial sweeteners erythritol and xylitol coupled with the determination of the heat of dissolution using a simple calorimetric set-up.

Four papers in the issue contain detailed advice on dealing with complications during structure solution and refinement. Parkin (2021) uses three case studies to provide hints and tips to deal with pseudo-merohedric twins. Milewski *et al.* (2022) alert us to the need to always examine critically the results of an automated structure determination. Vinaya *et al.* (2023) present a step-by-step guide to modeling whole-molecule disorder. Parkin, Cunningham *et al.* (2023) discuss in detail validation criteria for the structure determination of a mixed phosphine sulfide/selenide. These contributions contain excellent examples to use in schools and workshops, complemented by other articles across IUCr Journals dealing with, for example, pitfalls in the automatic determination of symmetry (Clegg, 2019), complex cases of disorder (Parkin, Glidewell *et al.*, 2023), validation (Linden, 2020; Spek, 2020), treatment of hydrogen atoms (Fábry, 2018), Hirshfeld surface analysis (Tan *et al.*, 2019), to name just a few.

Simoncic *et al.* (2023) give us an overview of the advances, applications and challenges of electron diffraction, a technique that will surely become of importance for the characterization of crystals less than 1 µm in size of pharmaceuticals and other materials with potential technological applications.

To conclude the issue, Massera & Helliwell (2023) share their list of 'Golden Oldies'. The authors suggest ten crystallography articles that must be read, reformulating the title of each paper to emphasize the importance of that concept and how it is perceived and applied today. With about 500 downloads on the day it was published (June 6, 2023) and more than 5100 downloads up to July 28, this article is attracting a great deal of attention and shows the appreciation that crystallographers have for the history of our field and their commitment to teaching.

Routine structure determination and refinement from powder and MicroED data, the implementation of artificial intelligence (AI) and machine learning (ML) tools, the availability of more powerful radiation sources, among many other advances in our field, will certainly require a sustained teaching effort. We considered that a special issue on teaching in *Acta Crystallographica Section E* was long overdue. We

hope this will be the seed of a permanent section dedicated to teaching, not only in *Acta E* but also across all IUCr journals. We look forward to further contributions.

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SPECIAL REPORT

Making your raw data available to the macromolecular crystallography community



Loes M. J. Kroon-Batenburg

A recent editorial in the IUCr macromolecular crystallography journals [Helliwell *et al.* (2019), *Acta Cryst.* D**75**, 455–457] called for the implementation of the FAIR data principles. This implies that the authors of a paper that describes research on a macromolecular structure should make their raw diffraction data available. Authors are already used to submitting the derived data (coordinates) and the processed data (structure factors, merged or unmerged) to the PDB, but may still be uncomfortable with making the raw diffraction images available. In this paper, some guidelines and instructions on depositing raw data to Zenodo are given.

1. Introduction

Advancement in science depends on the reproducibility of scientific results and therefore the sharing of research data is essential (Helliwell *et al.*, 2017). Open-science models aim at making research data available to the larger community. Open-science platforms have been established, for example the OpenAIRE project (https://www.openaire.eu) and the European Open Science Cloud (EOSC; Jones, 2015), promoting the sharing of data. Guidelines for proper data management are described in *The FAIR Guiding Principles for scientific data management and stewardship* (Wilkinson *et al.*, 2016), which requires research data to be Findable, Accessible, Interoperable and Reusable.

A recent editorial in the IUCr macromolecular crystallography journals (Helliwell *et al.*, 2019) called for the implementation of the FAIR data principles. Authors are encouraged to make their deposited original raw diffraction data publicly available when they submit an article describing a new structure or a new method tested on unpublished diffraction data. In addition, the availability of raw data will allow new science by reanalysis using enhanced methods and technology.

In a series of papers in *Acta Crystallographica Section D* (Terwilliger, 2014; Kroon-Batenburg & Helliwell, 2014; Guss & McMahon, 2014; Terwilliger & Bricogne, 2014), the possibilities and problems of archiving raw diffraction images have been discussed. Kroon-Batenburg & Helliwell (2014) estimated the costs of archiving raw diffraction images and brought forward the challenges in reprocessing the data as well as the need to capture and archive the metadata associated with the raw image data. Initially, the costs of raw data storage seemed to be prohibitive. An early initiative of raw crystallographic data archiving, the Store.Synchrotron service of the Australian Synchrotron (Meyer *et al.*, 2014), paved the way. After this, two large-scale repositories dedicated to diffraction proved that raw data archiving is feasible: the Integrated Resource for Reproducibility in Macromolecular Crystallography (IRRMC) currently has over

9600 data sets (Grabowski *et al.*, 2016) and the Structural Biology Grid Consortium (SBGrid) currently has 791 data sets (Meyer *et al.*, 2016). These are most frequently used by high-throughput genomics projects. Also notable is a Polish repository for macromolecular crystallography, MX-RDR (https://icm.edu.pl), that has 402 data sets and rich metadata. The ideal model was set up by the PDBj in 2021 by creating XRDa: an Xtal Raw Data Archive, which aims to collect raw crystal diffraction data for entries submitted to the PDB (Bekker *et al.*, 2022; https://xrda.pdbj.org/). It provides a complete data record consistent with the FAIR principles.

Large-scale facilities are developing their own data policies. 70% of facilities have a specific clause guaranteeing the long-term preservation of primary data from photon and neutron sources, which is often automatically released to the public after an embargo period during which access is privileged to the original researchers (Götz *et al*., 2021). However, with the highly brilliant sources of fourth-generation synchrotrons and X-ray free-electron lasers, as well as improved detector technologies, the data rates increase rapidly such that full data archiving may become impossible. Some raw data sets from XFEL serial crystallography and X-ray coherent imaging experiments can be found in the Coherent X-ray Imaging Data Bank (CXIDB) at https://cxidb.org/ (currently 215 entries). Also noteworthy is EMPIAR, the electron microscopy public archive, that stores raw images underpinning 3D cryo-EM maps and tomograms (https://www.ebi.ac.uk/empiar/) and currently contains 1426 entries and a total of 3.23 PB of storage.

Although raw data reanalysis is not (yet) carried out so frequently, we would like to give some examples of its usefulness.

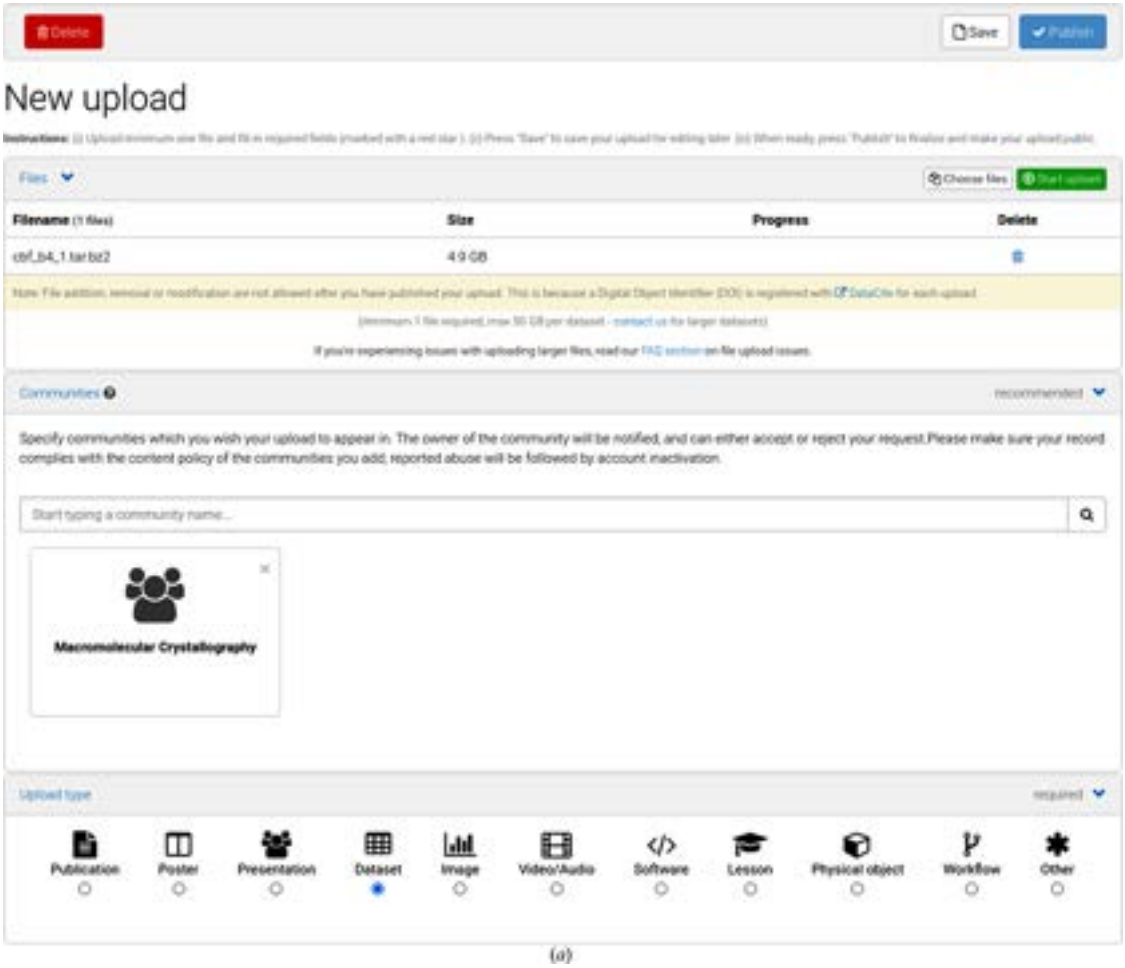


Figure 1. Upload page on Zenodo with the data items as filled in for the first *Raw Data Letter* (Neviani *et al.*, 2022). (*a*) The raw data file chosen will be uploaded after pressing the 'Start upload' button. The Macromolecular Crystallography community has been selected; the upload type is 'Dataset'.



Figure 1 (continued). (*b*) 'Reserve DOI' resulted in the DOI displayed. The publication date, title and authors and a description of the data set were filled in. Keywords and additional notes were given (see Fig. 2 for how this will appear on the Zenodo landing page).



Figure 1 (continued). (*c*) Select 'Open Access' and select your preferred license (CC BY 4.0 is the default) while keeping in mind the FAIR data principles. For this data set two related identifiers were given: the imgCIF file describing the metadata and the *Raw Data Letter* as published in *IUCrData*. At the time of uploading the data, the *Raw Data Letter* was not yet published. These identifiers were added at a later stage. Pushing the 'Publish' button will result in registration of the data with DataCite. The data can no longer be changed. A new version can be created, however, with the same concept DOI.

In a study on the effects of dimethyl sulfoxide on the binding of cisplatin and carboplatin to histidine, we used *EVAL* (Schreurs *et al*., 2010) to reanalyze the data from 11 different lysozyme crystals that were originally processed with *MOSFLM* (Leslie, 2006). We studied the possible effects of equipment and data processing on the calculated occupancies and *B* factors of the bound platinum compounds (Tanley *et al*., 2013). Using *EVAL*, we also reprocessed some of the data sets for 11 crystal structures of variants of the *Escherichia coli* enzyme *N*-acetylneuraminic lyase as they exhibited twinning and incommensurate modulation (Campeotto *et al.*, 2018). The reanalysis contributed to understanding why some of the structures were modulated. In the CommDat Workshop *Data Science Skills in Publishing* at ECM32 in Vienna (https:// www.iucr.org/__data/assets/pdf_file/0018/144009/07_KroonBatenburg _Rawdata.pdf) we gave two examples of indexing problems in raw data sets, one from SBGrid due to pseudo-merohedral twinning and one from IRRMC that had a second fragment and overlapping reflections.

The workflow of many crystallographers involves collecting data on a home source or a synchrotron facility. With the autoprocessing steps implemented on most beamlines, users have no need to download the data to a local computer but can simply use the resulting processed data in their research. The raw data will still be accessible if the facility has proper archiving and data-management systems in place. However, good documentation in a scholarly publication requires the research results to be supported by the original data.

Zenodo is an online repository that was developed and is hosted by CERN and OpenAire, with the support of the European Commission, and allows researchers to share publications and data facilitating open science. It is a highly sustainable solution to data archiving, as the data will be stored for as long as CERN

exists. Each data set is assigned a digital object identifier (DOI). Uploads can be made available online immediately. Although Zenodo is a general repository, communities can be established that group together certain types of data. Notably, there are the Macromolecular Crystallography (228 data sets) and Chemical Crystallography (44 data sets) communities.

The authors of papers describing research on a macromolecular structure are already used to submitting the derived data (coordinates) and the processed data (structure factors, merged or unmerged) to the PDB (via *OneDep* at https://www.wwpdb.org/), but may still be uncomfortable with making the raw diffraction images available. Below, we give some guidelines and instructions for depositing raw data to Zenodo.

2. How to

Zenodo (https://zenodo.org) is a general repository collecting publications, software, data sets, presentations, tutorials and some other types of data. To remove any barriers to publishing raw data, we give some simple instructions for depositing data with Zenodo. To be able to upload data one must first sign up. Once logged in, an ‘Upload’ button is available. The author’s previous uploads are shown, and by clicking ‘New upload’ a questionnaire follows. Choose the data file(s) on your computer and press the ‘Start upload’ button. Any file type is acceptable in Zenodo, although the use of a community standard is recommended (see below for what the preferred data formats may be). The maximum size of a data set is 50 GB. It is wise and convenient for data transfer if you pack your files as zip files or as a tar file compressed using gzip or bzip2. We recommended that you select a suitable community for the data, such as Macromolecular Crystallography. Click ‘Dataset’ as upload type, select ‘Reserve DOI’ and give the title and author details and provide a short description of the data, keywords and additional notes (see Fig. 1 for the steps in the Zenodo questionnaire). The DOI is registered with DataCite. The metadata will be exported to DataCite and will be searchable. By reserving a DOI, but not publishing, the future DOI can immediately be included in other materials, for example a draft publication or presentations. Also, the raw data content of the data publication can be freely adjusted. Once the ‘Publish’ button has been pressed the data files can no longer be changed. If you need to change the raw data after publication, a new version is created and the original DOI (called the ‘concept DOI’) will point to the most recent version. Additions or updates to the metadata collected by Zenodo (including the overall description) do not result in a new version and so can be freely changed. Related identifiers, such as your IUCr publication, can be given and will appear on the Zenodo landing page (see Fig. 2 for the resulting landing page for the example data in Fig. 1). If your paper is not yet published at the time of uploading the raw data, these identifiers can be added later. Although you can restrict access to your data, ‘Open Access’ is the only choice that is compatible with the FAIR principles. Zenodo suggests a CC BY 4.0 license for your data, but you can choose differently. Metadata may be freely reused under the CC0 waiver. Zenodo has Open APIs that allow software to freely access the metadata content (via OAI-PMH) and to deposit large amounts of data.

Raw diffraction data in macromolecular crystallography can come in many different data formats and with varying metadata quality. To ensure reusability, metadata should be accurate and complete or at least sufficient to be able to process the data. Large-scale facilities and diffraction-equipment manufacturers are becoming more and more aware of the FAIR data principles and the metadata content is thus increasing in quality. Recently, a gold standard was proposed by the HDRMX working group (Bernstein *et al.*, 2020). Noteworthy here are *Raw Data Letters*, which are a collaborative innovation of IUCr Journals with the IUCr Committee on Data, and are part of the journal *IUCrData* (Kroon-Batenburg *et al.*, 2022). *Raw Data Letters* are meant to describe interesting features in raw data sets that could be of interest to methods and software developers for purposes such as reanalysis by newer methods, or that may be relevant to the structural interpretation. The working group behind *Raw Data Letters* has developed methods to capture the metadata in imgCIF format (Bernstein & Hammersley, 2005; Hammersley *et al*., 2005) by reading the raw images or container files and asking for additional metadata details from the authors. The preferred data standards for *Raw Data Letters* are Nexus/HDF5 and imgCIF/CBF (Kroon-Batenburg *et al*., 2022).



Figure 2. Zenodo landing page for the raw data of the first *Raw Data Letter* (Neviani *et al.*, 2022). Data are published in the original HDF5 format as well as those converted to CBF.

3. Discussion

We highly recommend that authors make their raw data public so that the crystallographic community will move towards open science. Although in this paper we focus on Zenodo for raw data archiving, the macromolecular crystallography-specific SBGrid (https://sbgrid.org) and IRRMC (https://proteindiffraction.org) could be good alternatives. They both require an associated structure that is deposited in the PDB and both are open to the structural biology community. Some additional metadata are captured at the time of deposition, such as author names, affiliations, compound name, facility/beamline and additional processing details. SBGrid runs the data through an automatic processing pipeline which, when successful, shows the space group, unit cell and some statistics. Success indicates that the metadata are correct and sufficient. Failure is often related to an incorrect beam center. IRRMC provides a diffraction image for each scan, which is very useful if one is searching for data with specific features such as diffuse scattering. We believe that Zenodo is the most sustainable solution to data archiving, and authors can provide as much metadata and related information as they like. Finally, we would like to add that when using the *OneDep* system for structure deposition, authors can provide a DOI for their associated raw data, so linking the raw data to a PDB entry is straightforward.

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COMMENTARY

Using structural genomics depositions in undergraduate teaching of protein crystallography: everybody wins



Jon Agirre

Doing protein crystallography is easier than it has ever been thanks to advances in mechanics automation and software methods, but there is one step that remains tricky: obtaining crystals. Teaching the complete protein crystallography workflow requires having or growing crystals. And while some proteins do crystallize quite predictably within the time frame of almost any course, they are at this point almost devoid of the exhilaration that comes with stepping into the unknown. In this issue of *Acta Cryst. F, Structural Biology Communications*, a group led by Professor Krystle J. McLaughlin (Assistant Professor of Chemistry at Vassar College, New York, USA) shows how deposited but uninterpreted protein models from structural genomics consortia can be harnessed in undergraduate teaching to give students real-world research experience. The three leading authors on the article (Moorefield *et al.*, 2023) were undergraduate students at her course, and produced all the biochemical data and structure interpretation work presented there.

Professor McLaughlin is passionate about making the protein crystallography experience accessible to undergraduate students with a special focus on minorities currently underrepresented in research, all through the CURE (Course-based Undergraduate Research Experience) programme (McLaughlin, 2021). In the context of a biochemistry course underpinned by BASIL teaching modules (https://www.basilbiochem.org), McLaughlin got in touch with the Seattle Structural Genomics Center for Infectious Disease (SSGCID, funded by NIAID, NIH) in the USA to identify suitable targets for study. A good match right from the outset, the SSGCID specializes in microbial proteins, and wants to partner up with structural biologists to provide useful context to their structures. With their depositions currently sitting at 1656 structures (Fig. 1), they are sure to continue providing targets for generations of students to come. The SSGCID provided pure protein for the students to analyse; moreover, they would have supplied plasmids too, should they have been required for the study.

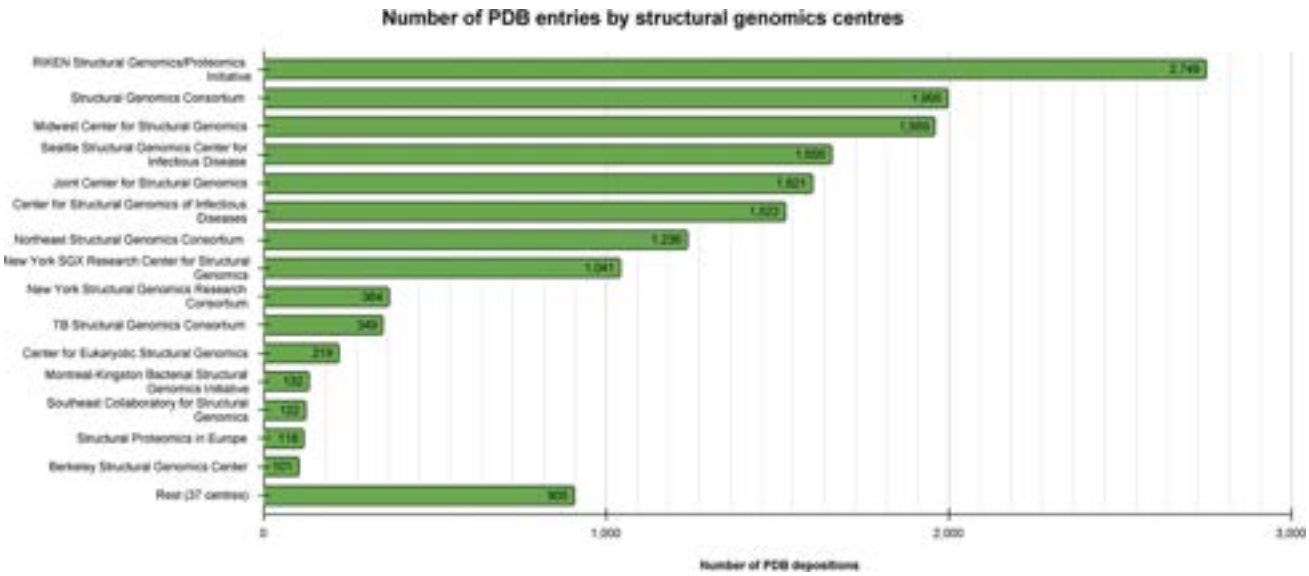


Figure 1. PDB depositions by 52 structural genomics centres around the world. Only centres with more than 100 depositions are named. Data: https://www.pdb.org.

Several undergraduate student groups took part in the course, but the one integrated by Moorefield, Konuk and Norman (lead authors on the article) managed to get the best data on the activity of their target enzyme, a family I inorganic pyrophosphatase from *Legionella pneumophila*. The ultimate deliverable of the research course was to produce a draft article in the style of *Structural Biology Communications*, which they did – McLaughlin fact-checked the draft and made some minor corrections prior to submission.

There are a number of important side-effects from this study. The importance of providing a controlled but meaningful research experience to undergraduate students comes across as critical to help avoid the disappointment some graduate researchers experience after starting a PhD; crucially, it might give students sitting on the fence a welcome push towards STEM research – this could be helpful in motivating students from disfavoured backgrounds who may feel discouraged by the current scarcity of visible role models. Underrepresentation of minorities is a problem that is most evident after the formative stage of career progression; bringing the *first article* event of scientific life forward by a few years – as opposed to doing it at the middle or end of a PhD – can only help increase diversity at the other end of the undergraduate-to-graduate gap. When asked about the aspirations of the three lead authors, McLaughlin (Fig. 2) sounded positively optimistic.



Figure 2. Professor Krystle J. McLaughlin (Vassar College, New York, USA).

The model presented here provides an excellent blueprint for establishing more collaborations between academia and any of the 52 structural genomics centres that have deposited structures in the Protein Data Bank, 15 of which are named in Fig. 1. However, this is just one way young researchers can contribute: another one could be submitting topical reviews by graduate/masters students who routinely survey the literature in support of their research project; or short software methods papers from those scripting workflows at their labs.

I should like to emphasize that *Structural Biology Communications* is open for business when it comes to processing submissions including undergraduate/masters students, and will handle and showcase their research the best it can. Finally, I would like to thank outgoing Section Editor Janet Newman (University of New South Wales, Australia), who championed the idea of encouraging younger authors to contribute their articles to this journal, and edited McLaughlin's manuscript.

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COMMENTARY

Commentary on 'Facing the phase problem' by Wayne Hendrickson



Figure 1. Wayne Hendrickson (front row, center) with former and current members of his research group at the Hendrickson Reunion Symposium, Columbia University, April 2022.

Janet L. Smith

The 2023 Ewald Prize honors Wayne Hendrickson for his many contributions to the field of macromolecular crystallography. His monograph, ‘Facing the phase problem’, is a beautifully written short history of crystallographic phasing, with a focus on experimental phasing. It begins in the early years of crystallography, with the dawning recognition that phase determination is a ‘problem’, and includes the contributions of Paul Ewald, for whom the Prize is named.

Wayne’s interest in the phase problem began when he was a PhD student at Johns Hopkins University in the laboratory of Werner Love. He and fellow PhD student Ed Lattman developed a method to represent the probability distribution for the phase of each reflection as four numbers, known as Hendrickson–Lattman or *ABCD* coefficients. Their landmark paper (published in *Acta Cryst. B*, 1970) appeared just after they received PhD degrees. The *ABCD* coefficients provided a simple means to combine phase information from sources as vastly different as isomorphous replacement, partial models, redundancy in the asymmetric unit, molecular replacement, and anomalous scattering. Phase combination became an essential tool of macromolecular crystallography as researchers tackled more challenging molecular systems that yielded crystals of increasingly poor diffraction quality.

Long before the explosive growth of macromolecular crystallography, Wayne continued his work on the phase problem as a postdoc with Jerome Karle at the US Naval Research Laboratory (NRL). There he sought to apply Karle’s direct-methods phasing to protein crystallography. However, he quickly became intrigued with an idea to solve the phase problem solely from the anomalous scattering of a few atoms in the protein crystal. This led to the famous crambin experiment. In a tour de force of data collection, Wayne recorded diffraction data from a crambin crystal using the Cu *K*α emission of a sealed-tube X-ray generator equipped with a four-circle diffractometer and a single-point scintillation detector. The data were punched on paper tape, one reflection at a time, as the tape unspooled onto the floor. Some time during the multi-day experiment, a staff member tasked with cleaning the floor ripped the precious unspooled tape from the punch device but, happily, did not remove it from the lab. Wayne processed the data and developed a method to solve the structure using the anomalous scattering of the six sulfur atoms in crambin. To do this, he started with Jerome Karle’s parameterization of the structure factor equation and formulated an observational equation relating the phase and phase probability for each reflection to the observed anomalous difference. This approach allowed him to combine phase

probabilities from anomalous scattering and from the sulfur partial structure (via *ABCD* coefficients!), yielding a lovely interpretable 1.5 Å electron density map for crambin.

Simultaneous with the crambin success, Wayne and NRL colleague John Konnert developed the first widely used software for crystallographic refinement of protein atomic models. Their major innovation was to include elements of protein stereochemistry (well established bond lengths, angles, *etc.*) as observations on an equal footing with diffraction data and to refine the atomic models by least-squares minimization. The Konnert and Hendrickson concept of stereochemical details as observables has been in continuous use since then, although today's software for refinement is far faster and more robust.

To crystallographers working today, Wayne is best known for his role in the breathtaking transformation of protein crystallography into structural biology, which occurred since the turn of the century. Anomalous scattering was prominent in this transformation. Wayne spurred the development of reliably tunable synchrotron beamlines to enhance the weak phasing signal in most anomalous diffraction experiments. He did this by solving novel structures of high biological impact using anomalous diffraction data from tunable beamlines at several synchrotrons. Ever fearless in deploying new technologies to the aid of protein crystallography, he led the development of a cutting-edge tunable beamline for macromolecular crystallography at the Brookhaven synchrotron. Ever motivated to improve crystallographic methods, Wayne developed the multi-wavelength anomalous diffraction method – with the memorable acronym MAD. For MAD, he extended the phasing formulation of the crambin experiment to multi-wavelength data. Arguably of broadest impact, Wayne envisioned a general method to incorporate selenomethionine (SeMet) in recombinant proteins. The ease of introducing an anomalous scatterer that does not interfere with the native structure or the function of a protein was truly transformative. By 2010, SeMet anomalous scattering had become the favored method for experimental phasing in protein crystallography, and so it remains today. When radiation damage from the bright X-ray beams of undulator sources challenged multi-wavelength experiments, MAD was quickly replaced by single-wavelength anomalous diffraction – with the equally memorable acronym SAD.

Wayne also sought to bring the results of protein crystallography to a broad audience at an opportune time. The Protein Data Bank grew by less than 100 entries per year before 1990 and exploded to nearly 700 entries per year in 1993. Correctly anticipating the rapid growth that followed, Wayne was founding editor of *Current Opinion in Structural Biology* (1991, with Aaron Klug), the annual volume *Macromolecular Structures* (1991–2000, with Kurt Wüthrich), and *Structure* (1993, with Carl Brändén).

Wayne's seminal contributions to macromolecular crystallography and his enthusiasm for protein structure have attracted many talented trainees to his lab. More than 50 current and former lab members (see Fig. 1) and many more friends, collaborators and colleagues gathered at the 2022 Hendrickson Reunion Symposium at Columbia University. The symposium followed a joyous reunion party and featured a full day of talks from several trainees among the many who went on to lead successful research groups in structural biology. The event was a fitting recognition of Wayne Hendrickson as a leading light of macromolecular crystallography, both for his development of seminal methods that now make X-ray crystallography a standard structural biology approach and his mentorship in training the next generation of creative scientists who continue to expand the reach of X-ray crystallography into the biological sciences. His article to accompany the Ewald Prize, published in this issue of **IUCrJ** (Hendrickson, 2023), is a terrific addition to our field.

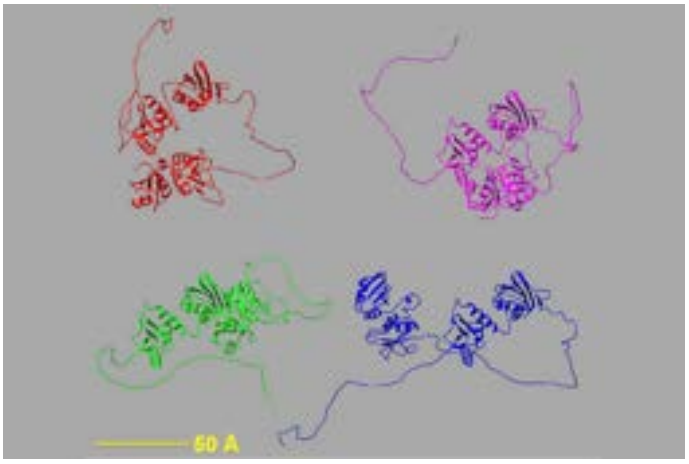
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COMMENTARY

AlphaFold, small-angle X-ray scattering and ensemble modelling: a winning combination for intrinsically disordered proteins



Véronique Receveur-Bréchot

Artificial intelligence has revolutionized many societal and scientific domains, and structural biology benefits from one of its most spectacular breakthroughs. The deep learning algorithm AlphaFold can predict with unparalleled accuracy the three-dimensional structure of folded proteins based solely on their sequence. In 1972, Christian Anfinsen was awarded the Nobel Prize in Chemistry for his groundbreaking work on ribonuclease which demonstrated that all the protein's folding information is encoded within its sequence. This ignited a surge of experimental and computational investigations into protein folding to unravel what was at the time referred to as the 'second half of the genetic code' and understand the mechanisms governing the protein's pathway towards its final three-dimensional conformation.

Now, half a century after Anfinsen's seminal article (Anfinsen, 1973), it appears that a long-awaited milestone has been reached and that one can now correlate a one-dimensional string of amino acids to an accurate three-dimensional structure. However, challenges still persist. The fundamental nature of artificial intelligence lies in its initial training using data that have accumulated over many years, the Protein Data Bank (PDB) in the case of AlphaFold. The PDB suffers from inherent biases: certain families of structures are under-represented due to the limitations of the methods used to solve the protein structures, in particular X-ray crystallization and cryo-electron microscopy (cryoEM). This is typically the case of proteins that exhibit a high conformational flexibility and cannot be described by a single three-dimensional structure. In particular, intrinsically disordered proteins (IDPs) or regions (IDRs) of proteins can adopt a tremendous number of conformations and this high dynamic is inherent to their function. Because of their flexibility, these polypeptides are often invisible in the structures solved by X-ray crystallization or cryoEM. Their flexibility may even preclude protein crystallization or lead to poorly diffracting crystals. In addition, a short disordered segment can undergo an induced folding upon binding to a partner, but may adopt different folds depending on the binding partner and the interface of interaction, further complicating accurate predictions. Therefore, AlphaFold could not train properly on disordered structures, which lack structural homologues in the PDB. Furthermore, AlphaFold uses multiple sequence alignments, while IDRs are very difficult to align because they are poorly conserved. For all these reasons AlphaFold cannot predict for now the 3D structure of long flexible disordered regions with accuracy and provides low confidence scores on these predictions. AlphaFold's creators

even suggest that the low confidence scores can be used as a method to predict protein disorder. Therefore, the single static representation of the structure of proteins containing IDRs provided by AlphaFold cannot convey all their structural and functional properties.

A very interesting strategy to circumvent this difficulty is to integrate AlphaFold predictions with ensemble molecular modelling and experimentally derived constraints, as proposed by Brookes *et al.* (2023) in their paper entitled *AlphaFold-predicted protein structures and small-angle X-ray scattering: insights from an extended examination of selected data in the Small-Angle Scattering Biological Data Bank*. Small-angle X-ray scattering (SAXS) is a particularly suitable experimental method for providing such constraints. SAXS data contain all the 3D information on the various conformations adopted by a macromolecule in solution. By calculating the SAXS profile from atomic coordinates and comparing it with experimental SAXS data, it becomes possible to select an ensemble of conformations that collectively contribute to the observed scattering spectrum. These conformers are generated through molecular modelling techniques that allow incorporation of information on the protein flexibility into the predicted structures.

To prove the effectiveness of this strategy, Brookes and co-workers utilized the Small Angle Scattering Biological Data Bank (SASBDB) as an additional resource. They selected monomeric AlphaFold models with a corresponding SASDBD entry, where the single AlphaFold model did not account for the collected SAXS data. The candidate proteins are composed of several folded domains connected by at least one long extended linker of more than 30 amino acids. These linkers are predicted to be unstructured by AlphaFold, with a low confidence score. Brookes and co-workers considered these regions as flexible and generated an ensemble of structures by exploring the conformational space of these regions using a Monte Carlo approach. They then selected the optimal ensemble of conformers and thus reached remarkable agreements with the SAXS data. Hence, by taking into account the conformational heterogeneity of the linkers, guided by the SAXS experimental data, they significantly improved the accuracy of the AlphaFold structural predictions (Fig. 1).

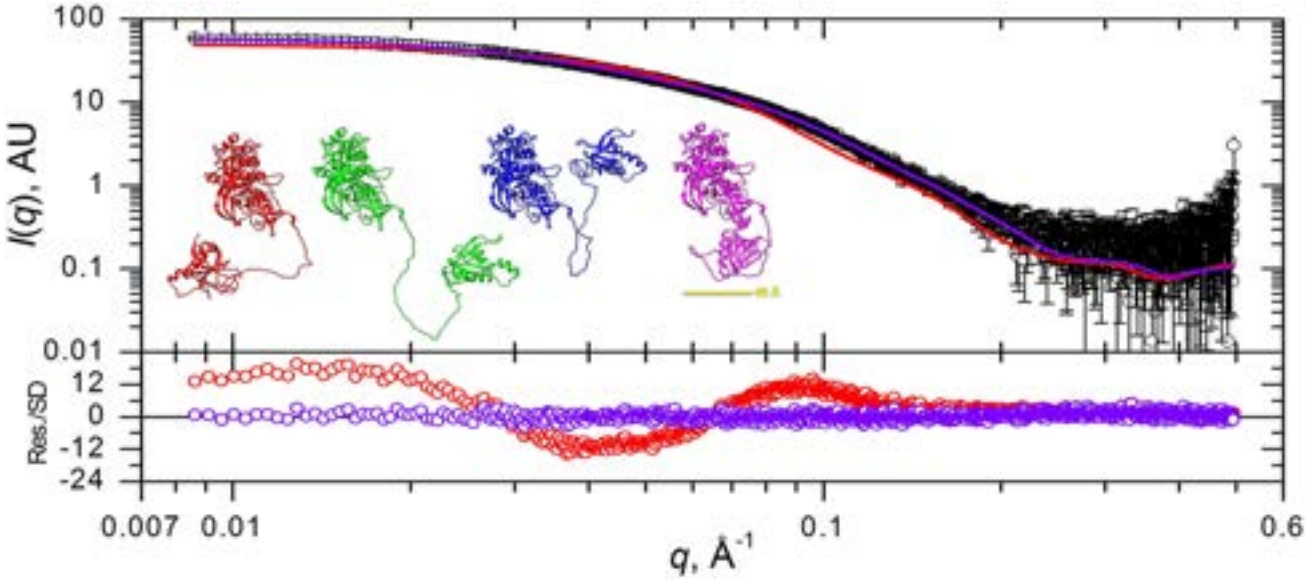


Figure 1. The fit to the experimental SAXS data is significantly improved when an ensemble of conformers is used (purple line) compared with the single predicted AlphaFold model (red line). Figure adapted from Brookes *et al.* (2023).

Besides the remarkable improvement in the structural description of the disordered domains, this article is striking for its rigorous analysis of the SAXS data. The authors are long-standing experts in small-angle scattering for structural biology, and they know all the strengths and limits of the technique (Trewhella *et al.*, 2022, 2017). In this new paper, Brookes, Rocco, Vachette and Trewhella explain with a lot of teaching the methodology, quality assessment, pitfalls and difficulties of SAXS data analysis that need to be known before any atomistic modelling, with an emphasis on the specific case of proteins with long IDRs. Their thorough approach and their valuable advice will undoubtedly inspire and guide structural

biologists struggling with SAXS experiments on IDPs, enabling them to confidently extract all the relevant information on their favourite protein from their data.

Finally, this paper successfully addressed the limitations of AlphaFold in predicting the structure of proteins with long IDRs, by incorporating adequate conformational flexibility. While AlphaFold has enabled considerable advances in structural biology, its next challenge is to accurately predict the conformations preferentially adopted by IDPs and IDRs. Efforts are currently being made to develop accurate predictions of conformational ensembles using machine learning with reduced computational cost (Zheng *et al.*, 2023). However, the conformational sampling of IDPs or IDRs is extremely sensitive to the environmental conditions, such as pH, temperature, redox conditions, crowding, ligand binding, post-translational modifications etc., and this is the motor of their activity. Experimentally derived constraints accounting for these conditions therefore remain necessary to accurately describe the dynamics and structural preferences that drive the functional properties of an IDP. SAXS, being one of the few experimental techniques that give access to the conformational sampling of proteins in solution, combined with ensemble modelling and AlphaFold predictions offers a promising strategy for adequately describing the structure and dynamics of IDPs and is expected to yield numerous successful advances in the understanding of these proteins.

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COMMENTARY

Counting on the future: fast charge-integrating detectors for X-ray nanoimaging

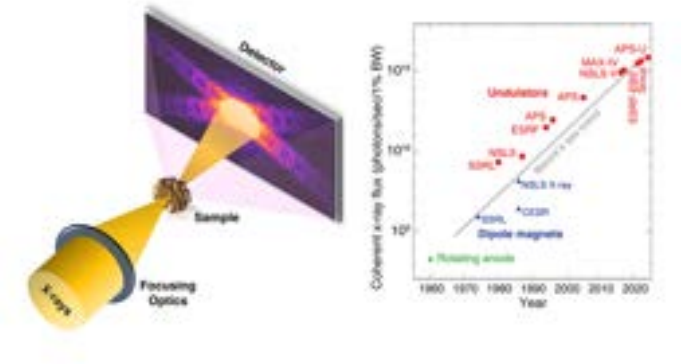


Figure 1. Schematic illustration of X-ray ptychography, where a coherent beam is scanned across the sample. Pixelated detectors record the far-field diffraction pattern, with beyond-optic, high-spatial-resolution information recorded at large scattering angles. This approach benefits tremendously from the historical increase in available coherent flux, which outpaces Moore's law for integrated circuits. Taking full advantage of these sources requires the development of advanced detectors, such as reported in this issue by Takahashi *et al.* (2023).

Junjing Deng, Antonino Miceli, Chris Jacobsen

X-ray nanoimaging is advancing quickly towards and beyond 10 nm resolution by scanning focused coherent beams and then collecting and iteratively phasing far-field diffraction data in a method called ptychography (Fig. 1). This yields phase and absorption contrast images and tomograms, sometimes with tensor information [such as magnetic field direction (Donnelly *et al.*, 2017)], beyond the efficiency and resolution limits of X-ray optics.

These rapid advances have been enabled by a steady increase in available coherent X-ray flux, as depicted in the inset of Fig. 1. Recent and noteworthy advancements have been propelled by the use of multi-bend achromat lattices in electron storage rings. Beyond these synchrotron light sources, X-ray free-electron lasers provide even greater coherent flux, but with such intense and spaced-in-time pulses that one must worry about possible destruction of the sample by the first pulse. Both source types are creating another challenge: photons in detector pixels can arrive so quickly that photon-counting circuitry cannot keep up, as the photon-generated voltage 'spikes' become difficult to separate from each other in time.

One viable solution to address this detector challenge is to move from photon counting to charge integration, where one simply measures the total charge accumulated in each pixel during a detector 'frame' time. With the knowledge of monochromatic illumination, one can then infer the number of detected photons. This was first done in charge-coupled devices or CCDs, where a voltage sequence was used to move per-pixel charge out to a collecting amplifier and digitizer. Through the implementation of multi-row parallelization, this approach has reached frame rates of around a kilohertz. Another approach has involved the utilization of bump-bonding to attach a sensor to per-pixel charge integration circuitry, sometimes with mechanisms to adjust the analog gain during a detector frame with frame rates increasing to several and even tens of kilohertz. This latter approach of using hybrid pixel array detectors

(HPADs) has seen widespread application (and commercial availability) first for photon counting but more recently for charge integration as well. Some variants of these detectors even store charge from each pixel for hundreds of frames at megahertz frame rates, with digitization and data transmission occurring in a burst afterwards.

In this issue of *Journal of Synchrotron Radiation*, researchers (Takahashi *et al.*, 2023) in Japan report an advance both in per-pixel photon arrival rate and in overall detector frame rate by using a single monolithic CMOS chip which both collects the charge (the sensor in HPADs) and incorporates per-pixel charge integration and digitization circuitry (the application-specific integrated circuit in HPADs). This CMOS approach can potentially offer greater flexibility in the choice of pixel size, and can reduce detector fabrication complexity (and perhaps lead to even faster frame rates, and lower cost) by eliminating relatively high capacitance bump-bonding between two chips with different processing requirements. This detector has been demonstrated for nanocrystal imaging at ESRF, an upgraded fourth-generation synchrotron source, with improved performance compared with a photon-counting detector (Grimes *et al.*, 2023). As reported in the paper by Takahashi *et al.* (2023), this detector is now being used for ptychographic imaging at 10 nm resolution over extended objects. A standout attribute showcased by this detector in this paper is its remarkable ability to record a peak intensity of approximately 250 million photons per pixel per second. This rate outperforms that of traditional photon-counting detectors, which typically encounter limitations around 1 million counts per pixel per second (with some correction possible to handle slightly higher rates).

The development of CMOS detectors with charge integration, and with fast-framing capabilities, will likely prove important as X-ray nanoimaging advances along with the development of X-ray sources with increasing coherent flux.

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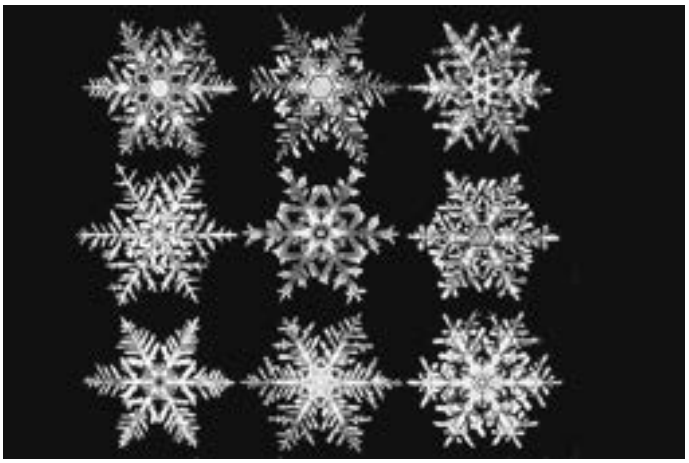
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FEATURE ARTICLE

Crystals humanized



Snowflake photomicrographs by W. A. Bentley from Bentley & Humphreys [12].

Istvan Hargittai, Magdolna Hargittai

We have collected a few textual and pictorial expressions that refer to crystals anthropomorphically (we based much of this contribution on material extracted from our monograph [1]). We dedicate this contribution to Alan L. Mackay on his 97th birthday. Alan has broadened our worldview of structures.

The Czech writer Karel Čapek (1890−1938) wrote about crystals following his visit to the mineral collection of the British Museum. To express his humility in front of these miracles of nature, he added a drawing to his description [2]:



Karel Čapek's drawing after his visit to the mineral collection of the British Museum [2] (the English translation of the source was kindly provided by Alan L. Mackay).

"...But I must speak again about crystals, shapes, colours. There are crystals as huge as the colonnade of a cathedral, soft as mold, prickly as thorns; pure, azure, green, like nothing else in the world, fiery black; mathematically exact, complete, like constructions by crazy, capricious scientists, or reminiscent of the liver, the heart ... There are crystal grottos, monstrous bubbles of mineral mass, there is fermentation, fusion, growth of minerals, architecture, and engineering art ... Even in human life, there is a hidden force towards crystallization. Egypt crystallizes in pyramids and obelisks, Greece in columns; the Middle Ages in vials; London in grimy cubes ... Like secret mathematical flashes of lightning, the countless laws of construction penetrate the matter. To equal nature, it is necessary to be mathematically and geometrically exact. Number and phantasy, law and abundance — these are the living, creative strengths of nature; not to sit under a green tree but to create crystals and to form ideas, that is what it means to be at one with nature!"

Aleksandr I. Kitaigorodsky (1914−1985) liked to ascribe anthropomorphic traits to crystals. He said when asked about his most important achievement in science: "I have shown that the molecule is a body. One can take it, one can hit with it; it has mass, volume, form, hardness. I followed the ideas of Democritos" [3]. Another version of this notion, attributed to Kitaigorodsky, that we heard repeatedly, reads: "The molecule also has a body; when it's hit, the molecule feels hurt all over." For Kitaigorodsky, this implied possible structural changes upon the molecules entering the crystal structure. This statement was the more remarkable because it signified a departure from his earlier views about the constancy of molecular shape and geometry regardless of whether the molecule was in the gas phase or in a crystal. One of us remembers a chemistry meeting in what at the time was East Germany — the German Democratic Republic — in some respects more Soviet than even the Soviet Union. There, Kitaigorodsky was quoted as referring to molecules as being free in the gas phase but no longer free in the crystal, and that loss of freedom would cause deformation. Part of the audience took it as a political statement as if reading

between the lines, equating the crystalline state with a rigid, regimented political system.

Maurits C. Escher (1898−1972), the Dutch graphic artist whose periodic drawings have been so helpful in discussing space-group symmetries, had romantic notions about crystals. The author Bruno Ernst, who wrote a book about Escher's art, quoted him [4]:

"Long before there were men on this globe, all the crystals grew within the earth's crust. Then came a day when, for the very first time, a human being perceived one of these glittering fragments of regularity; or maybe he struck against it with his stone ax; it broke away and fell at his feet; then he picked it up and gazed at it lying there in his open hand. And he marveled.

"There is something breathtaking about the basic laws of crystals. They are in no sense a discovery of the human mind; they just 'are' — they exist quite independently of us. The most that man can do is to become aware, in a moment of clarity, that they are there, and take cognizance of them."

Alan L. Mackay presented another anthropomorphic view that had its roots in his experience as a crystallographer. He expressed it in a poem [5]:

"My molecule is sick,
And I have caught the illness too.
Two atoms have temperatures,
Which are negative,
And two are not resolved at all.
How can I find a cure –
The *R*-factor is enormous,
And direct methods fail me?
Perhaps it is not my métier,
To be a structure analyst."

The female poet Anna Wickham (born Edith Alice Mary Harper, 1884–1947) in her poem *The Woman and Her Initiative* contrasted her 'colloid' self with her husband's 'crystalline' character, and the impression is that the latter’s demeanour left much to be desired [6]:

"Give me a deed, and I will give a quality.
Compel this colloid with your crystalline.
Show clear the difference between you and me.
By some plain symmetry, some clear stated line.
These bubblings, these half-actions, my revolt from unity.
Give me a deed, and I will show my quality."

In another poem, *Gift to a Jade*, it is unambiguous what she meant by her husband’s crystallinity [7]:

"For love he offered me his perfect world.
This world was so constricted and so small,
It had no loveliness at all,
And I flung back the silly little ball.
At that cold moralist I hotly hurled
His perfect, pure, symmetrical, small world."

Alan L. Mackay has done much to expand crystallography to embrace more among the structures of nature than merely the regular and the periodical. He pioneered handling systems with varying degrees of regularity in their structures, and he wrote about this not only in scientific treatises but also in his poetry. We quote here an example about flying through the clouds [5]:

"We cruise through the hydrosphere,
Our world is of water, like the sea,
But the molecules more sparsely spread,

Not independent, not touching,
But somewhere in between,
Clustering, crystallizing, dispersing
In the delicate balance of radiation
And the adiabatic lapse rate."

A beautiful example of imbuing crystals with human qualities is in the crystallographer Charles W. Bunn's (1905−1990) drawings [8] (reproduced in [1], 3rd ed., p. 495) and the writer John Ruskin's (1819−1900) words (cited here from [9]):

"And remember, the poor little crystals have to live their lives, and mind their own affairs, in the midst of all this, as best they may. They are wonderfully like human creatures − forget all that is going on if they don't see it, however dreadful; and never think what is to happen tomorrow. They are spiteful or loving, and indolent or painstaking, with no thought whatever of the lava or the flood which may break over them any day; and evaporate them into air-bubbles or wash them into a solution of salts. And you may look at them, once understanding the surrounding conditions of their fate, with an endless interest. You will see crowds of unfortunate little crystals, who have been forced to constitute themselves in a hurry, their dissolving element being fiercely scorched away; you will see them doing their best, bright and numberless, but tiny. Then you will find indulged crystals, who have had centuries to form themselves in, and have changed their mind and ways continually; and have been tired, and taken heart again; and have been sick, and got well again; and thought they would try a different diet, and then thought better of it; and made but a poor use of their advantages, after all.

"And sometimes you may see hypocritical crystals taking the shape of others, though they are nothing like in their minds; and vampire crystals eating out the hearts of others; and hermit crab crystals living on the shells of others; and parasite crystals living on the means of others; and courtier crystals glittering in the attendance upon others; and all these, besides the two great companies of war and peace, who ally themselves, resolutely to attack, or resolutely to defend. And for the close, you see the broad shadow and deadly force of inevitable fate, above all this: you see the multitudes of crystals whose time has come; not a set time, as with us, but yet a time, sooner or later, when they all must give up their crystal ghost − when the strength by which they grew, and the breath given them to breathe, pass away from them; and they fail, and are consumed, and vanish away; and another generation is brought to life, framed out of their ashes."

Death is an integral component of life, and the crystalline state is often associated with lifelessness and death. An eloquent description of the beauty and symmetry of snowflakes — water crystals — is given by Thomas Mann (1875−1955) in *The Magic Mountain* [10]. Here, in addition to their breathtaking beauty, Mann expresses also why their high symmetry is associated with a 'life-denying character':

"...Indeed, the little soundless flakes were coming down more quickly as he stood. Hans Castorp put out his arm and let some of them to rest on his sleeve; he viewed them with the knowing eye of the nature-lover. They looked mere shapeless morsels; but he had more than once had their like under his good lens and was aware of the exquisite precision of form displayed by these little jewels, insignia, orders, agraffes − no jeweller, however skilled, could do finer, more minute work. Yes, he thought, there was a difference, after all, between this light, soft, white powder he trod with his skis, that weighed down the trees, and covered the open spaces, a difference between it and the sand on the beaches at home, to which he had likened it. For this powder was not made of tiny grains of stone; but of myriads of tiniest drops of water which in freezing had darted together in symmetrical variation − parts, then, of the same inorganic substance, which was the source of protoplasm, of plant life, of the human body. And among these myriads of enchanting little stars, in their hidden splendour that was too small for man's naked eye to see, there was not one like unto another, and endless inventiveness governed the development and unthinkable differentiation of one and the same basic scheme, the equilateral, equiangular hexagon. Yet each, in itself − this was the uncanny, the anti-organic, the life-denying character of them all − each of

them was absolutely symmetrical, icily regular in form. They were too regular, as substance adapted to life never was to this degree − the living principle shuddered at this perfect precision, found it deathly, the very marrow of death − Hans Castorp felt he understood now the reason why the builders of antiquity purposely and secretly introduced minute variation from absolute symmetry in their columnar structures."

We augment this beautiful prose with the whaling captain and Arctic explorer William Scoresby's (1789−1857) drawings of snowflakes from Tom Stamp and Cordelia Stamp's little-known book [11] (see below), and a sample of photographs from W. A. Bentley and W. J. Humphreys' famous book of snowflakes [12] (see above).



William Scoresby's sketches of snowflakes from his 1806 logbook from Stamp & Stamp [11].

Scientists have expressed the same, perhaps less eloquently but most succinctly. According to Michael Polanyi (1891−1976), a perfectly ordered environment was not a suitable habitat (attributed to Michael Polanyi according to a private communication) [13]. The crystallographers Evgraf S. Fedorov (1853−1919) and J. Desmond Bernal (1901−1971) simply stated that "crystallization is death" [14, 15].

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FEATURE ARTICLE

Fifty years on: why macromolecular cryocrystallography has been so successful

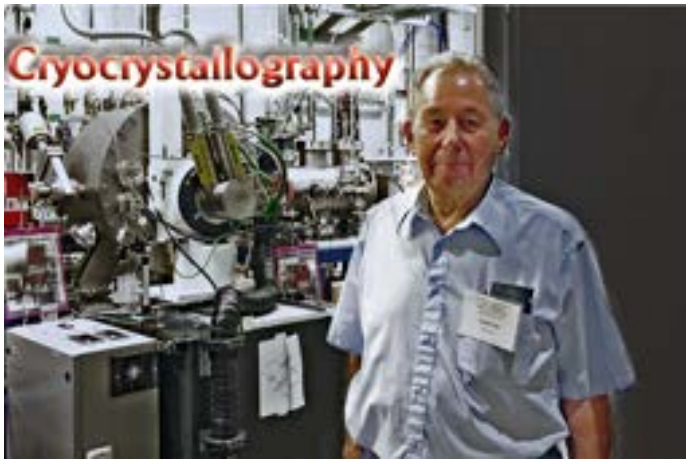


Photo taken at the 2018 Radiation Damage Conference, Brookhaven National Laboratory Synchrotron.

David J. Haas

Fifty years after publication, a scientific paper by Purdue researchers contributed to ending the 2020 COVID-19 pandemic by helping to quickly provide the three-dimensional structure of the SARS-CoV-2 spike protein for vaccine development (structure-guided drug design). This research project began in 1965, but the most important phase was performed in the Purdue University laboratory of Michael Rossmann between 1968 and 1969. The results were published in April 1970 (Haas & Rossmann, 1970), which described the *invention* of a means to cryocool protein crystals to near-liquid-nitrogen temperatures to reduce radiation damage. The paper also described the *discovery* that cryocooling of protein crystals actually reduced the radiation damage by more than ten times [today, cryocooling is now considered to reduce radiation damage by more than seventy times (Garman, 1997, 2005)]. Beginning 20 years later, around 1990, cryocooling technology grew into a key element when using synchrotron radiation for routine X-ray analysis. (The synchrotron was developed decades earlier but only perfected for protein crystallography after 1970, and produces X-ray beams millions of times greater than conventional X-ray tubes.) Today, with more than 50 synchrotrons operating worldwide, cryocooling is universally used to reduce X-ray damage during macromolecular crystallography X-ray data collection at every synchrotron. Synchrotrons and advanced cryocooling have been developed by brilliant scientists, enabling macromolecular cryocrystallography to become a routine method of structure determination. In addition, much of the credit for demonstrating the success of cryocooling goes to Michael Rossmann, who had the foresight and understanding of its potential! Thank you – once again – Michael.

Remarkably, as so often is the case, the 'primary' benefits of cryocooling macromolecular crystals were completely unforeseen by the Purdue scientists:

Cryocooling enables repeated X-ray data collection from a single crystal.

Cryocooling enables better crystal handling for synchrotron X-ray analysis and facilitates very rapid data collection with the intense X-ray beam (minutes, not weeks or months).

Cryocooling provides a host of operational and molecular/crystallographic benefits for structure interpretation not available at room temperature, such as better stability and easy transport.

Because of the remote access required by the X-ray shielded synchrotrons, robotic handling is used, and the synchrotron scientists have provided amazing technology just for this purpose. They are to be congratulated, big-time!

The personal story behind the April 1970 scientific paper

With the 1970 published scientific results, I left the field of crystallography to enter industry. In 2004, I had a brief demonstration of cryocrystallography by Elspeth Garman, but it completely overwhelmed me after 30 years – unfortunately, I did not pursue it. However, in 2015, I attended the ACA Meeting in Philadelphia and then the X-ray Macromolecular Crystallography Course at Cold Spring Harbor Laboratory in 2017, which finally opened my eyes to the subject. I was invited by Stephen Burley to present a seminar at Rutgers PDB on 24 April 2019, and this preparation led to the 'History of Science' paper published in 2020 detailing this subject (Haas, 2020). Surprisingly, I only realized recently that it is the 50th anniversary of this event. Eureka!

Being able to perform this 'proof of principle' research on cryocooling protein crystals in the Rossmann Laboratory was more than just fortuitous. I doubt that I would have been able to perform this experiment anywhere else, first because Michael Rossmann had substantial insight into the future of crystallography, which led him to agree to support the work (and me), and second, the Rossmann Laboratory and Purdue University had all the proper apparatus and personnel that were needed. Hence, I was able to complete the task, which might otherwise have been delayed by years, perhaps decades.

This project began two years earlier (1965) when I arrived for my first postdoctoral fellowship position with David C. Phillips at the Royal Institution of Great Britain. He had constructed the very first automated X-ray diffractometer and, while collecting data on myoglobin and lysozyme protein crystals a few years before, found that this radiation damage problem proved to be serious. From this work, he experienced how the X-rays used to analyze the crystals caused them to deteriorate – the same problem that all other protein crystallographers had observed (and lived with!), except with his automatic diffractometer, he could observe the problem in real time [he wrote a scientific paper on this topic: Blake & Phillips (1962)]. Therefore, when I arrived, David Phillips suggested that I investigate this issue and see if I could reduce the radiation damage. That was the fortuitous beginning of the 'Radiation Damage Project' in September 1965.

I worked on it by myself at the Royal Institution for more than a year without any success. Then during the summer of 1966, David Phillips told me that the crystallographic group was leaving the Royal Institution and that I would need to transfer my work to another laboratory. He had already inquired as to available locations, and the one he suggested was the Weizmann Institute of Science in Rehovot, Israel. My wife, Sandra, and I agreed, and a few months later, we drove to Israel in late December 1966 with my research supplies in our car, so I could just continue the project there. Little did I know that this was to provide a major breakthrough for the invention of macromolecular cryocrystallography.

The Weizmann Institute Crystallography Laboratory was excellent, and the Director, Wolfie Traub, provided everything I needed. However, after several more months, I realized that I had to change the direction of the project, so Wolfie and I made a list of possible alternatives. Only one seemed realistic. If I froze (cryocooled) the protein crystals with liquid nitrogen, then this could possibly prevent the X-rays from damaging the protein crystals. In addition, to my surprise, Wolfie had constructed the exact apparatus I needed several years earlier – a liquid nitrogen 'gas-jet' cooling apparatus just sitting in the rear of the laboratory – unused. I immediately began the cryocooling experiments.

Within a few weeks I was able to cryocool the lysozyme crystals that I had brought with me. And then when I continued the X-ray exposure for several days to create the radiation damage I had always observed on dozens of crystals, the X-ray diffraction photographs showed little or no changes, indicating possible radiation damage protection. This was the first time I had observed this, and it proved to be a Eureka moment in my research! I spent the next few weeks performing additional experiments to better understand the phenomena, but this was already May, and the Six-Day War hysteria had already begun

in Israel. On 5 May 1967, the American Embassy announced that all Americans should leave Israel because, if a war begins, there would be no transportation out. So, that same day I drove my wife with our six-month-old son to the airport so they could fly to London to stay with our English friends. At the airport, we booked the next flight, and they were safely away within hours. Without my family and most of the staff and personnel at the Weizmann Institute, I was kept from performing all the experiments I had planned.

However, I continued with some of the work even though I had to collect the liquid-nitrogen supply from the Weizmann Institute supply building myself. I was the only person in the entire chemistry building, and there was basically no one on campus. I just continued on my own, preparing all my meals and telephoning Sandy every day in London. With the war imminent, the Weizmann Institute was essentially closed, so any chance of completing the research at the Weizmann Institute was dashed.

The war began on the morning of 5 June 1967, but we only saw a few military aircraft overhead that day. Sometime in the morning of this first day, a group of Weizmann security personnel came around and instructed the group that they had assembled as to what we were to do during this time of war. I was told I would be in charge of fire protection for the Stone Administration Building. They showed me where the fire hoses were within the building. In a 15-minute training session, I was 'fully' trained, more or less, in how I was to fight any fire that should develop and whatever I needed to do if the building was damaged. With my portable radio and a bunch of books, I camped out on the porch of the building, sleeping there for the next three nights. Some of the security staff came by occasionally, but on the third day, they said the war had progressed sufficiently that there was no danger of aircraft, so I could return to my apartment.

The war was over in just six days, but in conversations with the few Weizmann staff that remained, they indicated that the Institute would not be reopened for many months, as everyone would remain in the military forces until the peace negotiations ended. I realized that I would need to make an immediate decision on the matter.

As I had previously arranged for a position with Michael Rossmann at Purdue University (during my previous year's job search in September 1966), I only needed to check that the position was still available. I contacted Michael to confirm this. He said I could return at any time, as he was certainly aware of the Six-Day War situation. Hence, I decided to return to the United States as soon as possible. This proved a good decision, so I packed all our belongings into our car, said goodbye to several individuals I knew who were still around the Institute, and drove to the Port in Haifa. Remarkably, within minutes, I located a ship sailing directly to London (Tilbury), and so I purchased the ticket, drove to the side of the ship where they loaded our car onto the deck with a crane, and wow – I was in England within days. What luck!

If not for these fortuitous events, the proof experiments of reduced radiation damage by cryocooling crystals would probably have been delayed for decades. In addition, my final phase of work with Michael Rossmann would probably not have occurred elsewhere as Michael was only convinced by the 'perfect' lysozyme X-ray precession photographs from the Weizmann Institute. He quizzed me extensively and studied all the precession photographs as if it were my final exam. Still, I was sure that the work at Purdue would provide quantitative evidence (proof) for reduced radiation damage. And that is precisely how it happened!

The Rossmann Laboratory was a state-of-the-art crystallography laboratory and there were a host of postdocs and graduate students: Margaret Adams, Alan Wonacott, Michael Schevits and Alex McPherson. They were all working on the lactate dehydrogenase (LDH) protein project (Wonacott *et al*., 1968). The laboratory was very pleasant, and the group was always willing to help me learn the new methods. I had written a short paper describing my Weizmann Institute findings for reduced radiation damage at –50°C on the return trip to the United States, so this was distributed to Michael and the other members of the Rossmann group for their support of my project proposal (Haas, 1968).

Everyone was certainly skeptical of the benefits of possibly extending the useful life of the crystals, but I was adamant that it was worthwhile even though the 'perceived' complexity and difficulty of building, installing and operating cryo-apparatus may be a barrier. I think everyone assumed that the radiation-damage reduction would be only a few hours, certainly not the hundreds of hours that resulted. (No one could even imagine the importance of cryocooling crystals with synchrotron-radiation sources.) Again, the only convincing demonstrations of reduced radiation damage were the lysozyme precession photographs from the Weizmann Institute, but the general notion at the time was that cooling protein crystals would damage them to a point where the X-ray data could not be collected.

After weeks of discussion, Michael agreed to loan me one of the Picker automated X-ray diffractometers for three months (and no more!) in the spring of 1968, and he would fund the purchase and construction of the most primitive cryocooling apparatus if I put the system together myself. (It probably would only be used once for my project anyway.) The Purdue supply department arranged for liquid nitrogen to be delivered and provided me with several large Dewar flasks. The Purdue glass workshop fabricated a coaxial gas-delivery jet for directing the nitrogen gas onto the crystal with a dry-air outer barrier jet surrounding the nitrogen stream. I made it to exactly match the Weizmann Institute apparatus. Initially, the single crystals were each mounted in a Lindemann glass vial in the conventional manner along with a small amount of mother liquor exactly as had been done for more than 30 years, but soon after that, I froze the crystals positioned near the end of a single glass fiber where it remained attached by a small amount of frozen liquid. This was a major step forward. Michael wanted the work to be performed on his protein (LDH, not lysozyme), and enough of his crystals were available for me to use (this proved to be an important decision!). Sucrose was tested as a cryoprotectant to prevent ice formation in the LDH crystals as soon as the cryo-equipment was ready – it worked perfectly.

A temporary setup was rigged up for the precession camera, which successfully obtained precession photographs of cryocooled LDH crystals. Therefore, after Michael approved the project in late 1967, the cryo-apparatus was ready to perform the data collection in the spring of 1968. The Purdue glass making facility and laboratory supply group were invaluable. With the cryo-gas tube assembly ready, simple control circuits were fabricated, and we purchased a suitable air dryer and several bathroom scales for tracking the weight of the liquid-nitrogen-filled Dewars (the scale weight indicates the remaining liquid nitrogen in the Dewar). Three months of work were required for the data-collection portion of the project, and I began the work in April 1968.

We found that initially cooling the protein crystals in a cold gas jet was unsuitable because the crystal faces nearest the gas jet froze more rapidly and asymmetrically. Thus, the usual mounting procedure consisted of placing a single LDH crystal (approximately 0.5 mm of each edge) on a strip of filter paper with a dropper to remove excess liquid, scooping the crystal up on the end of a 0.25 mm diameter glass fiber, and immediately plunging it into liquid nitrogen. The crystal was instantly frozen isotropically to the glass fiber and immobile. As the glass fiber tip had previously been mounted and aligned to the center of the goniometer head, the crystal was also nearly centered for the diffractometer. Finally, the fiber with the protein crystal was transferred quickly from the Dewar full of liquid nitrogen to the diffractometer, where a streaming jet of cold nitrogen gas prevented thawing. Ice formation was prevented using a coaxial dry nitrogen jet around the cold jet and by surrounding the whole diffractometer with a polyethylene bag filled with dry-nitrogen gas. A statement in our 1970 paper says that a thermocouple placed near the end of the cold jet provided a (nearly) continuous record of the crystal temperature, approximately –75°C.

The data collection proceeded from the first day, with only a few interruptions when mechanical issues with the Picker diffractometer occurred. We also collected data from LDH crystals at room temperature to prepare a comparison graph of a radiation-damage reference reflection (showing data collected at both 273°C vs –70°C). Punched cards controlled the Picker diffractometer, and it was run 24 hours a day with only a few delays. Otherwise, I fell into a routine for several months of loading the punched cards, filling the Dewar flask with liquid nitrogen and regularly checking the intensities of the two reference reflections to ensure that the crystal was aligned correctly. The experiment continued unimpeded for three months –

this was a very exciting time.

We processed the data during the late summer and fall of 1968, and Michael spent several months analyzing the electron-density maps from our collected data (Haas & Rossmann, 1970). The data produced nice results, with the most important graph from these experiments showing a comparison of the reduced X-ray spot intensity decay of the two reference reflections. This radiation-decay graph [Fig. 3 in Haas (2020)] indicated that the X-ray damage in cryocooled LDH crystals was reduced more than tenfold at –75°C compared with room-temperature data. It was the first quantitative measure of radiation-damage reduction (finally, quantitative proof!). Michael wrote the final draft of the paper and submitted it to *Acta Crystallographica* in July 1969. The tenfold reduction was low compared with the 70-fold number that is now accepted, probably because of the higher temperature and temperature variations due to the nitrogen gas jet on the crystals. Reduced radiation damage on cryocooling crystals was independently confirmed by Gregory Petsko in his 1975 study on protein crystals at subzero temperatures (Petsko, 1975). This certainly contributed to the recognition of the benefits of cryocooling.

In 1969, after interviewing for positions at several universities and pharmaceutical companies, a perfect industrial position became available. I left basic scientific research in 1970 and joined the electronics industry as an X-ray scientist in May 1970 (Philips Electronic Instruments in Mount Vernon, New York), ending my protein crystallography career. I regret not being more diligent with my brief encounter in 2004 at the Chicago ACA meeting and in Oxford with Elspeth Garman and Louise Johnson; but finally, in 2015 when at lunch with Fran and Alex McPherson, Alex explained to me that cryocooling of protein crystals had become a universal technology for X-ray synchrotron data collection. He said it was used at all 50 synchrotrons around the world and used regularly by all protein crystallographers. I was amazed! I have now concluded that in 1970 I had so rejected and repressed any thoughts of cryocrystallography that this explains why I was totally unaware of the subject for 30 years.

Cryocooling was slow to be implemented, even though several crystallographers experimented in the field between 1975 and 1990. After 1970, it appears that crystallographers generally knew the benefits of cryocooling. After 1995, most protein crystal structure data were collected at synchrotrons from cryocooled crystals. (This is because the synchrotrons produce X-ray beams millions of times more intense than the older conventional vacuum X-ray tubes and destroy the protein crystals within seconds.) In addition, the development of structure-guided drug design became widely used (see Goodford, 1984) and was developed rapidly during the early 1980s. Structure-guided drug design has been a motivating force for the pharmaceutical industry, and with the AIDS epidemic in the 1980s, protein crystallography, synchrotrons and cryocooling had already become a major force for attacking these issues.

In early 2017, I was fortunate to be invited to attend the Cold Spring Harbor X-ray Macromolecular Crystallography Course, which had been given for more than two decades. In addition to this being my first direct exposure to modern crystallography after more than 45 years, I was able to participate in laboratory work employing cryocrystallography. I never thought much about this until I began reading about the 'AIDS Lazarus effect' (Cold Spring Harbor Laboratory, 2016). The AIDS Lazarus effect is just one example of the successes of structural biology. Later that year, on being invited by Stephen Burley to give the weekly Rutgers Protein Data Bank Seminar on 24 April 2019, I reviewed the extensive literature regarding the history and chronology of macromolecular cryocrystallography. For more than 30 years, synchrotrons have been successfully used for the X-ray data collection on thousands of protein crystals. This is clearly demonstrated by the fact that more than 94% of all FDA-approved drugs used PDB protein structures employing cryocooling [see the Garman figure in Haas (2020)]. The cryocooling invention developed and demonstrated in the Rossmann Laboratory at Purdue University has proven itself in real-world drug design and as one of the main technologies of the structural and molecular biology fields today. Furthermore, personally, my life is being extended because of one of these pharmaceuticals – Eureka!

I cannot thank enough the many scientists and groups who have enabled me to fill in this 50-year knowledge gap, and in particular, Elspeth Garman, whom I am privileged to know.

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OUTREACH

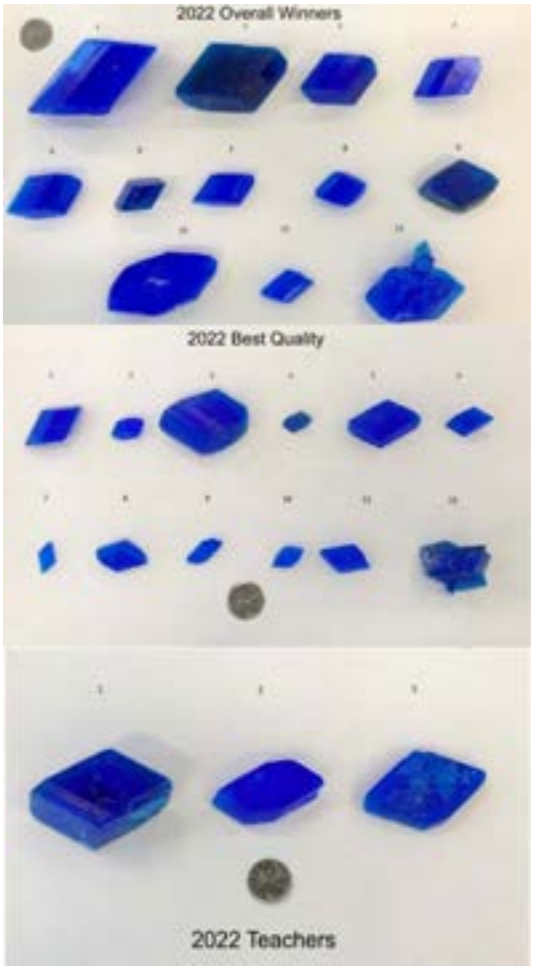
Sparking interest in STEM: the National Crystal Growing Competition in Canada



Michelle Dao, Joy-Lynn Kobti, V. Nicholas Vukotic

The Chemical Institute of Canada (CIC), a non-profit association of professionals in the chemical sciences, hosts outreach events every year across the country, such as the National Crystal Growing Competition. The goal of the competition is to promote chemistry, chemical engineering and chemical technology to the youth and to inspire the next generation of scientists and crystallographers through an exciting, educational and interactive competition. The National Crystal Growing competition has been active for over 30 years. This occurs every fall semester and is open to almost all students, including those who are home-schooled plus teaching staff. Individuals or teams can enter the competition whose aim is to grow the largest and highest-quality crystal possible. The task at hand can be challenging, as many factors affect the crystal growing process (*i.e.* temperature, vibrations *etc.*), which will likely result in students performing trial and error to succeed. This allows the students to develop critical problem-solving skills and to have basic laboratory experience by using various equipment and glassware. After a few weeks of waiting, the crystals are then submitted and evaluated on a regional, provincial and national level. Students and their teachers can win various prizes ranging from textbooks and swag to cash prizes, with the first prize historically being ~CAD$350 cash.

Last year, in 2022, many schools participated across Canada. The 2022 winners for best overall crystals were Rebecca Rouhana, Paulina Abou-Nehme and Zackary Hamwi from Collège Catholique Samuel-Genest (Ottawa, ON). The runner-ups for second and third place were Mathis Poirier-Larouche from École d'éducation internationale de Laval (Laval, QC) and Samuel Giguère from École secondaire Veilleux (St-Joseph-de-Beauce, QC), respectively. The 2022 winners for the highest-quality crystals were Tyson Bergen, Owenn Flaming and Kailee Tait from Leamington District Secondary School (Leamington, ON). The second place and third place winners were Amélia Barriault and Tina Scherrer from École Monseigneur-Labrie (Havre St-Pierre, QC) and Heather Tocher and Selina Liu from Fleetwood Park Secondary (Surrey, BC), respectively.



The 2022 winning crystals of copper(II) sulfate pentahydrate.

The competition has resulted in various high-school and university news stories, which showcase the dedicated outreach efforts of the regional coordinators across Canada. These include highlights from schools such as Polyvalente des Abénaquis, the Conseil des écoles catholiques du Centre-Est, the University of Waterloo and the University of Windsor. A science department head at the Catholic Central High School in Windsor, ON, notes, "*During COVID time, when there was limited availability of extracurricular activities, this competition gave some of my chem students a great opportunity to do something exciting and fun*." Windsor regional coordinator and professor from the University of Windsor, Nick Vukotic, says it was fun to be part of the event, and he looks forward to doing it again and highlights that "*it is a great way to get students involved in chemistry and excited about science in general*."

Another high-school teacher from the Laval School of International Education also shared that the "*competition is very educational for someone who loves science and intends to pursue this field further. Crystal growth is a long-term endeavor that requires precision, patience, and perseverance. Choosing the right "crystal seed," nurturing its growth, and regularly changing the growth solution – these tasks all take time and develop essential qualities for any aspiring scientist*."



Kailee Tait, Tyson Bergen and Owenn Flaming are 10th graders at Leamington District Secondary School who won the Best Quality award at Canada's 2022 National Crystal Growing Competition (left image). Jessica Fisher, Damien Sharpley and Jasmine Vo are from Jacob Hespeler Secondary School and were part of a group of students who came in tenth at the National Crystal Growing Competition in 2012.

The CIC's National Crystal Growing Competition is an engaging event that promotes chemistry to students and the public, sparking interest in STEM. By taking part in STEM outreach, we can play a pivotal role in shaping young minds, fostering curiosity and making a lasting impact. Participation and support are not only welcomed but actively encouraged. For more information about how to get involved in the Canadian competition, check out https://www.cheminst.ca/discover/national-crystal-growing-competition/. Readers are invited to immerse themselves in the exciting realm of STEM outreach, embracing opportunities such as the National Crystal Growing Competition.

OUTREACH

2022 US Crystal Growing Competition



Jason Benedict

"*We really appreciate the contest and prizes. My students love growing crystals, some of them even got kits so that they can grow crystals at home. Thanks so much.*" – Haley Metcalf, 6th grade Science Teacher at Franklin Park Middle School in Salem, IL

2022 was another great year for the US Crystal Growing Competition (USCGC, Fig. 1)! Once again, thousands of kids, parents and educators from all over the country participated in the #2022USCGC! None of this would be possible without the tremendous efforts of the USCGC Crystallites: Fernando Uribe-Romo (University of Central Florida, UCF), Michael Nippe (Texas A&M University, TAMU), Karah Knope (Georgetown University, GU), Tasha Benedict (University at Buffalo, UB) and Jeffery Rack (University of New Mexico, UNM)! A HUGE thank you to all of their wonderful students, and mine too who helped make the #2022USCGC happen!



Figure 1. Hand of Travis Nelson examining a submission during judging of the 2022 USCGC. Photo credit: University at Buffalo | Meredith Forrest Kulwicki.

The 2022 USCGC began during National Chemistry Week in mid-October and concluded in early December. Hundreds of kilograms of alum went out, and over 160 crystals were sent to UB for judging – a new record (Fig. 2)!!! For an awesome photo-essay of the judging, check out https://ubuffalo.exposure.co/the-challenge-of-crystal-growing.



Figure 2. Entries from the 2022 USCGC on display in the Department of Chemistry at the University at Buffalo. Photo credit: Jason Benedict.

There was an exciting addition to the line up of 2022 judges this year! Two local educators and USCGC participants joined the panel: Dana Pepe (Olmstead School #64) and Jeff Yap (Williamsville South High School). It was so fun and rewarding to help get educators more involved in the contest! As judges, they had the opportunity to see all of the submissions firsthand and take new ideas and the experience back to their classrooms!

Holding the judging back at UB (Fig. 3) meant a return for many veteran judges including Andrea Markelz (UB, Physics), David Lacy (UB, Chemistry), Travis Nelson (UB, Geology), Luis Velarde (UB, Chemistry) and Jeff Rack (UNM, Chemistry). But we were certainly happy to welcome many new judges too: Luis De Jesus-Baez (UB, Chemistry), Andrew Murkin (UB, Chemistry). And lastly, we were so glad that Jacob Furst (UCF), a graduate student in the lab of Fernando Uribe-Romo, made the trip to judge!



Figure 3. Lots of judges hard at work scoring the entries for the 2022 USCGC. Photo credit: Meredith Forrest Kulwicki.

"*Thanks so much again. Students love participating in this kind of active hands-on learning and it lets me teach them not only about the crystallization process, but also about science concepts like controlling variables, solubility, impurities, chemical sedimentary rocks and cave formations*." – Haley Metcalf, educator at Franklin Park Middle School

Winners once again came from across the country! For grades K-8, the Derby North Middle School Science Club with students in grades 6–8 led by Kimberly Norden won both 1st place overall (US$200), and 1st place highest quality crystal (US$100)! Zacia Emniser, Hunter Williams, Shanelle Pruden and Teagan Lobek, a team of 6th graders from Mrs Haley Metcalf's class at Franklin Park Middle School (Salem, IL), won 2nd place Overall (US$100, Fig. 4). And Charles Rambo, a 5th grader from the Geauga Engineering and Robotics 4-H club in Novelty, OH, took home 3rd place Overall (US$50).



Figure 4. Hunter and Zacia (back) and Teagan and Shanelle (front) winners of 2nd place Overall for grades K-8 from Franklin Park Middle School (Salem, IL). Photo credit: Haley Metcalf.

"*The kids absolutely love this contest. Every year. Every kid. Thank you so much for all the time and energy you put into it. It is so fun to do with them*." – Lucy Walter, educator at Lyme/Old Lyme High School

In the 9–12 grade division we also had another dual category winner from the same school: Susan Schmidt's class at Somerville High School in Somerville, MA!! 1st prize Overall (US$200) went to a team of 10th graders Jameer Perez Sinclair, Camden Pereira and Brian Rodriguez (US$200, Fig. 5) and 1st place Highest Quality crystal (US$100) went to Sebestian Ungar. Chase Calderon, Eli Goldberg and Andrew (Quinn) Sprankle, 10th graders from Lucy Walter's class at Lyme/Old Lyme High School in Old Lyme, CT, won 2nd place Overall (US$100, Fig. 6). Lucas Watts, Daniel Armendariz-Huang and Ayomi Odetoyinbo, 10th and 11th graders from Jim Burdick's class at HC Williams High School in Canton, NY, won 3rd place Overall (US$50, Fig. 7).

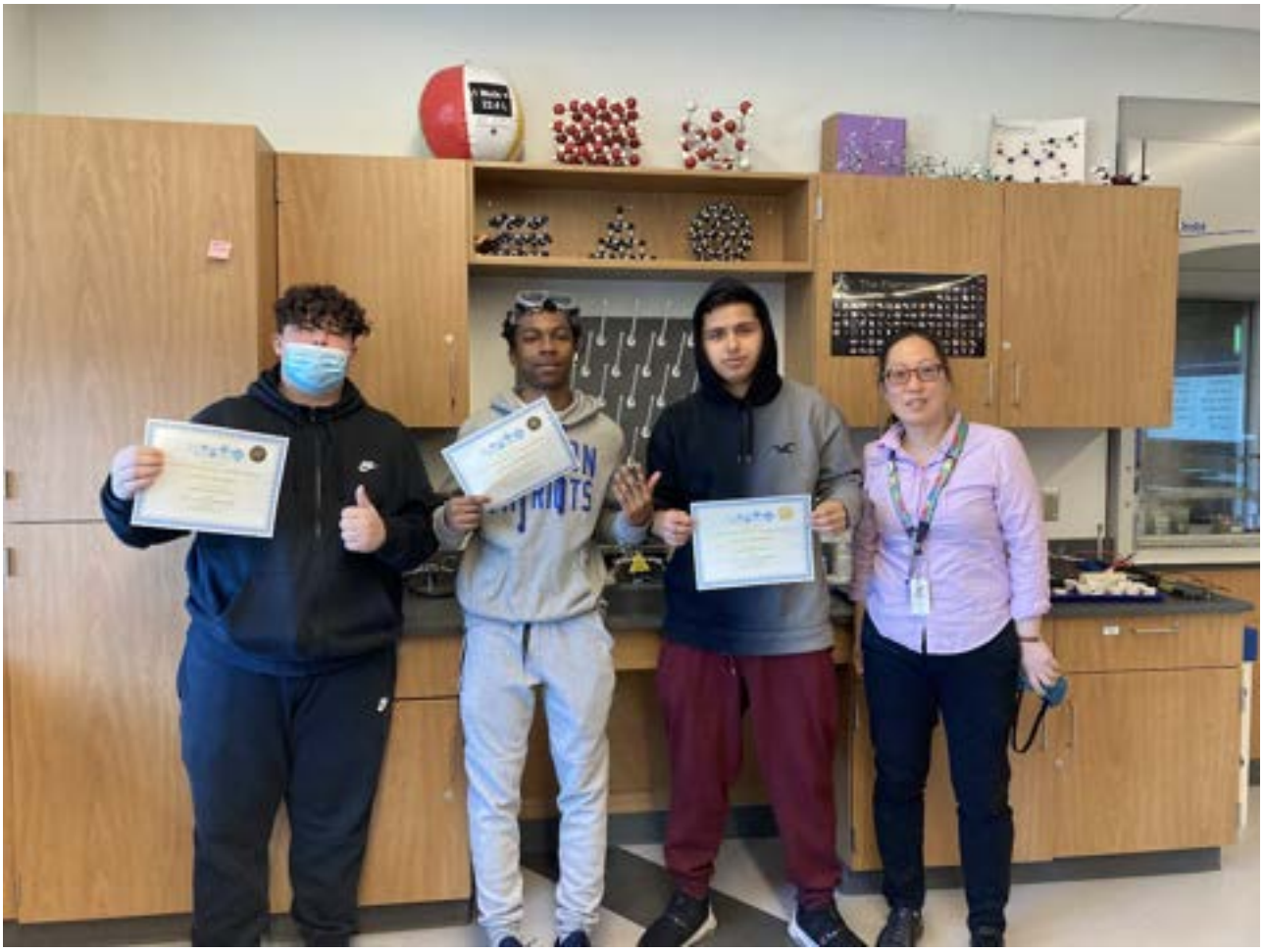


Figure 5. (Left to right) Camden, Jameer and Brian, and their teacher Susan Schmidt, winners of 1st place Overall for grades 9–12 from Somerville High School (Somerville, MA).



Figure 6. (Left to right) Eli, Quinn and Chase, winners of 2nd place Overall for grades 9–12, from Lyme/Old Lyme High School (Old Lyme, CT). Photo credit: Lucy Walter.



Figure 7. (Left to right) Daniel, Ayomi and Lucas, winners of 3rd place Overall for grades 9–12 from HC Williams High School (Canton, NY). Photo credit: Jim Burdick.

"*Every year, my students say that growing crystals was one of their favorite activities of the year. I connect it to ionic bonding and how the arrangement of ions affects the properties and shape of the macroscopic crystal. Thanks for running this contest every year – my students are thrilled to have won 1st place. You have helped spark interest in chemistry, and I hope more and more schools participate each year!*" – Susan Schmidt, educator at Somerville High School in Somerville, MA

"*The contest gives me a bit of a mission to focus on in the fall before each week starts getting interrupted with delays and snow days. Very excited we finally cracked the top 3!*" – Jim Burdick, educator at HC Williams High School in Canton, NY

The 'Best Teacher Crystal' was won by Karen Metcalf from Cornerstone Learning Community in Tallahassee, FL. Coolest Crystal? This year there were 40 submissions to this category! With so many submissions and growth in this category, we may need more than 'coolest'! Once again, a "super dark purple – nearly black crystal" won!!!! It was sent in by Kate Bryson and Gavin Michaels, 8th graders from Mrs Lisa Matejka's class at Trinity Lutheran School in Bloomington, IL. I've said it before, and I'll say it again. I never tire of seeing what happens when kids and their imaginations combine with crystals (Fig. 8)!!!



Figure 8. Top ten “Coolest Crystals” for 2022 viewed in white light (upper) and black light (lower). (1) “super dark purple – nearly black crystal” sent in by Kate and Gavin from Mrs Lisa Matejka’s class at Trinity Lutheran School in Bloomington, IL. Photo credit: Jason Benedict.

“*It just grew this way. I have never done this before, and it is awesome!*” – Ke’asia Thompson from Margaret Beeks Elementary (Blacksburg, VA) assisted by Elizabeth Larsen (Margaret Beeks) and Amanda Morris (Virginia Tech)

All of the winners were once again announced Academy Award Style on TikTok:

K-8: https://www.tiktok.com/@uscrystalcomp/video/7192622823288868142

9–12: https://www.tiktok.com/@uscrystalcomp/video/7192626792765607211

Teacher: https://www.tiktok.com/@uscrystalcomp/video/7192627430119591211

Coolest: https://www.tiktok.com/@uscrystalcomp/video/7192643357506555179

Please check out all the winners and some great participant posts on the contest website and at #2022USCGC on Twitter!

The USCGC helps raise public awareness of the importance of crystal-based research and the organizations, including the ACA, that promote and support these important activities. The USCGC gratefully acknowledges the support of our sponsors: ACA, National Science Foundation, Ward’s Scientific/VWR, Pritzker School of Engineering at the University of Chicago, Bruker AXS, Rigaku, Krackeler Scientific, Cambridge Crystallographic Data Centre, the Western New York section of the American Chemical Society, the Departments of Chemistry of UB, GW, UCF, UNM and TAMU. Please consider making a tax-free donation to the 2023 contest! For more information, please visit the USCGC website or e-mail Jason Benedict at jbb6@buffalo.edu.

This article was first published in *ACA Reflexions*, the Newsletter of the American Crystallographic Association.

MEETING REPORT (IUCR SUPPORTED)

AICS2023 – Electron Crystallography: A deep dive into nanocrystals



Group photo.

Annalisa Guerri, Paolo Pio Mazzeo

The annual school of the Italian Crystallographic Association (AICS2023) was held in Pisa, Italy, from 3 to 6 July 2023. The Organizing Committee, all members belonging to the University of Pisa (Marco Taddei, Enrico Mugnaioli, Francesca Nerli, Giulio Bresciani, Gabriele Paoli, Michele Alderighi), selected 34 students from 9 different countries: Austria (1), Denmark (4), India (2), Italy (21), Poland (1), Sweden (1), Slovenia (1), Spain (1) and UK (2).

The program of the school was organized with theoretical lessons and practical sessions so that students could learn the basis of electron diffraction theory and then apply it during the workshops, which involved the use of different software packages (*SIR2019*, *SHELX*, *PETS*, *JANA* and *OLEX2*).

During the school a get-together dinner was organized at the beginning of the event to allow people to get to know each other and a social dinner close to the end of the course. All the students were satisfied with the concepts learnt during the school.

Funds from the IUCr provided subsistence support for 6 PhD students and 5 postdocs from Austria (1), Denmark (3), Italy (3), Poland (1), Slovenia (1), Spain (1) and Sweden (1).

MEETING REPORT (IUCR SUPPORTED)

Fifth Summer School on Mathematical Crystallography



Massimo Nespolo

The fifth edition of the Summer School on Mathematical Crystallography in Nancy, France, was held from 12 to 16 June 2023 on the campus of the Faculty of Sciences and Technologies of the Université de Lorraine. It welcomed 28 participants (16 males, 12 females) from 19 countries and 4 continents, representing 26 institutions from 13 countries and 4 continents. Lodging and restoration were provided on-site.

The program included group theory, exercises on *International Tables for Crystallography* and on the Bilbao Crystallographic Server, as well as tutorials on the *Jana2020* software package. The lecturers were Professor Massimo Nespolo (Université de Lorraine), Professor Mois Ilia Aroyo (Universidad del País Vasco, Bilbao, Spain; editor of Volume A of *International Tables for Crystallography*), Dr Michal Dušek (Czech Academy of Sciences, Prague, Czechia) and Dr Andrey Zameshin (Malvern Panalytical), supported by Dr Isabella Pignatelli (Université de Lorraine) as tutor. Poster presentations from the participants were on display during the five days of the school.



The school benefited from the generous financial support of the IUCr, the European Crystallographic Association, the Association Française de Cristallographie, the Société Française de Minéralogie et Cristallographie, the Université de Lorraine (via the Doctoral School of Chemistry, Materials and Physics and the Pôle scientifique CPM), the Grand Nancy Metropolitan Government, and Malvern Panalytical as industrial partner. More than half of the budget was used to help students and young scientists to attend the school by partially covering their expenses.

This school was organized in the framework of the activities of the IUCr Commission on Mathematical and Theoretical Crystallography, which had been slowed down by the SARS-CoV-2 outbreak.



Details on the school and the list of participants can be found on the school website.

MEETING REPORT

72nd Annual Denver X-ray Conference



Stephanie Jennings

The 72nd Annual Conference on Applications of X-ray Analysis, more commonly known as the Denver X-ray Conference or DXC, was held 7–11 August 2023. The week-long conference returned to the Chicago area, visiting The Westin Chicago Lombard (Lombard, IL, USA). X-ray and materials scientists gathered at the conference to discuss various techniques, applications, software, instruments and products for XRD and XRF analysis. The combination of attendees and exhibitors brought the attendance to over 375 X-ray scientists, with over 30% from outside the United States.

DXC workshops

The technical program began with 16 half-day tutorial workshops held on Monday and Tuesday of conference week. Topics were categorized as XRD, XRF or 'special topic', and focused on both beginner and advanced levels. In total, 45 specialists were invited to participate as workshop instructors, and many provided handouts that were posted on a private website for attendees only. Topics included the following:

What the APS Upgrade will bring to X-ray Analysis – Parts I & II

Cultural Heritage

Basic to Intermediate XRD

Basic XRF

In situ Battery Measurements

Quantitative XRF

Sample Preparation for XRF

Intro to GSAS-II

Advanced Topics in GSAS-II

Texture

Micro XRF

XRF of Layered Structures

XRD Methods for Complex Multi-Phase Identification

How to Get the Best from Your Handheld XRF Spectrometer

XRF Trace Analysis

Plenary Session and DXC awards

The Plenary Session, *Energy Storage*, was held on Wednesday morning as the opening session for the oral talks that were presented during the next three days of conference week. Scott Misture (Alfred University, NY, USA) chaired the plenary, which began with an awards presentation.

The Barrett Award, given biennially to recognize outstanding contributions to the field of powder diffraction, was presented to Ashfia Huq (Sandia National Laboratories, Livermore, CA, USA). Dr Huq received the award for her commitment to and leadership in the advancement of spallation neutron powder diffraction and for her service to the neutron powder diffraction community.



Barrett Award winner Ashfia Huq (left; Sandia National Laboratories, Livermore, CA, USA) pictured with Conal Murray (IBM Thomas J. Watson Research Center, Yorktown Heights, NY, USA).

The Jenkins Award, given biennially to recognize scientists who exhibit lifetime achievement in the advancement of the use of X-rays in materials analysis, was presented to Tim Elam (University of Washington, Seattle, WA, USA). Dr Elam received the award for his contributions to X-ray fluorescence spectrometry in the development of instrumentation and methods of X-ray analyses in challenging environments, including the PIXL micro-XRF spectrometer on the Mars rover Perseverance. The award also recognized his many contributions to educating and teaching others in the field of X-ray spectroscopy.



Jenkins Award winner Tim Elam (left; University of Washington, Seattle, WA, USA) pictured with Tim Fawcett (ICDD, Newtown Square, PA, USA).

Also presented during the DXC Plenary Session was the 2022 ICDD Hanawalt Award, recognizing distinguished, recent work in the field of powder diffraction. The Hanawalt Award was presented to Karena Chapman (Stony Brook University, NY, USA). Dr Chapman received the award for her contributions to developing X-ray diffraction capabilities in the study of challenging materials problems in sustainable energy and environmental remediation.



Hanawalt Award winner Karena Chapman (left; Stony Brook University, NY, USA) pictured with Tom Blanton (ICDD, Newtown Square, PA, USA).

Eight outstanding young scientists received the 2023 Robert L. Snyder Student Grant Award. The awardees and the works they presented at the conference were as follows:

Dana Alramahi (Illinois Institute of Technology, Chicago, IL, USA): *High Entropy Oxide Tungsten Bronzes as Anodes for Lithium Ion Batteries*, XRD Poster Session

Karen Castañeda Marin (Illinois Institute of Technology, Chicago, IL, USA): *Synthesis and Characterization of MoP Nanoparticles Used As a Catalyst in CO_2 Reduction Reaction*, XRF Poster Session

Sven Hampel (Clausthal University of Technology, Germany): *Successful Picoliter Printing of 65 Elements for TXRF Analysis and Related Methods,* XRF Poster Session; *Investigation of the Genesis of Spinel Solid Solutions in Recycling Slags,* Energy Storage and Harvesting Session; and *Determination of Diffusion Coefficients of Vanadium Inside Polymer Electrolyte Membranes*, General XRF Session

Benjamin Hulbert (University of Illinois at Urbana Champaign, IL, USA): S*pecimen Displacement Correction for Powder X-ray Diffraction in Debye-Scherrer Geometry with a Flat Area Detector,* General XRD Session, and *Crystal Structure Solution and Thermal Expansions of $CaZr_4(PO_4)_6$ and $SrZr_4(PO_4)_6$*, XRD Poster Session

Hao Lin (Illinois Institute of Technology, Chicago, IL, USA): *Exploring the Structural Evolution in Li-Rich Layered Materials via Operando XRD*, XRD Poster Session

Benard Lawer Patawah (Illinois Institute of Technology, Chicago, IL, USA): *XAS Study Local Atomic Environment Mn-Edge in MnO_xGO Nanocomposites as Air-Cathode for Metal-Air Battery Application*, XRF Poster Session

Himihami Mudiyanselage Senevirathna (Illinois Institute of Technology, Chicago, IL, USA): *In Situ EXAFS Study on Pd–Ni(OH)$_2$ during Electrocatalytic CO$_2$ Reduction Reaction*, XRF Poster Session

Philipp Ziegler (TU Wien, Austria): *Tackling Low-Z Element Quantification with TXRF*, XRF Poster Session.



2023 Robert L. Snyder Student Grant Award winners.

Following the awards presentation, the Plenary Session continued with three fascinating talks by keynote speakers Y. Shirley Meng (Argonne National Laboratory, Lemont, IL, USA), Karena Chapman (Stony Brook University, NY, USA) and Will Chueh (Stanford University, CA, USA). Dr Meng presented the talk *Designing Better Materials for Future Batteries*. Next was Dr Chapman's presentation on *X-ray Visions: Operando Insights into Functional Energy Materials*. Lastly, Dr Chueh presented on *Dynamic Electrochemical Phenomena at the Mesoscale*. The session was very well attended and offered great insight into future advancements in science and technology.



2023 Plenary Speakers (left to right) Karena Chapman, Y. Shirley Meng, Scott Misture (session chair) and Will Chueh.

Special sessions

From Wednesday afternoon through Friday morning, 16 half-day oral sessions were held. Over 100 presentations were organized in the oral sessions, with 30 presentations given by invited speakers, experts in their respective fields. Topics included the following:

New Developments in XRD and XRF Instrumentation

Imaging

Stress and Texture Analysis

Trace Analysis

Machine Learning Techniques in X-ray Analysis – Parts I & II

Synchrotron Applications in XRD

Industrial Applications of XRD

General XRF

Industrial Applications of XRF

General XRD

Quantitative Analysis of XRF

Energy Storage and Harvesting

Cultural Heritage

Applications of Rietveld Analysis

Micro XRF and Synchrotron Applications

Poster sessions

Posters were presented on Monday and Tuesday evenings during the XRD and XRF Poster Sessions. Two E-poster stations were also set up in the exhibit hall. Attendees were given the opportunity to preview electronic copies of the posters at the E-poster stations or through the mobile app *Whova*. Respected judges chose the best posters, and the competition was strong.

Ultimately, the following presenters were named winners:

XRD Best Poster Awards

James Kaduk, T. Ens, N. Boaz (North Central College, Naperville, IL, USA), T. Blanton and A. Dosen (ICDD, Newtown Square, PA, USA) for their work: *Crystal Structures of Large-Volume Commercial Pharmaceuticals*

Benjamin S. Hulbert, J. E. Brodecki and W. M. Kriven (University of Illinois at Urbana-Champaign, IL, USA) for their work: *Crystal Structure Solution and Thermal Expansions of* $CaZr_4(PO_4)_6$ *and* $SrZr_4(PO_4)_6$

Dana Alramahi, O. Marques and C. Segre (Illinois Institute of Technology, Chicago, IL, USA) for their work: *High Entropy Oxide Tungsten Bronzes as Anodes for Lithium Ion Batteries.*



XRD Poster Session Award winners (left to right) Ercan Cakmak (poster judge), James Kaduk, Dana Alramahi, Benjamin S. Hulbert and Tom Watkins (poster judge).

XRF Best Poster Awards

Ruthmara Corzo (NIST, Gaithersburg, MD, USA), J. Stallworth and T. Gluodenis (Lincoln University, PA, USA) for their work: *Elemental Characterization of 3D-printed Polymers Using Micro X-ray Fluorescence Spectrometry for Forensic Applications*

Sven Hampel, F. Sand, U. E. A. Fittschen (Clausthal University of Technology, Germany) and G. Pepponi (Fondazione Bruno Kessler, Italy) for their work: *Successful Picoliter Printing of 65 Elements for TXRF Analysis and Related Methods*

Karen A. Castañeda, I. Senevirathna, C. Segre and M. Asadi (Illinois Institute of Technology, Chicago, IL, USA) for their work: *Synthesis and Characterization of MoP Nanoparticles Used as a Catalyst in CO_2 Reduction Reaction.*



XRF Poster Session Award winners (left to right) Ruthmara Corzo, Karen A. Castañeda, Diane Eichert (poster judge), Sven Hampel, Maggi Loubser (poster judge) and Poulami Dutta (poster judge).

We would like to thank two of our exhibitors for sponsoring additional Best Poster Awards during the XRF Poster Session: Amptek, Inc. and XOS.

Amptek Award for Best Student XRF Poster

Alyssa Tovar and M. Schmeling (Loyola University Chicago, USA) for their work: *Environmental Sampling of Chicago Industrial Corridors.*

XOS Innovation Award™

First place: Donald Windover (NIST, Gaithersburg, MD, USA) and K. J. Kim (KRISS, Daejeon, Korea) for their work: *Thickness Monitoring Using X-ray Fluorescence in Hafnia Films*

Runner up: Sven Hampel, F. Sand, U. E. A. Fittschen (Clausthal University of Technology, Germany) and G. Pepponi (Fondazione Bruno Kessler, Italy) for their work: *Successful Picoliter Printing of 65 Elements for TXRF Analysis and Related Methods.*

Exhibits and sponsorships

The exhibition hall accommodated 36 companies with displays of products and services for the X-ray community. See a complete listing of exhibitors and their product descriptions in the 2023 Onsite Program. The Denver X-ray Conference is very appreciative of their support this year.

Many of the exhibitors also supported the conference as sponsors, including Amptek, Inc.; Anton Paar; Bruker; ICDD; KETEK GmbH; Materials Data; Petrick GmbH; Rigaku Americas; Xenocs and XOS. The generosity of our sponsors helps to keep attendee costs low and the quality of the conference high. We are grateful for their support!

Website and proceedings

To view the complete DXC Program, please visit the ‘Past DXC’ page of the conference website, located under the ‘About DXC’ tab. The conference proceedings, *Advances in X-ray Analysis*, Volume 67, will be published in the summer of 2024. Select papers will also be published in the *Powder Diffraction* journal. Please also visit the ‘Resources’ tab on the ICDD website for free full access to manuscripts published in Volumes 40–66 of *Advances in X-ray Analysis*.

The Conference Services team at ICDD would like to thank the many people who volunteered their time and efforts to organize this event. Members of the DXC Organizing Committee, session chairs, workshop instructors, invited and contributed speakers, and exhibitors all played a role in bringing the community together again. Special thanks also to the attendees who joined us as well. The success of the event is attributed to each and every individual who participated, and we send our genuine thanks to all of you!

2024 Meeting

Save the date! DXC will return to Colorado, 5–9 August 2024, at The Westin Westminster, Westminster, CO, USA.

MEETING REPORT

Hatfest!



Marjorie Senechal

This summer's Hatfest at Oxford University, UK, was a seamless hybrid of conference and festival. For two joyous days (20 and 21 July), we celebrated the Hat, while papers were presented, arguments percolated and research plans laid.

Just four months before, David Smith, a retired printer and tiling hobbyist in Yorkshire, UK; Joseph Myers, a combinatorics specialist in Cambridge, UK; Craig Kaplan, a computer scientist at the University of Waterloo, Canada; and Chaim Goodman-Strauss, a tiling theory expert at the Museum of Mathematics in New York, USA, had posted a jointly authored 89-page preprint, *An Aperiodic Monotile* [1], on arxiv.org. The Hat, as the tile was dubbed, made world headlines at the speed of light.

The search for a single shape that tiles the plane, but never periodically, goes back to the early 1970s, when Sir Roger Penrose's tilings by kites and darts showed that 'order' and 'translation' are not synonyms. And if two shapes can tile aperiodically, what about one? Several monotile candidates were proposed over the ensuing years whose features (periodic layers, discontinuities) prompted mutterings: *that's not what we were looking for!* But now here's the Hat, a simple 13-sided polygon nestling in a periodic tiling of the plane (Fig. 1).

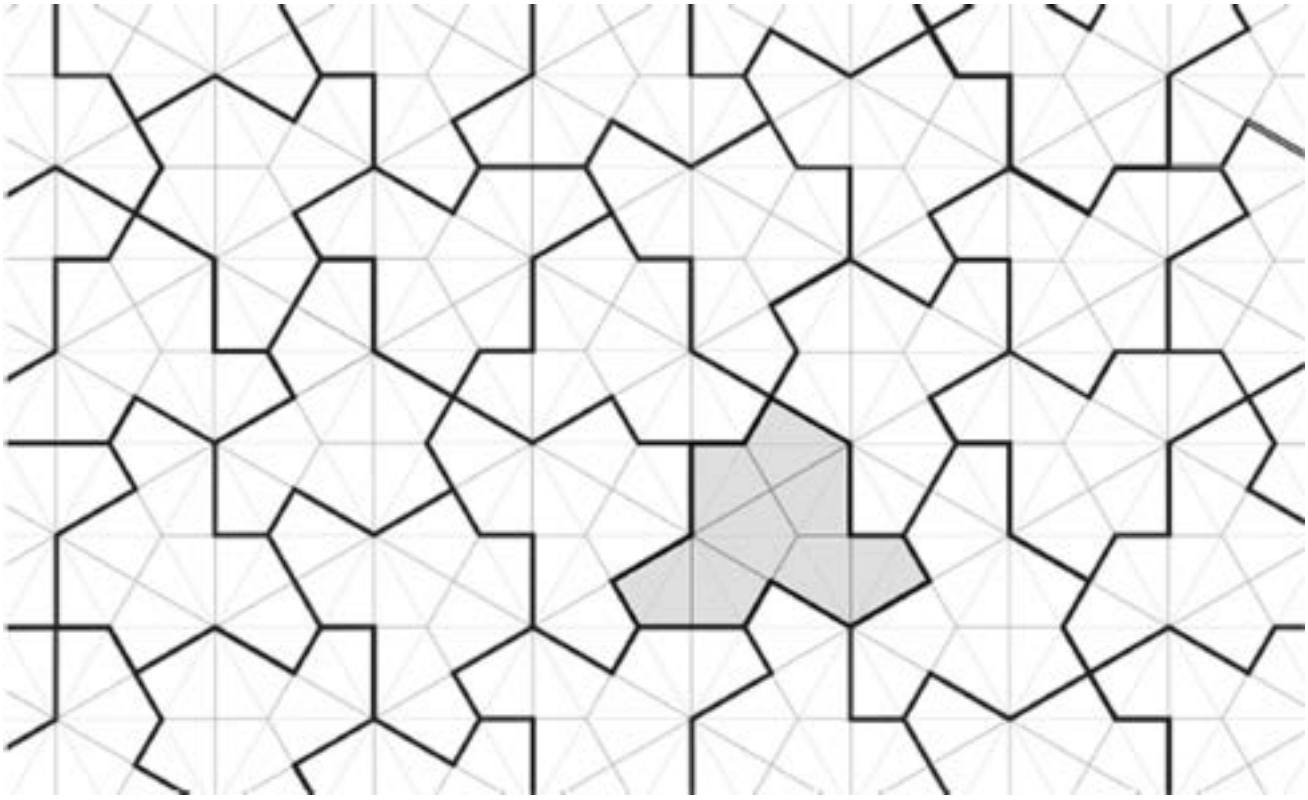


Figure 1. A small portion of an infinite Hat tiling (Fig 1.1 of [1], reproduced with permission).

David Smith (Fig. 2) discovered the Hat while 'messing about' with the *PolyForm Puzzle Solver* app (https://www.jaapsch.net/puzzles/polysolver.htm).



Figure 2. David Smith at the Hatfest. Photo by Stan Sherer.

He knew that an aperiodic monotile was a tiling holy grail, and as the regions he tiled grew larger and larger with no translations in sight, he thought he might have found one. He contacted Kaplan, who contacted Myers and Goodman-Strauss. Together, the quartet proved that

(*a*) the Hat is indeed a tile (its copies fill the plane without gaps or overlaps);

(*b*) all Hat tilings are nonperiodic (they proved this in two very different ways);

(*c*) the Hat is just one of an infinite family of aperiodic monotiles obtained from it by increasing or decreasing the lengths of its edges (see Fig. 3 and https://cs.uwaterloo.ca/~csk/hat/).

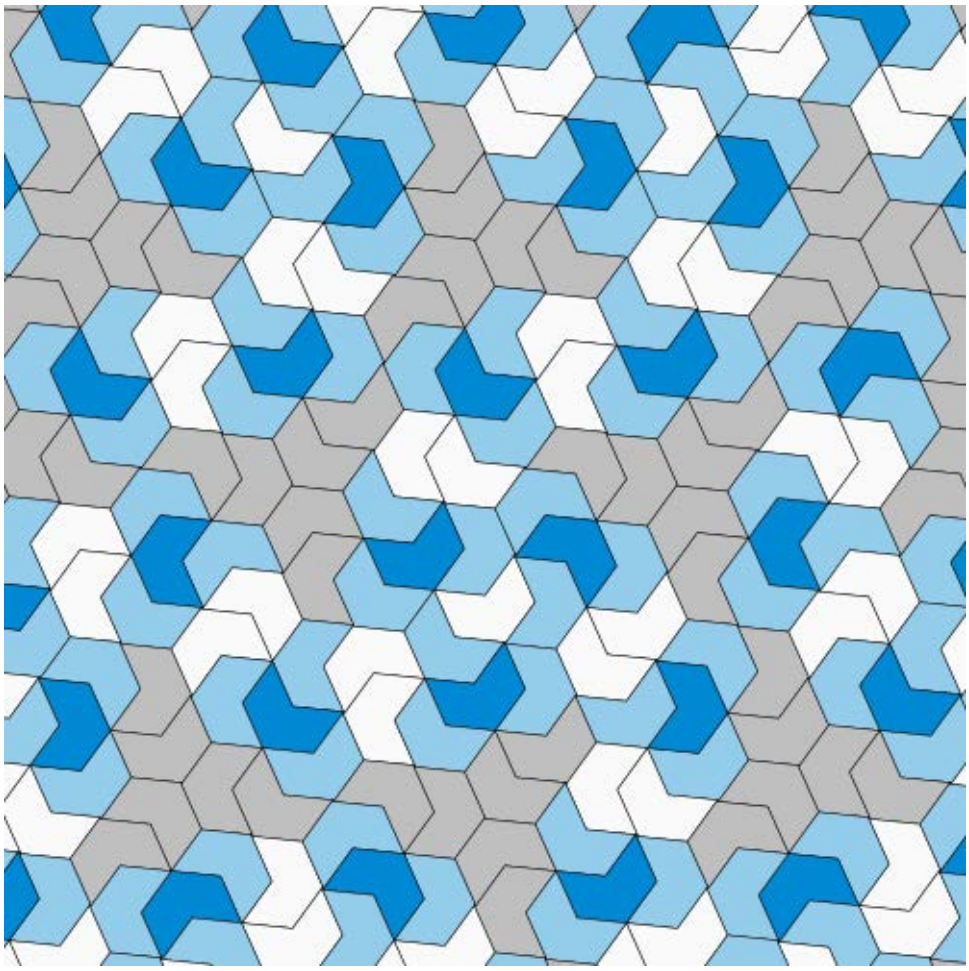


Figure 3. Craig Kaplan's animation of the Hat family (for the link and details, see https://cs.uwaterloo.ca/~csk/hat/).

Moreover, in those four months between the posting and the Hatfest, other scholars showed that Hat tilings are aperiodic crystals (*i.e.* their diffraction patterns consist of sharp Bragg peaks), that the diffraction patterns have sixfold rotational symmetry (Fig. 4), and that Hat tilings can be generated by cut-and-project methods like those used for Penrose and other aperiodic tilings [2, 3].

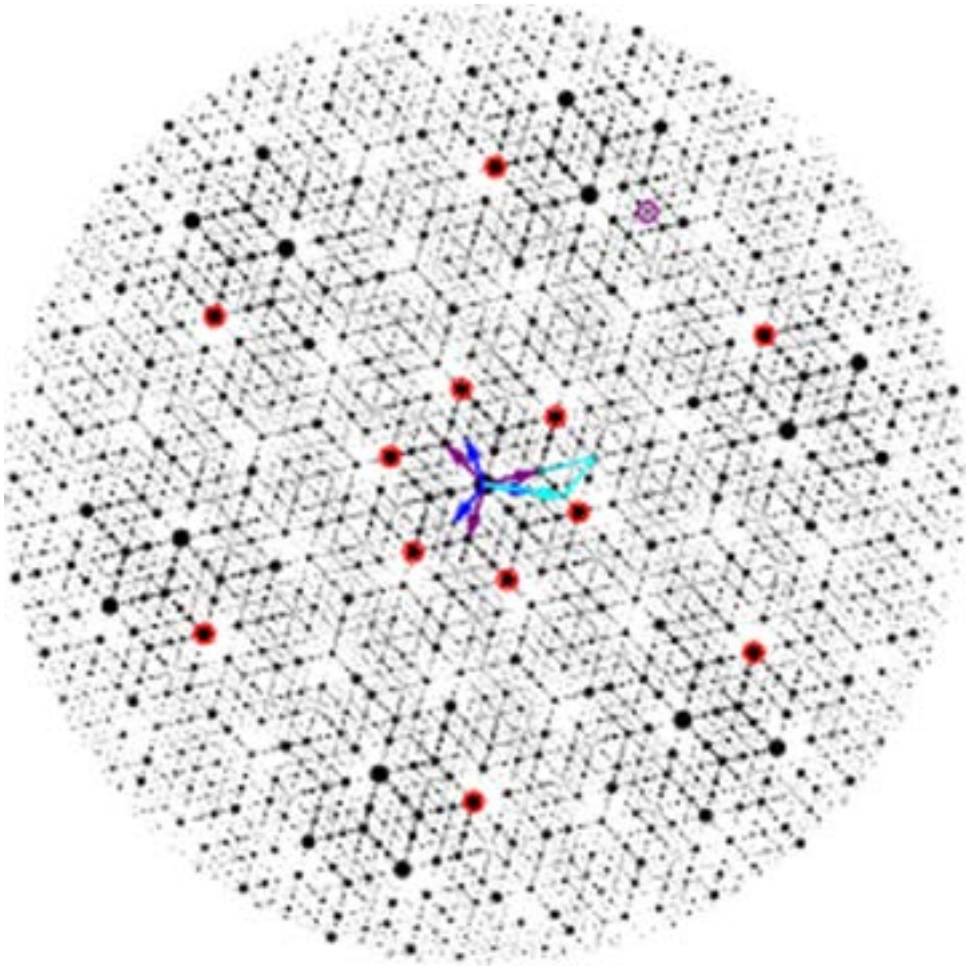


Figure 4. Diffraction pattern of a Hat tiling [2, 3].

Still, some muttered: *that's not what we were looking for!* Hat tilings include – and must include – both the hat and its mirror image, *but those are two different tiles!* Or are they? Euclid considered them to be the same, and so does the authoritative *Tilings and Patterns* [4]. Objection overruled! Nevertheless, the four authors quickly tweaked a member of the Hat family into an aperiodic monotile (which they called a spectre) that tiles the plane *without* its mirror image [5].

The Hatfest was organized by four British scientists: Felix Flicker (physics, Cardiff University), Nick Jones (Oxford Mathematical Institute), Henna Koivusalo (mathematics, University of Bristol) and Mike Whittaker (mathematics, University of Glasgow). Fittingly, it was held in Oxford's Mathematical Institute, whose splendid courtyard is paved with a Penrose tiling (Fig. 5).



Figure 5. Entrance to the Andrew Wiles Building, home of the Mathematical Institute at the University of Oxford. Photograph by Alain Goriely, 2013. (Creative Commons Attribution-Share Alike 3.0.)

The unprecedented excitement over the Hat is due to its remarkable properties, the internet and the generosity of the authors, who freely shared their ideas and software. It was also due to its accessibility from several vantage points. As everyone at the Hatfest could attest, understanding the Hat draws on the full discovery–justification spectrum, from hands-on 'messing about' to case-by-case computation to hefty theory. Everyone could, and did, jump right in.

The first day of the festival was designed for the broadest of audiences. Natalie Frank (Vassar College, Poughkeepsie, NY, USA) brought the audience up to speed on the math. Sir Roger Penrose (University of Oxford) described the development of his two aperiodic tiles and asked whether there might be a completely different type of aperiodic monotile, one that's *not* situated in a periodic tiling. In my talk, I showed how paradigms baked into tiling theory and crystallography over the centuries had ingrained the periodicity paradigm. Craig Kaplan told the inside story of the discovery of the quartet's collaboration.

There were hands-on workshops, too. David Smith and Jean-Marc Castera (Paris, France) led one on the Hat, and Lorenzo Sadun (University of Texas, Austin, TX, USA) led another on origami. Hatfest participants assembled a Hat tiling (Fig. 6 and Fig. 7) during a reception and discussion with artists. The first day concluded with a public lecture by Chaim Goodman-Strauss and a panel discussion with the day's speakers, chaired by Henna Koivusalo. At one point, I think during Chaim's talk, Felix Flicker told me later: "I looked back over the full lecture theatre (we had around 330 people signed up in the end) and saw people from all walks of life delighted to be hearing about this fascinating discovery. One person was wearing a Hat hat, while another was wearing a Hat dress. People were drinking Hat beer. Outside the theatre, the walls were lined with Hat artwork, including a hand-sewn quilt that had taken thousands of hours to make. People are thrilled about it in a way I haven't seen before for other discoveries."



Figure 6. Participants in the Oxford Hatfest creating a tiling with paper hats. Photograph by Stan Sherer.

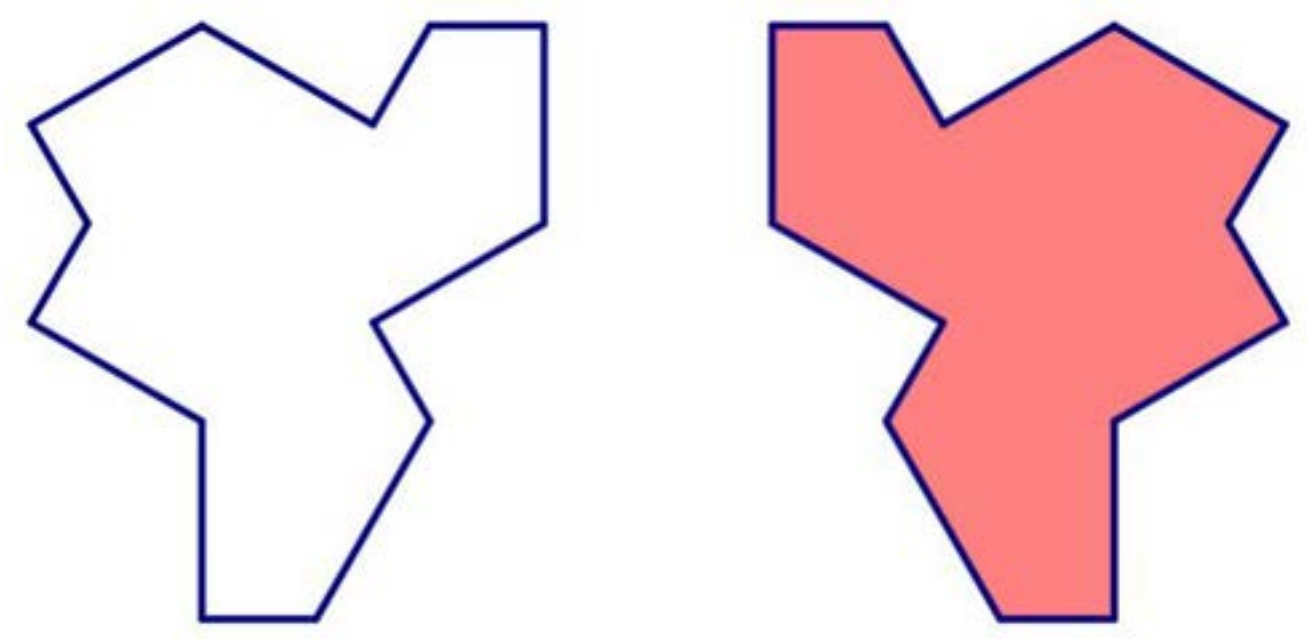


Figure 7. The red paper hats in Fig. 6 are mirror images of the white hats.

Talks on the second day – see https://sites.google.com/view/thegrimmnetwork/hatfest for the full list of speakers, affiliations, lecture titles and abstracts – situated the Hat in up-to-the-minute tiling theory and in the growing field of aperiodic order. And Adolfo Grushin (CNRS, Grenoble, France) discussed joint work with Felix Flicker on possible applications in physics and materials science, in which they found that Hat tilings sit "in a previously unoccupied place in crystallography between quasicrystals and crystals." And, by looking at the behavior of electrons in tight binding models based on the Hat, they found properties remarkably similar to those of the 2D-periodic crystal graphene. (Other properties lie closer to those of models of disordered materials and quasicrystals.)

The Hatfest was the second meeting of the Grimm Network (https://sites.google.com/view/thegrimmnetwork/hatfest), founded by the four organizers to honor the

memory of the mathematician and physicist Uwe Grimm (Open University, UK), who died unexpectedly in 2021. "Uwe was always really welcoming, bringing together as broad a range of people as possible to create an international community interested in aperiodic tilings," Felix Flicker explained. "We sought to continue his legacy by bringing together mathematicians, physicists, artists, hobbyists, and more. I think Uwe would have been very proud of the event and his legacy."

I am pleased to dedicate this note to Uwe, who was my colleague and friend. I hope that future meetings of the Grimm Network will keep us up to date on this rapidly burgeoning field.

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MEETING REPORT (IUCR SUPPORTED)

20th International Conference on Crystal Growth and Epitaxy



Group photo.

Annalisa Guerri

The 20th edition of the International Conference of Crystal Growth and Epitaxy (ICCGE20) was held at the University Campus of S. Giovanni a Teduccio, Naples, Italy, from 30 July to 4 August 2023. The Conference should have been held in 2022 according to its triennial schedule but due to the pandemic, it was postponed to 2023.

Almost 600 participants from 40 different countries attended, and the presence of female participants was around 35%. Also, the student attendance was significant. All the scientific sessions were well populated.

At the end of the conference, several prizes were awarded:

Frank Prize to Peter Vekilov (University of Houston, TX, USA) and Juan Manuel García-Ruiz (Instituto Andaluz de Ciencias de la Tierra, Granada, Spain) for significant fundamental contributions to the field of crystal growth

Laudise Prize to Peter Rudolph (Crystal Technology Consulting, Schönefeld, Germany) for significant technological contributions to the field of crystal growth

Schieber Prize to Bharat Jalan (University of Minnesota, Minneapolis, MN, USA) to recognize the outstanding value of his scientific publications in the field of crystal growth

Rostislav Kaishev Prize to Isha Bade (Imperial College London, UK) and Artur Tuktamyshev (University of Milano-Bicocca, Italy) for the best oral presentations by young scientists.

Seven young scientists received IUCr bursaries to support their attendance (see photo below).



Awardees of the IUCr grants, from left to right: Arnab Kar (Department of Physics, IISc, Bangalore, India), Durgesh Singh Sisodiya (HBNI, Mumbai, India), Adhikari Abinash (Institute of Physics, Polish Academy of Sciences, Warsaw, Poland), Annalisa Guerri (LOC), Veronika Grigoreva (RAS, Novosibirsk, Russia), Hanna Dabkowska (IUCr President), Charlotte Vernozy-Trouillet (École Polytechnique, Paris, France) and Andrea Zappettini (Conference Chair). Missing: Ekaterina Kochetkova (Leibniz Institute for Solid State Research, Dresden, Germany) and Nerith Rocio Elejalde-Cadena (Institute of Physics UNAM, Mexico City, Mexico).

AWARDS AND PRIZES

Structural biologists elected to National Academy of Sciences



Left: Helen Berman delivering her keynote lecture "What the Protein Data Bank tells us about the past, present and future of structural biology" at the 2008 IUCr Congress in Osaka (photo contributed to the IUCr gallery by the Osaka Local Organizing Committee). Right: Catherine Drennan in the Drennan Research and Education Laboratory at MIT (photo by Kalman Zabarsky).

In recognition of their distinguished and continuing achievements in original research, Helen Berman (Rutgers University, Piscataway, NJ, USA) and Catherine Drennan (MIT, Cambridge, MA, USA) were elected to the US National Academy of Sciences (NAS) in May 2023. The NAS is a private, nonprofit institution that was established under a congressional charter signed by President Abraham Lincoln in 1863. It recognizes achievement in science by election to membership, and — with the National Academy of Engineering and the National Academy of Medicine — provides science, engineering and health policy advice to the federal government and other organizations. Current NAS membership totals approximately 2,400 members and 500 international members, of which approximately 190 have received Nobel Prizes.

Helen M. Berman is Board of Governors Distinguished Professor Emerita of Chemistry and Chemical Biology at Rutgers University. She played a key role in founding the Protein Data Bank (PDB) in 1971 and was the Director of the Research Collaboratory for Structural Bioinformatics (RCSB) PDB, a member of the Worldwide PDB, from 1998 to 2014. In her capacity as Director of the PDB, Professor Berman served as an *ex officio* member of the IUCr Commission on Biological Macromolecules, and has contributed many articles to IUCr journals.

Catherine (Cathy) L. Drennan is professor of chemistry and biology at the Drennan Research and Education Laboratory at MIT. The Drennan lab combines X-ray crystallography and cryoEM with other techniques to understand enzyme mechanisms, an approach they term “structural metalloenzymology”. Earlier this year, Professor Drennan won the American Society for Biochemistry and Molecular Biology’s 2023 William C. Rose Award for her outstanding contributions to biochemical research and commitment to training younger scientists.

AWARDS AND PRIZES

Hao Wu to receive 2024 Gregori Aminoff Prize



The Royal Swedish Academy of Sciences has decided to award the Gregori Aminoff Prize in crystallography 2024 to Hao Wu (Boston Children's Hospital, Harvard Medical School, MA, USA) for her *discoveries by crystallography of the assembly mechanisms of large oligomeric signaling complexes in innate immunity, a paradigm-shifting concept in signal transduction.*

The innate immune system provides the body with its first line of response to dangerous bacteria, viruses and hazardous substances, and consists of proteins on the cells' surface and inside them. Once the system is activated, large protein complexes are built for the purpose of neutralising the attacking organisms. Professor Wu has used protein crystallography and cryoEM to establish how these protein complexes form, as well as their structures. Her research has led to an entirely new and improved understanding of how the innate immune system functions.

"Professor Wu is a master at identifying important biological issues and solving them using advanced structural and biochemical methods. Her discoveries may be of huge importance in understanding the causes of inflammatory diseases, their progression and treatment," says Björn Dahlbäck, professor emeritus at Lund University and a member of the Prize Committee at the Royal Swedish Academy of Sciences.

The Gregori Aminoff Prize in crystallography recognises a documented individual contribution to the field of crystallography, and has been awarded to Swedish and foreign researchers since 1979. See previous laureates here.

REGIONAL NEWS

Crystallographic reflections: A history of the Society of Crystallographers in Australia and New Zealand



Crossing the Nullarbor Plain from Perth, Western Australia, on the 1,700 km long Eyre Highway to attend the Crystal 5 meeting at Monash University, Victoria, in August 1967. Left to right: Biswanith Mukajee, Syd Hall and Ted Maslen. Photo credit: Syd Hall, using a time delay on the camera exposure, judging from the shadow of the tripod. Image reproduced from the IUCr photo gallery.

Roderick J. Hill

I joined the (then) Society of Crystallographers in Australia (SCA) soon after its formation in 1976 and was privileged to serve as its Honorary Secretary for three terms from 1982. However, work eventually took me away from direct participation in crystallographic research, and I lost touch with the Society. Many years later, after reconnecting, I realized that crystallography and the Society had changed significantly. The original pioneers of the Society, to whom it owed a great debt, were greatly diminished in number, and unless its rich and illustrious history was soon recorded, it would be lost forever. In early 2022, I contacted the then President (Megan Maher) and the Council of the now Society of Crystallographers in Australia and New Zealand and offered to write its history. To my delight, they accepted my offer; some snippets from the resultant manuscript are provided below.

The Society of Crystallographers in Australia and New Zealand (SCANZ) has existed in three configurations over the last 60+ years. The first version is generally recognized as emerging in May 1961 in association with the first 'open' (*i.e.* not just internal institutional) meeting of Australian crystallographers (since dubbed 'Crystal 1') at the University of Sydney. This meeting of what later became known as the 'Bush Crystallographers' was the initiative of Hans Freeman, then Professor of Chemistry at the University of Sydney. Hans was also central to the movement in 1973 to establish the Society of Crystallographers in Australia (SCA) and was elected as its inaugural President at the Crystal 10 meeting in Richmond, NSW, in April 1976. In acknowledgment of the major and long-term engagement of colleagues from 'across the ditch' (aka New Zealand), the name was changed to the Society of Crystallographers in Australia and New Zealand (SCANZ) at the Crystal 21 meeting in Thredbo, NSW, in February 2000.

The original Bush Crystallographer 'members' were a small group of individuals who, for the most part, had learned their trade as postgraduate or postdoctoral students overseas, working with some of the icons of crystallography in the early post-WWII period (*inter alia* Kathleen Lonsdale, Linus Pauling, Dorothy Hodgkin, Edward W. Hughes and J. Monteath Robertson). Among these, first-generation

Australian pioneers in the early 1950s and 1960s may be counted: Hans Freeman (Sydney University); ‘Sandy’ Mathieson, Barrie Dawson and Dave Wadsley (CSIRO); Jack McConnell and Nev Stephenson (University of NSW); Maureen Mackay (La Trobe University); Alan White, Jim Graham and Ted Maslen (University of Western Australia); Bryan Gatehouse (Monash University) and Terry Sabine (Australian Atomic Energy Commission, now ANSTO).

They established the first tranche of significant crystallography laboratories in Australia and were key players in the organisation of the early Crystal meetings and the formation of the SCA. Their graduate students, in turn, established second-generation groups at other universities and research institutions in Australia and overseas. A corresponding group of New Zealand crystallographers founded major laboratories at Industrial Research Lower Hutt (George Patterson), University of Auckland (F. J. Llewellyn), University of Canterbury (Bruce Penfold) and University of Otago (A. J. Ellis). Fig. 1 shows some of these key players at Crystal 1 at Sydney University in 1961, and Fig. 2 shows several others, probably at Crystal 4 at Lucas Heights in 1966.



Figure 1. The photo possibly shows some of the participants likely to have been present at the first Bush Crystallographers Meeting (Crystal 1), organised by Hans Freeman at Sydney University, 25–26 May 1961. Left to right: John E. W. L. Smith, Janet and Max Taylor, Anne and Gordon Robinson and John Cowley, annotated with their (later) SCA connections. Photo contributed to the IUCr gallery by Syd Hall.



Figure 2. Prominent pioneers of crystallography in Australia, pictured around 1966, perhaps at Crystal 4 at the AAEC, Lucas Heights. Left to right: Dave Wadsley, Sandy Mathieson, Janis Friedrichsens and Barry Dawson. Photo contributed to the IUCr gallery by Syd Hall.

Throughout its existence, both as a collective and through its individual members, SCANZ has played a very significant role in the development of the crystallography landscape in Australia, New Zealand and overseas. It was a foundation partner in the Federation of Scientific and Technological Societies (FASTS), the political lobby group for increased funding for Australian science and technology; it was a major actor in the push for funding for Australian access to major synchrotron and neutron facilities overseas (the so-called ‘suitcase science’/‘Small Country Big Science’ initiative). Its members were prime movers in the establishment of the Australian National Beamline Facility (ANBF) at the Tsukuba synchrotron in Japan, and they were also key advocates for the establishment of the Australian Synchrotron and the new OPAL research reactor. They also led or participated in many of the technical committees advising on the type and design of beamlines for those facilities. Along with the Crystallographic Society of Japan, the Society was a strong proponent and prime mover in the establishment of the Asian Crystallographic Association (AsCA) in 1987 and, until recently, one of only four Regional Associates of the International Union of Crystallography (IUCr).

Through the Society’s *ex officio* representative (and other independent members) on the National Committee for Crystallography of the Australian Academy of Science, the Society is (in practical terms) the primary link for Australia’s engagement with the IUCr. Society members have acted as President and Vice-President of the IUCr, served on its Executive Committee, and occupied seats on all 22 Commissions of the IUCr at one time or another, often as Chair. It has been the organiser of two of the IUCr Congresses and General Assemblies held since 1948, the 14th in Perth in 1987 and the 26th in Melbourne in 2023, and it devoted considerable resources to the Australia-wide celebration of the International Year of Crystallography in 2014. It maintains a strong supportive presence (both financial and participatory) in AsCA meetings.

Since 1961, its series of regular national meetings (to date, 34 and counting; Fig. 3) and, since 1980, its Newsletters (79 and counting) have provided critical and effective platforms for the exchange and dissemination of scientific information, science politics and personalia, past, present and future in the domestic and international crystallographic domains.



Figure 3. The approximate locations of all 34 meetings of the Bush Crystallographers, SCA and SCANZ, and the two IUCr Congresses and General Assemblies organised by SCANZ from 1961 to 2023. Map reproduced with permission from Rand McNally.

The Crystal meetings and newsletters continue to provide an important and fertile connection point for professional and student crystallographers in Australia and New Zealand. They have served to celebrate and encourage the achievements of members and to engender a sense of a crystallographic community across both nations. From interviews with some of the early participants in these meetings (and from my own recollections), they were certainly memorable affairs, often showcasing (aside from science) the musical, singing and raconteurial talents of otherwise quite often shy and retiring scientists. Not to be missed, as evidenced by the small groups of crystallography lecturers from the University of Western Australia and their students who were willing to endure a road trip over 3–4 days (with rotating drivers and sparse accommodation) of more than 3,400 km, in part across the Nullarbor Plain on the then unsealed (dirt) Eyre ‘Highway’, from Perth to Melbourne to attend the meetings, and back again (see top photo).

Along with the Crystal and IUCr meetings, SCANZ has organised several significant one-off events, including the Bragg Symposium in Adelaide in 2012 to mark the centenary of the founding of X-ray crystallography by W. Lawrence Bragg (born and educated in Adelaide), a field in which he and his father, William H. Bragg, made pre-eminent contributions recognised by the award of the Nobel Prize for Physics in 1915. Another event was the 1991 dedication ceremony for the ‘A.D. Wadsley X-ray Laboratory’, held at the CSIRO Division of Mineral Products, Port Melbourne, in recognition of David Wadsley's pioneering contributions to crystallography and solid-state chemistry (Fig. 4). Participants included David’s family and many of his friends and colleagues (most of whom were foundation members of the SCA) from around the country and overseas.



Figure 4. Standing, left to right: David Scaife, Jim Graham, John Watts, Bruce Hyde, Alex Moodie, Jeff Wunderlich, Gus Mumme, Bob Roth, Terry Sabine, Alan Reid, Hans Freeman, Judge Bevan, ??, Sir Alan Walsh, M. Fehlmann, Bryan Gatehouse, ?? and Ted Ringwood. Seated: Joy Bear and Sandy Mathieson. Photo credit: Rod Hill.

The structure and culture of the Society have gone through several major changes over its 60+ years, from an *ad hoc* small informal grouping of most of the early crystallographers in Australia funded by local organising institutions to its present position as a formally incorporated entity with active global engagement and a membership of nearly 300 people, around 50% of whom are students. Its financial resource is now more than AUS$2.3M, the investment returns from which allow it to offer travel scholarships to prominent overseas speakers and students to attend national and international meetings. These funds also enable awarding of the Bragg and Mathieson Medals to outstanding mature and early-career researchers at each Crystal meeting.

Diversity and gender equity was introduced in 2020 as a formal policy of the Society, applied in particular to Office Bearers and speaking and session-chair roles at all its meetings. It has also instituted a policy of encouraging young researchers through its Rising Stars Awards at each national meeting, along with an allowance for carer’s provisions.

From its initial focus (typical of the time) on the crystallography of inorganic materials and minerals, the Society has embraced increasing focus on structural biology as humanity responds to the need for greater understanding of the nature and function of molecules essential to life. It is also adjusting to the massive change in the ‘face’ of the science of crystallography over the years, from a unique and important discipline in its own right to a still extremely important but now largely enabling discipline underpinning the broader biological, materials, chemical and physical sciences. Emerging technologies and software, such as cryo-EM and massive protein folding algorithms based on artificial intelligence for the solution of macromolecule structures, are also providing new challenges.

Although crystallographic data collection and structure solution is now, for most compounds, largely automated, the need for advances in crystallographic science and equipment to deal with ever larger and more complex materials (especially in the biological domain) has ensured that the discipline remains as important and rewarding for researchers as ever. The Society has greatly assisted adaption to these changes through its generous financial support for student attendance at national and international

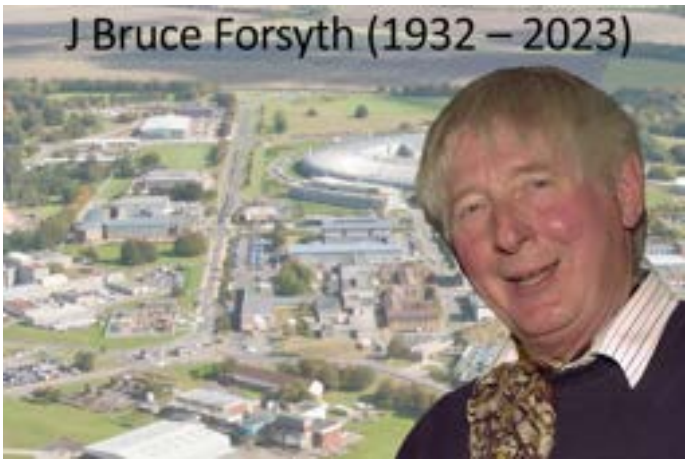
crystallography meetings and its continued commitment to the teaching of crystallography through its Australian Crystallography Schools (in partnership with the Australian Synchrotron), which have operated since 2008.

As a result of all these actions, the Society’s meetings remain relevant and exciting, and continue to attract the best speakers from home and abroad by showcasing the most relevant and exciting science of the day.

Dr Roderick J. Hill DSc FTSE FRACI FAusIMM was Secretary of the SCA 1982–1987. He is a former Chief Research Scientist at CSIRO and PVC for Industry Engagement and Commercialisation at Monash University, Victoria, Australia.

OBITUARY

J. Bruce Forsyth (1932–2023)



Mike Johnson, Bill David, Andrew Taylor, Jane Brown

From Mike Johnson, Bill David and Andrew Taylor

Bruce Forsyth was a renowned research scientist who made significant contributions to the study of the atomic structure of magnetic materials through his development of the technique of polarised neutron scattering.

Following a PhD in Cambridge (UK), Bruce moved to Harwell, where he designed and built diffractometers on the Dido and Pluto reactors as part of Harwell's expanding user programme providing access for academic researchers.

He joined the Neutron Beam Research Unit (NBRU) at the Rutherford Appleton Laboratory (RAL) in 1972. The NBRU, under the leadership of Leo Hobbis, had been set up initially to support the development of a research reactor to replace Dido and Pluto. However, with the closure of the NIMROD synchrotron on the RAL site, the opportunity presented itself to build a world-leading pulsed neutron source based on the accelerator infrastructure and expertise at the RAL, which eventually became the ISIS Facility.

Bruce played a key role in developing the scientific case for ISIS as secretary of the 'Structure Determination' working group (led by Brian Fender), which assessed the range of science that could be achieved by the new source and outlined the key parameters for a number of crystallographic instruments, including the High-Resolution Powder Diffractometer (HRPD) and the Single-Crystal Diffractometer (SXD).

Promotion to an Individual Merit post soon followed, and Bruce's career developed in instrument building in science and in computing, both at the RAL and the Institut Laue-Langevin (ILL, Grenoble, France). His computing skills were key to defining the new facility's computing and data acquisition system, and his acronym PuNCH (Pulsed Neutron Computer Hierarchy) lives on at ISIS today. He also co-authored the specification-of-requirements document issued to companies bidding to supply the control and analysis computers.

His main scientific contribution was in crystallography, principally magnetic structures, and specifically exploiting the scattering of polarised neutrons, where he made many innovations in tandem with his long-time collaborator, Jane Brown of the ILL. As well as authoring scientific papers on the subject, he was instrumental in producing the Cambridge Crystallographic Subroutine Library (CCSL) suite of software, which is still widely used in the international scientific community.

Bruce retired from the RAL in 1997 after 25 years on the international scene but continued to be active with honorary positions at the Clarendon Laboratory, Oxford, and the University of Warwick, as well as collaborations in Grenoble.

Bruce brought enthusiasm and energy to all his work throughout his career – engaging and positive and always sporting a cravat! He was a 'light touch' manager, allowing and encouraging his team to develop and flourish. He and his wife, Janette, made team members welcome and were generous in making their holiday home in East Portlemouth available to colleagues. Bruce was a class act and a true polymath.



From Jane Brown

Bruce and I first met in 1955 when he joined the alloys group of the Crystallographic Laboratory of the Cavendish Laboratory in Cambridge as a research student. Although Bruce was my elder by a couple of months, he was a year junior in the lab because of the 18 months he spent doing National Service in the RAF. We both worked, under the supervision of Dr W. H. Taylor, on a project sponsored by the American Airforce to study the crystal and electronic structures of aluminium-rich intermetallic compounds. This led to our efforts to determine the electron distributions in these compounds and to the development of one of the very first automatic X-ray diffractometers, 'MAXIM', which received its instructions on punched paper tape from the EDSAC 1 computer.

After completing his PhD in the field of X-ray diffraction, Bruce moved on to neutron diffraction at the Atomic Energy establishment at Harwell. There he was responsible for building their first (and only) polarised neutron diffractometer on the Pluto reactor. He was closely involved with the establishment of the university user programme at Harwell and finally moved to the RAL when a Neutron Scattering group to support university users was created there.

When the British joined the ILL associates in 1973, Bruce immediately became involved in the plan to redirect three diffractometers, already ordered for the user programme, to the ILL. He had already been planning to upgrade and automate the Pluto polarised neutron diffractometer. He was rapidly able to adapt these plans, and proposed that one of the three diffractometers become a polarised neutron instrument. His ideas were accepted, and he became responsible for installing and programming the D3

polarised neutron diffractometer on the H8 beam of the ILL reactor.

He and his family spent the year 1974–1975 in Grenoble while the installation was underway. In the following years at the RAL, he was a staunch supporter of the UK Neutron Scattering Programme and a frequent visitor to the ILL, where we did many experiments together. Many of these were on D3, but he also exploited several other instruments. Over the years, we developed an increasing interest in the possibilities offered by neutron polarization analysis. After several less-than-satisfactory experiments using conventional techniques, Bruce became a valued collaborator in many of the exploratory experiments to establish methods for carrying out polarization analysis with the zero-field polarimeter Cryopad.

I will remember Bruce as a good friend and close collaborator with a constantly cheerful and outgoing personality.

Dr Forsyth served on the IUCr Commissions on Charge, Spin and Momentum Densities (1987–1996) and Neutron Scattering (1993–1999). For a list of his papers in IUCr journals click here.

OBITUARY

John William White (1937–2023)



Photo of Professor White published with permission of the Research School of Chemistry, Australian National University, Canberra, and David White.

Richard Welberry

It is with sadness that we report that Professor John White, whose name will be familiar to many in crystallography and neutron science circles, passed away at his home in Canberra, Australia, on 16 August 2023 at the age of 86. Our thoughts are with his wife, Ailsa, his four children and their extended families, and many friends and colleagues. He will be sorely missed by all who knew him.

John William White AO CMG FRS FAA FAIP FRACI (born 25 April 1937) was a Professor of Physical and Theoretical Chemistry in the Research School of Chemistry at the Australian National University in Canberra. He was a past president of the Royal Australian Chemical Institute and President of the Australian Institute of Nuclear Science and Engineering. He held the Argonne Fellowship (University of Chicago, IL, USA) and was for many years a Fellow of St John's College, Oxford, UK. Between 1975 and 1981, he was director of the Institut Laue-Langevin (ILL), Grenoble, France. He was a founding member of the International Society for Science and Religion.

John was born and grew up in Newcastle, NSW. He was born on Anzac Day – an important day for all Australians. He was proud of this coincidence and made a point of attending the Anzac Day Parade (held at dawn) whenever he was in Australia. He was the eldest child of George and Jean White and had two younger sisters, Wendy and Gina. Both his parents were immensely supportive and proud of him. He was the first in the family to go to university – at the age of 16. John graduated from the University of Sydney in 1957 with First Class Honours in chemistry and won the Frank Dixon Prize. He went on to obtain his MSc in 1959 and then won a prestigious 1851 Scholarship to continue his studies in Oxford, where he obtained his DPhil and subsequently became a Lecturer and Fellow of St John's College (at the tender age of 26). He remained in Oxford until 1985, apart from a five-year period between 1975 and 1981, when he moved with his family to Grenoble to take up the appointment of joint director and then director of the ILL. He returned to Australia in 1985 to take up the appointment of Professor of Physical and Theoretical Chemistry at the Research School of Chemistry in the Institute of Advanced Studies at the Australian National University. He maintained his links both with St John's in Oxford and with the ILL in Grenoble and frequently visited both, usually managing to do some experiments, either at ILL or at the Rutherford Appleton Laboratory Neutron Source (ISIS) near Oxford. He kept his house in Grenoble.

John was very proud of his association with St John's College, and it has been said that since that time, the only tie that he ever wore was his St John's tie. His time in Oxford affected him in many ways, and he valued every moment. His family recalls with affection that he met his wife-to-be, Ailsa, during his early

days at Oxford, and he would often relate the story of their first meeting and maintained that it was the single most important and best thing that ever happened in his life. John and Ailsa shared an incredible bond through 57 years of marriage.

Perhaps John's most significant contribution to Australian science has been his role in getting both the OPAL Neutron Source (in Sydney) and the Australian Synchrotron (in Melbourne) funded by governments and built to the highest international standard. Together, these two research facilities represent at least a AUS$500M investment in the country's scientific and technological future, and they have accelerated the internationalisation of Australian science, in addition to decelerating the brain drain. Although not in the direct management chain, John served on many important committees and used his position in the Australian Academy of Science to help make the political, scientific and business case for both OPAL and the Australian Synchrotron. This has given the next generation of Australian researchers in many fields of science and engineering "the opportunity of a generation" and has allowed them to do their research in Australia rather than to have to travel overseas.

From an early age, John liked to experiment in the laboratory himself. His family recalls that as a schoolboy, he set up a laboratory in his grandmother's house. Every week, he obtained a new chemical from the local pharmacy, on which he experimented using a textbook his father bought him. He claimed never to have had a fire or an explosion! Later, even when he had a large group of students and postdocs working with him, he would still like to be involved himself. He led from the front!

One of the marks of John's career has been the talent that he nurtured and grew at Oxford and the Australian National University in Canberra, where he has played a leading and influential role for the last 30 years or so. Several of his protégés have become directors of leading international research centres around the world. The Bragg Institute at the Australian Nuclear Science and Technology Organisation (ANSTO) employs at least three of John's students or postdoctoral fellows from the Australian National University. He has deeply influenced the careers of many more.

John was the second President of the Asia-Oceania Neutron Scattering Association and was one of the leading players in its formation (along with colleagues in Japan and Korea). As recently as July 2015, he was awarded the AONSA Prize in recognition of his leadership across the Asia–Pacific. He has advised many overseas laboratories, including the CCLRC in the UK and several others in the USA. Most significantly, he was chair for many years (2002–2012) of the International Advisory Committee for the Japan Proton Accelerator Research Complex, the other leading facility (along with OPAL) of its type in our region.

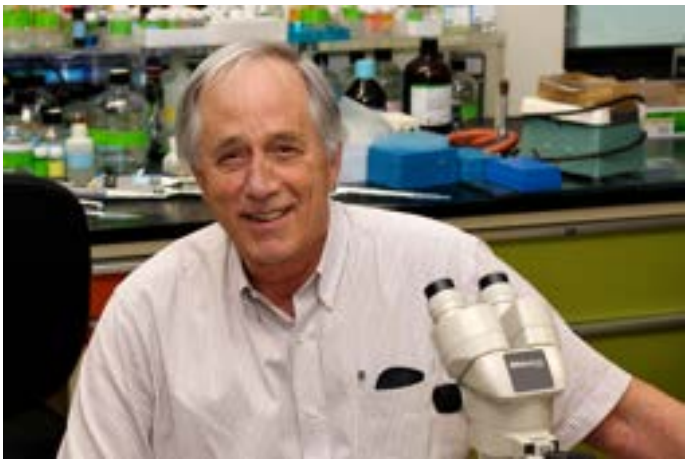
John has made huge contributions to global science: most notably, I think he must have been the first to open up the new method of neutron scattering (using neutrons from research reactors) to chemistry in the 1960s. This gave British and Australian chemists a leadership position they have never relinquished. In addition, he was a prime mover in using specific deuteration of molecules to change the contrast in such experiments, which now turns out to be the "killer application" of neutron scattering worldwide. Indeed, it was a key factor in Australia's decision in 1997 to build the new OPAL Reactor and later on to fund the world-leading National Deuteration Facility at ANSTO.

Another aspect of John's legacy to Australia was his involvement in the setting up of the Oxford Australia Scholarship fund over 20 years ago. This Fund was initiated to endow scholarships each year for academically top Australian graduates to go to Oxford University for study and research. John took the lead in raising the endowment, which now totals AUS$4,500,000, and for those 20 years, he chaired the committee that awards the scholarships annually. So far, about 100 young Australians have benefited from this scheme.

On a personal level, I have enjoyed many stimulating interactions with John, covering a wide range of mutually interesting topics, which I will greatly miss.

OBITUARY

Michael James (1940–2023)



Michael at the laboratory bench in 2010.

J. N. Mark Glover, Cyril M. Kay, Joanne Lemieux, Randy J. Read

Michael James liked to tell a story from his childhood when he was fascinated by rockets and their propellants. After walking over to the local branch of Canadian Liquid Air in Winnipeg he asked for some liquid oxygen. ‘Sure, kid’ they said, and put some in his bucket. (Attitudes to health and safety were different in those days.) As he walked home, he realized that liquid oxygen boils pretty quickly, so he ran the last part of the way and carried the rapidly emptying bucket into the basement. There was only a bit left and there wasn’t time to do anything fancy, so he splashed in some methanol to make a lox/alcohol propellant and tossed in a match. When he picked himself up from where he had been thrown by the explosion, he heard picture frames crashing down upstairs and his mother shouting ‘Michael, what have you done this time?’. He never lost this childhood enthusiasm for science (though his experiments became less dangerous) and was active in research until the end of his life.

Michael James was born in Vancouver and grew up in Winnipeg, Manitoba on the Canadian prairies. After high school, he studied chemistry at the local University of Manitoba, where he was excited to learn that it was possible to see the 3D structures of molecules using X-ray crystallography. Aiming to get the best possible background for a future working in this area, he applied to do a DPhil at Oxford with Dorothy Hodgkin in 1963. It was a time of great advances in crystallography, with Dorothy about to win the Nobel Prize for her ground-breaking structures of penicillin and vitamin B_{12}, and the first protein structures having recently been determined in Cambridge. Michael’s thesis project was to determine structures of antibiotic peptides. While there, he was exposed to protein crystallography through the work going on at the same time to determine the 3D structure of insulin.

After completing his DPhil in 1966, Michael took a postdoctoral position determining small-molecule structures in the Department of Chemistry at the University of Alberta in Edmonton, Canada. He remained at the University of Alberta for the rest of his life. However, his career took a quick turn when he learned that the Biochemistry Department was seeking to set up a protein crystallography laboratory. With his move to Biochemistry he became the first protein crystallographer in Canada, determining the first 3D protein structure (that of *Streptomyces griseus* protease B, a serine protease) in 1974 (Delbaere *et al.*, 1975). That same year, Michael joined Larry Smillie, Cyril Kay, Brian Sykes, Robert Hodges and Robert Fletterick in forming the Medical Research Council (MRC) Group in Protein Structure and Function, later to be joined by Wayne Anderson, Charles Holmes and Zygmunt Derewenda. The Group became internationally known and respected for its multi-disciplinary approach to problems in protein chemistry as well as a superb environment for research training. During its tenure (1974–2000), the Group published over 1600 research papers and trained some 250 graduate students and postdoctoral fellows,

many of whom went on to distinguished independent careers of their own.

In his research, Michael brought the same expectations of high precision to proteins that he had learned in small-molecule crystallography, and his group became known for the quality of the structures it produced, becoming early adopters of least-squares refinement (Sielecki *et al.*, 1979) and computer-graphics techniques. In the earlier years, Anita Sielecki (a member of the group since 1976 who eventually became his second wife) played a pivotal role in many aspects of the research including the development of optimal refinement protocols, as well as guiding students and creating a warm and supportive group atmosphere.

Initially, Michael concentrated his group's efforts on understanding the structure and function of proteases, an area that remained important to him through the rest of his career. The group worked on a variety of serine proteases and their complexes with both small molecules (Brayer *et al.*, 1979) and protein inhibitors (Fujinaga *et al.*, 1982). They determined the first structure of an aspartyl protease, penicillopepsin (James *et al.*, 1977), setting the stage for the understanding of key members of this family such as renin (Sielecki *et al.*, 1989) and the HIV protease.

Eventually, the James laboratory turned its interest to the proteolytic enzymes from picornaviruses. Members of the laboratory determined the structures of the 3C proteinases from hepatitis A virus (Allaire *et al.*, 1994) and polio virus (Mosimann *et al*., 1997), as well as the 2A proteinase from rhinovirus (Petersen *et al*., 1999). All of these molecules are potential targets for antiviral drug development.

Prior to 2004, five families of proteolytic enzymes were known. A sixth family, the glutamic peptidases, was discovered in a collaboration between the James laboratory and Professor Kohei Oda of Kyoto, Japan (Fujinaga *et al.*, 2004).

Branching out into other areas, Michael's group carried out structural studies of a variety of biochemically and medically important proteins. The structure of troponin-C (Herzberg & James, 1985) shed light on how muscle contraction is regulated. Structures of TEM-1 β-lactamase (Strynadka *et al*., 1994) and its complex with the inhibitor protein BLIP (Strynadka *et al.*, 1996) gave new insight into antibiotic resistance and how it might be prevented. He also became interested in a structural understanding of inherited metabolic diseases, with a series of structures shedding light on Sandhoff (Mark *et al*., 2003) and Tay–Sachs (Lemieux *et al.*, 2006) diseases, as well as mucopolysaccharidosis I (Bie *et al.*, 2013).

In collaboration with the Canadian company ViroChem Pharma, members of the James laboratory determined the structures of allosteric inhibitors of NS5B, the RNA-dependent RNA polymerase from hepatitis C virus (Wang *et al.*, 2003). The company took several of these non-nucleotide inhibitors to Phase II clinical trials.

His last published paper, on a protease from a virus that causes porcine epidemic diarrhoea, was special in having his daughter Michelle as a coauthor (Shamsi *et al.*, 2022).



Michael with former laboratory members at a celebration of his career in June 2017, at the University of Alberta in Edmonton. From left to right, back row: Bret Church, Stanley Moore, Randy Read, Kathy Bateman, Amir Khan, Helen Blanchard, Ken Ng, Michael James, Natalie Strynadka, Maia Cherney, Nina Bernstein, Cathy McPhalen, Marie Fraser; front row: Steve Sprang, Rabih Farraj, Joanne Lemieux, Chunying Niu, Jiang Yin, Pravas Kumar Baral, Haiying Bie, Meitian Wang.

Michael received many honours during his long and distinguished career. He was elected as a Fellow of the Royal Society of Canada in 1985 and as a Fellow of the Royal Society of London in 1989. He was presented the Martin Buerger Award of the American Crystallographic Association in 2009. In 2010, he received an honorary doctorate of science from his undergraduate alma mater, the University of Manitoba. In June of 2023, the month before he died, he was appointed an Officer of the Order of Canada, one of Canada's highest honours.

In his approach to science, Michael's passion was always to move closer to the truth. As a consequence, he took as much pleasure in the scientific advances of others in the MRC Group and the Department of Biochemistry as he did in his own group's breakthroughs. He wanted to contribute and to understand, but was always unassuming; he could laugh at himself and never dominated or inflated his ego at the expense of others. Beloved by members of his laboratory, Michael was an inspirational friend and mentor to his students, postdoctoral associates and colleagues, and a joyous companion to those lucky enough to know him.

Michael James died on the 24 July 2023 after a short admission to the University of Alberta Hospital. He is survived by his three children, Daphne and Marcus from his first marriage to Pat, and Michelle from his third marriage to Deborah.

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OBITUARY

S. K. Sikka (1942–2023)



Nandini Garg

Dr S. K. Sikka breathed his last on 21 June 2023 while visiting his children in Boston. This news saddened not only us high-pressure physicists but also the entire department of atomic energy India. He was not only an eminent scientist but was also a very wonderful and simple person. He was a great mentor and his enthusiasm even at the age of 80 was infectious.

Dr S. K. Sikka was born in November 1942 in the city of Jhang in undivided India. After his graduation from Punjab University he joined Bhabha Atomic Research Centre (BARC) when he was only 18 years of age. He started his scientific career under the mentorship of Dr R. Chidambaram. He held several key positions and went on to become the director of the Atomic and Condensed Matter Physics Group at BARC. In 2002, he chose to move to the office of Principal Scientific Advisor to the Government of India as its Scientific Secretary and later became a Homi Bhabha Chair Professor.

Dr Sikka was well known for his pivotal contributions to Pokharan-I and -II. He set up a laboratory with facilities for static pressure generation employing diamond anvil cells and shock wave generation with gas guns, which was the first such laboratory in India. Dr S. K. Sikka was not only an ace experimentalist but also an accomplished theoretician.

His early interests were in the crystal structure determination of hydrogen-bonded materials using neutron diffraction, neutron resonance scattering and neutron anomalous dispersion. His studies of the phase problem employing anomalous and direct scattering methods have been incorporated in the teaching aids of the IUCr. Some of his significant early work was on single-crystal neutron diffraction studies on potassium oxalate monohydrate at the CIRUS Reactor at Trombay BARC, India. It had been shown that this compound was the only reported structure in which neither of the lone pairs of the hydrogen-bonded water molecules was specifically directed despite the availability of metal ions in that structure. In fact the classification of the hydrogen-bonded water molecules with respect to their lone-pair coordination, proposed by his team [*J. Chem. Phys.* (1964). **41**, 3616], is the most extensively used classification in related literature. Based on a modified Lippincott–Schroeder potential for the hydrogen bond, he explained why the shorter hydrogen bonds are less bent on average than the longer ones. His structure solutions of $Cd(NO_3)_2.4D_2O$ and $Sm(BrO_3)_3.9H_2O$ using anomalous neutron scattering and neutron resonance scattering using two wavelengths were the first reported applications of the use of thermal neutrons in the determination of the phase problem.





Due to his brilliance, Dr Sikka was requested to work in areas relevant to the departmental programs and thus started working on high-pressure behavior of materials. In the initial days the main interest was in the EOS data of materials. Based on the Saha ionization theory, he and his colleagues developed a model to compute the EOS of solids in the intermediate pressure region (500–1000 GPa) [*Phys. Rep.* (1983). **102**, 121]. He worked on the high-pressure behavior of several actinides. However, apart from this, he also worked on basic research problems in the area of high-pressure science. He has a volume of work on the formation of omega phase in alloys and *d*-rich transition elements under static and shock pressures. His review article [*Prog. Mater. Sci.* (1982). **27**, 245] on the "Omega Phase in Materials" is considered to be a textbook by researchers in condensed matter physics/materials science. He worked extensively on high-pressure-induced crystal to amorphous phase transitions [*Prog. Mater. Sci.* (1996). **40**, 1]. Notable amongst his studies are those on negative thermal materials, quartz-like materials and different forms of carbon and silicon.

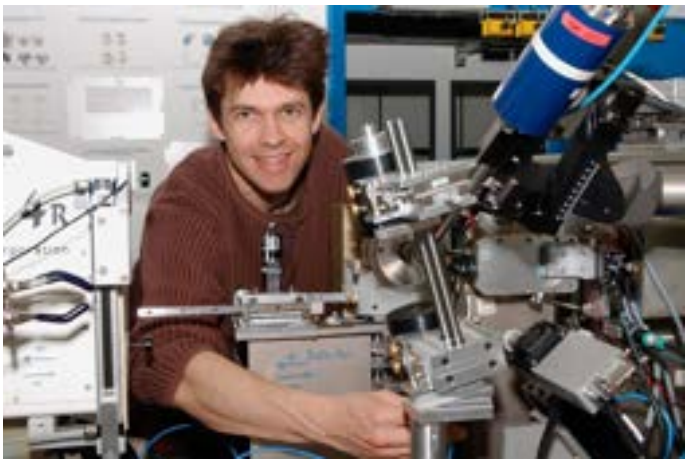
Dr Sikka served as a member of the Executive Committee of the International Association for Advancement of Research and Technology under High Pressure, and as a consultant to the IUCr Commission on High Pressure. He chaired the INSA committees for the IUCr and Committee on Data for Science and Technology and served as a member of the Asia Pacific Academy of Materials and on the editorial board of the journal *High Pressure Research*.

He was the recipient of several awards; notable among them were the H. K. Firodia award for Excellence in Science and Technology, M. M. Chugani Award for Excellence in Applied Physics by the Indian Physics Association and the fourth highest Indian civilian award, the Padma Shri. He was an elected fellow of the Indian National Science Academy, Indian Academy of Sciences and the National Academy of Sciences, India.

Dr Sikka was a former Chair of the Indian National Committee on Crystallography. For a list of his papers in IUCr journals click here.

OBITUARY

Raimond B. G. Ravelli (1968–2023)



Raimond on beamline ID14-4, ESRF, Grenoble, France, 2002/2003. Photo credit: EMBL, Grenoble.

Elspeth F. Garman

On 11 July 2023 in a beautiful and full chapel in Maastricht, the Netherlands, we remembered and bade farewell to a much-loved colleague and friend, Raimond Ravelli, who died on 30 June after a sudden unexpected 10-week illness. Raimond was a highly creative structural biologist who contributed hugely to the field. The bare facts of Raimond's far too short 55-year life give no indication of the profound impact of his innovations in X-ray crystallography and electron microscopy methodology, and make it easy to underestimate his own seminal contributions in answering numerous scientific questions in structural biology. More importantly though, facts cannot tell of the profound inspiration he gave to those fortunate to be his colleagues, collaborators and mentees.

Raimond was born in De Bilt, near Utrecht, the youngest of three children. His nickname was 'Kikvors' ('frog') because he was always ready to jump and to surprise. He loved to read and build with LEGO (a fascination he retained all his life), but at school it soon became clear how intelligent he was. His scientific talent and passion surfaced as a teenager and at the age of 18 he participated in the finals of the Netherlands National Chemistry Olympiad. He performed best under pressure and in fact he later seemed to seek that pressure in his research life too. He loved to perform experiments, so it was no surprise to his family when he decided to study chemistry at the University of Utrecht, graduating in 1992 despite his extensive commitment to his rowing crew. Raimond stayed in Utrecht for his PhD research under the supervision of Henk Krabbendam and Jan Kroon, working on X-ray data-collection techniques, particularly Laue methodology (Ravelli *et al.*, 1999). His PhD was awarded in 1998 for a thesis entitled *Laue Diffraction and Fast Monochromatic X-ray Data Collection Techniques*. One of his thesis projects was to write the brilliant *STRATEGY* software program (Ravelli *et al.*, 1997) which allowed efficient X-ray diffraction data-collection strategies to be computed and utilized. This was widely adopted by the worldwide crystallographic community, making Raimond's name well known to many. While writing his thesis, Raimond also developed a keen interest in the structure and mechanism of the acetylcholinesterase enzyme, in close collaboration with the groups of Joel Sussman and Israel Silman at the Weizmann Institute of Science in Rehovot, Israel, which bore fruit on a number of joint projects (Ravelli, Raves *et al.*, 1998; Ravelli, Hezemans *et al.*, 1996; Harel *et al.*, 1995), and continued to attract his interest for many years afterwards (Harel *et al.*, 2004, 2007).

Following his move in 1998 to the EMBL Outstation in Grenoble, France, first as a postdoctoral fellow, then as a staff scientist and ultimately as a Team Leader, Raimond grew to be a widely recognizable expert in crystallographic data collection. As a member of the ESRF–EMBL Joint Structural Biology Group, under the guidance of Sean McSweeney he undertook the careful optimization of the first undulator

beamline at the ESRF dedicated to macromolecular X-ray crystallography: ID14-4. Their efforts resulted in this beamline becoming the first choice for data collection runs for many crystallographers, to the extent that, to my knowledge, it is the only beamline to have a day-long symposium or 'wake' organized for it in February 2014 after it had sadly been dismantled. This event reflected the great respect of the community for both the technical achievements and the significant impact of the scientific results that had been obtained on ID14-4. For instance, the beamline was instrumental in determination of the structure of the 30S ribosome, which was awarded the Nobel Prize for Chemistry in 2009. In fact, two of the three Nobel awardees used ID14-4: Ada Yonath privately tutored Raimond on ribosomes and Venkatraman Ramakrishnan acknowledged Raimond in his seminal Nobel article. Raimond was the *beamline responsible* and he worked very hard, day and night, with great patience and good humour to help numerous colleagues collect high-quality diffraction data at the highest scientific standard. He instigated the installation of the first on-line microspectrophotometer (McGeehan *et al*., 2009), and then oversaw its redesign and improvement, making it possible for less expert users to take measurements. He also steered the development of the 'Mini Kappa goniometer head' with Florent Cipriani and colleagues at the EMBL (Brockhauser *et al*., 2013) to allow users to orient crystals for optimal X-ray diffraction results. He thus put his exceptional scientific gifts and experimental talents to good use for many colleagues.

From his observations of diffraction degradation suffered by cryo-cooled crystals on the beamline, Raimond developed a keen interest in radiation damage (RD). With Sean McSweeney and Joel Sussman they investigated the phenomenon in detail, publishing two seminal papers entitled *The 'fingerprint' that X-rays can leave on structures* (Ravelli & McSweeney, 2000) and *Specific chemical and structural damage to proteins produced by synchrotron radiation* (Weik, Ravelli *et al*., 2000). Raimond also analysed and published a paper on unit-cell expansion effects (Ravelli *et al.*, 2002) in the first *Journal of Synchrotron Radiation* special issue on RD, combining papers collected together following the Second International Workshop on RD in crystalline biological samples. Raimond was a very regular contributor to this series of workshops, held biennially from 1999 (1st) to 2020 (11th), and was one of the Organizing Committee members from 2003 onwards, reviewing the RD landscape in 2006 (Ravelli & Garman, 2006).

It became evident from RD investigations at the ESRF that the damage rate to cryo-cooled crystals was dependent on the absorbed dose, a parameter which can be estimated from knowledge of the beam conditions and crystal constituents but cannot be measured. Raimond thus wrote a computer program called *RADDOSE* to calculate absorbed dose, and this was further developed in collaboration with us and then released to be used by many researchers (Murray *et al*., 2004). It was later rewritten in Java and released as the current *RADDOSE-3D*.

Raimond was a lateral thinker of great originality, and always thought outside the box. His scientific curiosity and enthusiasm were contagious and inspirational to many of us, and were the seed of many new projects. Often, Raimond's ideas went beyond his core scientific interests, thereby fertilizing and connecting different disciplines and various areas of research. He recognized that the RD effects led to specific changes in the structure factors measured, leading him to contribute to data-reduction methods, particularly zero-dose extrapolation (Diederichs *et al.*, 2003). Furthermore, he realized that the specific RD to disulfide bonds and acidic amino acids in cryo-cooled crystals could be used as a phasing signal if data sets before and after an X-ray (or UV laser) 'burn' were collected. Thus Radiation damage Induced Phasing (RIP) was born (Ravelli *et al*., 2003; Nanao *et al*., 2005; Ravelli *et al.*, 2005) and contributed to some important structure solutions (*e.g.* Rudiño-Piñera *et al*., 2007). There were two features of ID14-4 that made it particularly suitable for systematic radiation damage studies: the beam had an approximately top-hat profile and the X-ray flux was continuously monitored using an in-line foil with a diode above it, with the values being written into the image headers. As well as studying RD to protein crystals, Raimond also investigated RD to DNA using Raman spectroscopy (McGeehan *et al*., 2007).

During his time at EMBL, in conjunction with developing novel methods, Raimond led and participated in a number of exciting structural biology projects. Notable among these was work on the assembly of tubulin and its mechanism of regulation (Dorléans *et al.*, 2009), featuring two papers published in *Nature*

(Ravelli *et al*., 2004; Gigant *et al*., 2005). The crystal structure determination of the rabies virus nucleoprotein-RNA complex (Albertini *et al*., 2006) published in *Science* and of the human Slit-Robo complex (Morlot *et al.*, 2007) were among other impactful results. Clearly, he was often called upon to tackle the most challenging, seemingly intractable, and thus to Raimond the most interesting, problems.

It was a joy to work with Raimond but it could also be tough, especially when there was some sort of deadline involved, since he had rather a 'flexible' approach to deadlines. He would speak up when he agreed, but also when he disagreed; in both cases with a wide and sincere smile. Consequently, differences of opinion were met head on and discussed with disarming honesty in a determined effort to sort out the issues for the good of all parties. Thus, any misunderstandings could be sorted out, resulting in very strong and productive collaborations which often developed into equally strong and enduring friendships.

Grenoble sits in a cradle of spectacular scenery, and Raimond loved to be outdoors on bike rides and mountain hikes. When he was not working crazy day- and night-time hours, he made the most of these opportunities and there are many stories of adventures experienced by visiting researchers when they went on outings with Raimond. A special feature of trips with him was that he absolutely refused to come back the same way that he went. Legendary were his 'shortcuts', defined as the least straightforward way to connect two points on the map. A very particular such shortcut was related by Martin Weik at the memorial service: 'Whoever worked with Raimond needed to be prepared for adventure, not only in, but also outside the lab. Legendary were the sledging hikes, during which Raimond took colleagues and friends through deep snow in the alps, inviting them to sledge down on little plastic sledges for children. When I realized that the slope felt almost vertical, I politely declined and offered to drive the car down the mountain to greet them there. On my way down, all of a sudden, a huge cloud of snow fell in front of my car, but luckily, I just stopped in time. In the middle of the road, there was Raimond with a colleague, excited that he found this adventurous shortcut down the mountain.'.

Raimond moved back to the Netherlands in 2007 after being awarded a prestigious VIDI award (a personal grant reserved for the most promising young research leaders) by the NWO (The Dutch Research Council). He took up a position as an Assistant Professor at Leiden University Medical Center (LUMC). The impetus for this move was that with amazing predictive power and vision, and well before the current revolution in electron microscopy (EM), he realized that the focus of his research should be redirected from crystallography to cryo-EM, even while maintaining his abiding interest in structural biology. Making this change years before many others also judged this to be a wise move, he was well 'ahead of the pack' (much like his position during many cycling tours in the Grenoble mountains). He made significant contributions and became a very well respected member of the new community, making important progress in optimizing the new capabilities of cryo-EM. This included methods to characterize the new CCD cameras (Vulovic *et al.*, 2010) and to control the rate of RD (Karuppasamy *et al*., 2011), since this is also a limiting factor in cryo-EM structure determination.

One of Raimond's major achievements during his time at the LUMC was to combine 20 000 EM images to obtain an entire, very detailed multi-scale image of a zebrafish embryo (Faas *et al.*, 2012), earning him a place in the Guinness Book of World Records for the largest digital image (281 gigapixels!). It was on display for some years in the Naturalis Biodiversity Center in Leiden.

In 2014 he moved as an Associate Professor to Maastricht University in the newly formed Maastricht Multimodal Molecular Imaging Institute (M4I), to continue his work in cryo-EM and help build the Institute of Nanoscopy (IoN). He developed improved approaches for optimizing cryo-EM studies, inventing several advanced techniques to allow efficient sample preparation such as pin printing to substantially reduce sample waste, and reducing sample evaporation using dewpoint control feedback loops (Ravelli *et al*., 2020). He was particularly proud of the development of Vitrojet, a highly original device for automated cryo-EM sample preparation, and he held several patents for his inventions.

During his time at Maastricht University, Raimond elucidated the structure of beta-amyloid fibrils (Gremer *et al*., 2017), and was part of the team who showed that SARS-CoV-2 can productively infect

human gut enterocytes (Lamers *et al*., 2020), both studies being published in *Science*. Raimond also pursued tomographic methods (Berger *et al*., 2023), putting to use his earlier experience on ID14-4 to image crystals (Brockhauser *et al*., 2008), and he continued his radiation damage investigations particularly on the effects of dose in single-particle cryo-EM (Zhang *et al*., 2021).

In November 2022, Raimond was appointed to a Full Professorship in Structural Biology at Maastricht University. His inauguration speech (Oratie) was the occasion to showcase his talent as speaker and communicator to a wider audience. His speech, given to a packed auditorium of colleagues, family and friends, is a *Musing on Nanobiology* and is available at https://www.youtube.com/watch?v=Gv3pKRp5S2Y&t=667s. Raimond's enthusiasm and passion for science emanated from him and was an inspiration to all those present. The Oratie included the first showing of his SARS-CoV-2 lifecycle animation, made in collaboration with Kèvin Knoops, Montserrat Barcena and Jeroen Claus; the animation has already won 15 different awards for design and science education. It can also be found here: https://www.youtube.com/watch?v=XlOi2hVGtg0. However, the voice on YouTube which describes the lifecycle is of course not Raimond's but is my own: I was most honoured when he asked me to go to London and record it at a professional studio. Raimond's attention to detail when writing the script was, as always, particularly impressive.



Raimond on 18 November 2022 at his Oratie, Maastricht University.

Raimond was not only a brilliant scientist but also a thoughtful and inspiring mentor and a much-appreciated colleague at the EMBL, ESRF, LUMC and Maastricht University, as well as in the wider structural biology community. His students remark on his exceptional mentorship and teaching skills; his colleagues know him for his enormous enthusiasm and passion for science, his generosity, inclusivity and humility. He will be greatly missed by his colleagues and collaborators, and also by his many friends around the world, for whom knowing him was a privilege and inspiration. Raimond's legacy to those he trained and mentored throughout his career will certainly live on.

Raimond leaves behind him his partner Maaike de Backer, and their son Seppe and daughter Noé. The structural biology community extend their deep sympathy to them for their loss.

Postscript: personally, I will remember Raimond as firstly a very kind, treasured and supportive friend who happily attended my daughter's orchestral concerts in Leiden and London, and who came to Oxford both for my husband's funeral and also for my retirement event. Secondly, I will never forget his great integrity and high standards as a scientist, even if that meant spending two hours in the middle of my night on a phone call with him to finish editing one of our joint papers when I was in Australia. Rest in peace, dear Raimond, the world is a better place because you were in it.

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IUCR SUPPORTED EVENTS

IUCr supported meetings

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



11th Oct 2026 - 16th Oct 2026

Indaba10

Skukuza, Kruger National Park, South Africa



5th Dec 2026 - 10th Dec 2026

African Materials Research Society (AMRS 2026)

Nairobi, Kenya

MEETINGS CALENDAR

Meetings calendar

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



Indaba10 South Africa 11th Oct 2026 - 16th Oct 2026



Synchrotron Radiation: Science, Knowledge, Innovations, Future (SKIF-2026) Russian Federation 18th Oct 2026 - 23rd Oct 2026



CCP-EM/Diamond Icknield Workshop United Kingdom 9th Nov 2026 - 13th Nov 2026



Instruct-ERIC hands-on workshop on Advanced cryo-FIB-SEM methods Germany 9th Nov 2026 - 13th Nov 2026



Crystal36-AXAA 2026 Meeting Australia 26th Nov 2026 - 2nd Dec 2026

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

Joint Polish-German Crystallographic Meeting 2027 Germany 15th Feb 2027 - 18th Feb 2027