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LETTER FROM THE PRESIDENT

Enthusiasm makes the world go round



Sven Lidin

People impress me.

Perhaps I'm a guy who is easy to impress, but I've always been impressed by others and this has in no way abated lately. I've always been aware that people are smart, resourceful and innovative and possess all the other virtues that makes life and science progress, but lately I've come to realize that there is another human attribute that tops all the rest in terms of usefulness and in terms of magnificence. It's enthusiasm.

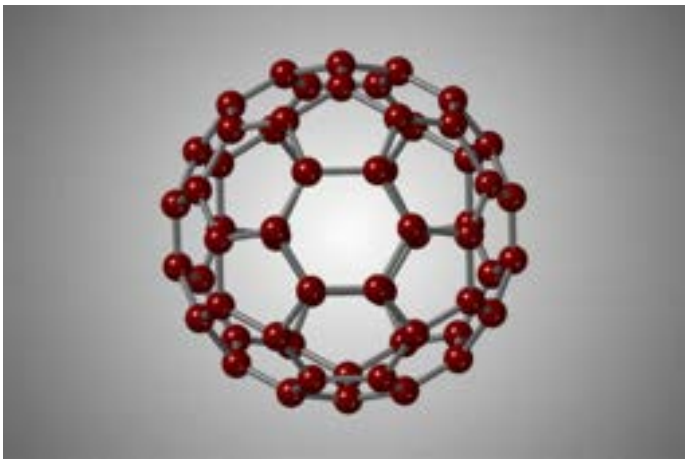
Being part of a partial university lockdown where only necessary tasks are to be performed on-site and physical human contact is essentially zero, I sometimes find it a little difficult to get my own levels of enthusiasm above the waterline. I basically meet only myself, and while I can be as charming as the next guy in a brief encounter, I wear a bit thin as company over time. I've known myself for over 60 years now, and the novelty has worn off. No surprises there. I need people to function and I need people to feed my enthusiasm.

In the past few months, I've been struck by the enthusiasm that has reached me through conferences in which I've participated online. This is where people impress me. Sitting in my flat, contemplating whether to do something about the piles of dust quietly gathering in the corners of the room and in the recesses of my mind, I'm struck by the enthusiasm conveyed to and conferred to me by other participants. This year, I've been electronically to conferences in Dakar and Novosibirsk and late last year, I was teleported to Mexico City for the same purpose. I came away enthused and refueled. Certainly, online meetings are not the real deal. The energy levels are not those of a physical meeting, and above all, the coffee-break revelations and the collaborations that start over beers after the day is done just don't happen, but you still get to listen to real people and you get reminded of all the exciting things others do that make this world, despite it all, a fun place!

The IUCr Congress and General Assembly that was postponed from last summer will definitely take place this summer organized from Prague. The organizers are presently working very hard to arrange what right now looks to be a hybrid meeting. There are many practical challenges to schedule all the sessions and meetings that are to take place given that a fair proportion of the attendees will sit in time zones far from Central European Time. I want to thank everyone who is working to organize meetings around the world to bring people together. It has never been more challenging. It has never been more important. By being smart, resourceful and innovative you help us all find our way back to that enthusiasm that makes the world go around. Thank you! See you soon at a screen close to you. Now I'll go and do a bit of dusting …

EDITORIAL

Editorial



Mike Glazer

COVID continues to rule the world, and many of us live in countries in which there is a severe lockdown. No-one knows when any of this will end. Here, in the UK, the lockdown is quite strict and all foreign travel has been banned. So it is difficult to not feel trapped. I was lucky enough, though, because of my age, to receive a vaccine injection in January, which I hope will give some protection. That was a relief, to be sure. The speed with which all the vaccines have been developed is mind-blowing, and much of it is due to our own area of science, in which a great deal of work has been done to determine the structural characteristics of the SARS-CoV-2 virus. As members of the crystallographic community, I think we can be proud of the role that our subject has played.

Harald Reichert has written an important article for us describing the new EBS source for the ESRF synchrotron, which has a performance far exceeding the designers' expectations. The EBS has a small and bright source, enabling very fast data collections as well as excellent spatial resolution. For instance, it will be possible obtain diffraction information from individual grains in a powder, thus enabling single-crystal structural solution. This promises to be a major advance, enabling all sorts of exciting, new experiments to be carried out.

I was deeply saddened to hear of the death of Judith Milledge. I met her when I and Howard Flack became PhD students in Kathleen Lonsdale's group at University College London. She was a remarkable person in many ways, bursting with ideas, some of which were truly brilliant, a sharp brain, a clever scientist and a thoroughly nice person. She did have the unfortunate habit of getting bored quickly with projects that she had started before moving on to other topics before finishing. I recall Kathleen Lonsdale admonishing her at coffee time, in front of all of us in the group, for not completing anything she started. But this had no effect on Judith. Her warm personality shone through, and she continued to bubble with fresh ideas. Perhaps I can take this opportunity to tell an anecdote (I have many more!) from those times.

Next to my desk was a huge electromagnet in a wooden case (I was told that it had belonged originally to Faraday). One day, Judith had an idea that I should use the magnet to study the diamagnetic susceptibility of my crystals. To do this one had to suspend a crystal on a fine glass fibre between the poles of the magnet, and set it into oscillation. I really didn't want to do this, but how could I refuse? I hatched a plan to delay things. I made a set of glass fibres and placed them on my desk in readiness. Now, my desk backed onto the sink where we used to make our coffee and tea, and at coffee time, one of our female members (if I recall correctly it was June Sutor, famed for her work on hydrogen bonding) came in and put her handbag down on the edge of my desk, crushing my glass fibres. Of course by this time, Judith had moved onto some other ideas and so I never did use the magnet.

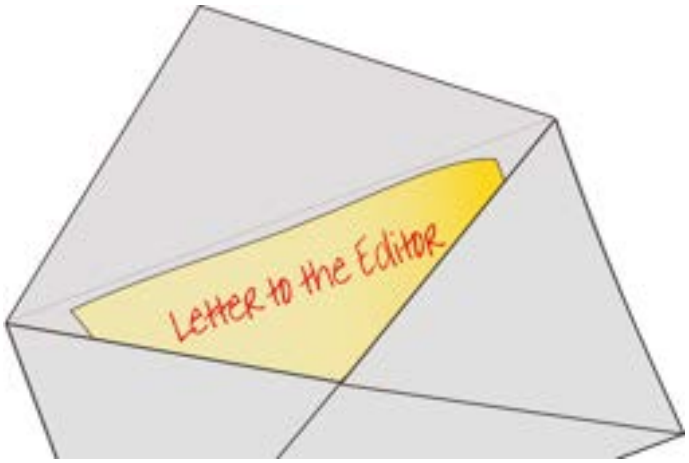
In this issue, we publish an article by Piero Macchi on an important topic. Normally, when we solve crystal structures, we assume that all the atoms in a crystal can be treated as being spherical. This is obviously incorrect as the atoms are not isolated from one another, and so their electron densities are spread out. Over the years various methods have been devised to modify this assumption, mainly using local multipolar corrections. However, quantum mechanics was developed at roughly the same time as X-ray crystallography and for the last 100 years or so has become increasingly tied in with structure solution. Today we call this quantum crystallography.

Another area of advance is demonstrated by Brian Toby's article where he reports on Rietveld powder analysis in 100 picoseconds. This has been achieved by Bob Von Dreele, Samantha Clarke and James Walsh and opens the door to studying reactions and fast changes in materials. There is no end to the advances being made in crystallography!

We also have another short article from Istvan Hargittai, reminding us of the work of Caroline MacGillavry, who discovered the work of the artist Maurits Escher and how it related to crystal symmetry. He also brings our attention to the work of Khudu Mamedov, from Azerbaijan, who also developed a similar type of artwork.

LETTER TO THE EDITOR

Protecting science from politicisation



Hanna Dąbkowska

It was with great interest and curiosity that I read Mike Glazer's article about Jan Czochralski – the Polish chemist, engineer, inventor and creator of the popular crystal growth technique (the Czochralski Method) – in a recent issue of the *IUCr Newsletter*.

In 1978 I was involved in the process of acquiring a Czochralski apparatus (produced by Malvern in Cambridge, UK) for the newly created crystal growth laboratory in the Institute of Physics, Polish Academy of Science. It was 25 years after Jan Czochralski's death. I was then a newly graduated chemist from Warsaw University and had not realised that Jan Czochralski was a Pole, working in Warsaw (he was a former professor at Warsaw Technical University). I was aware that the name was Polish – who else could pronounce the famous “cz” letter combination? – but somehow I was left to believe that he was an American of Polish origin. His name never appeared in any Polish records. It was not until about 10 years later, after the Solidarity movement changed the political direction of Poland dramatically, when Paweł Tomaszewski and Anna Pajączkowska dared to uncover the tragic Czochralski story. It is all reported in Glazer's paper.

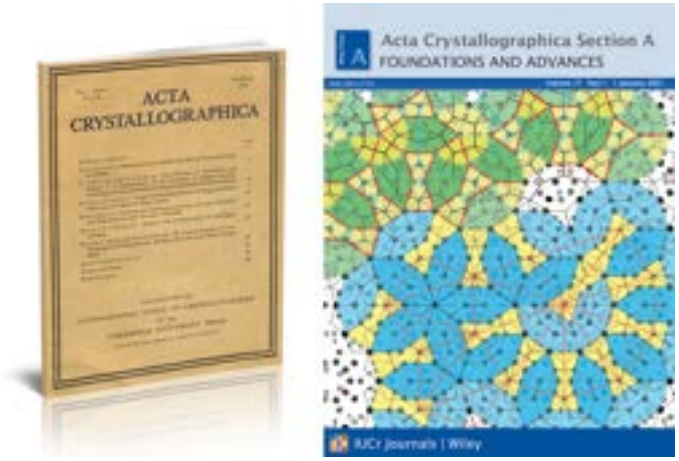
Since then, the recently established Polish Society for Crystal Growth took Jan Czochralski as its patron, the medal in his name is awarded every year and even a short movie about this most cited Polish scientist was created. Now we know that Jan Czochralski goes down in the history books as a great achiever and a patriot, not as a despised traitor.

I am immensely grateful to Professor Glazer not only for reminding the crystallographic community of Jan Czochralski's story but also for his steady support for young, Polish crystallographers whom he traditionally hosted in his laboratory in Oxford in those difficult times, when visitors from behind the iron curtain were not so easily accepted in the free western scientific world.

It is good to be reminded again that science can be dampened – or even destroyed – in an unfavourable political environment. Some of us have nearly forgotten it can happen, some have never experienced it. This article makes us all aware that protecting science from being politicised is extremely important. Always was, always will be.

EDITORIAL

Modern crystallography and its foundations



Angela Altomare, Simon J. L. Billinge

Acta Crystallographica Section A: Foundations and Advances (*Acta A*) has been the premier journal (see Billinge & Miao, 2015) for foundational work in crystallography for the past 72 years (if we include the years when there was only one *Acta Crystallographica*). As we move into its 73rd year, we seek to maintain its prominence and impact, and this editorial is designed to share with you how you can help.

First, as described in our aims and scope (as captured at https://journals.iucr.org/a/), we remind our authors that, although ‘crystal’ is in the title of the journal, we accept articles about structural studies from a much broader array of materials, whether crystalline or not. For example, we welcome articles developing methodologies for single-particle imaging, studies of diffuse scattering and direct imaging of atoms. If you are reading this you already know this, but please share this with your colleagues!

We would also like to remind authors that, beyond the mathematical foundations of the subject, we also welcome articles that describe software and computational platforms that implement those algorithms. For example, analysis algorithms are moving in the direction of powerful but computationally demanding AI (artificial intelligence) and machine learning (ML), the data moving from tables to databases, and the analysis tools moving into the cloud (see, for example, Fig. 1), and we welcome articles in these areas.

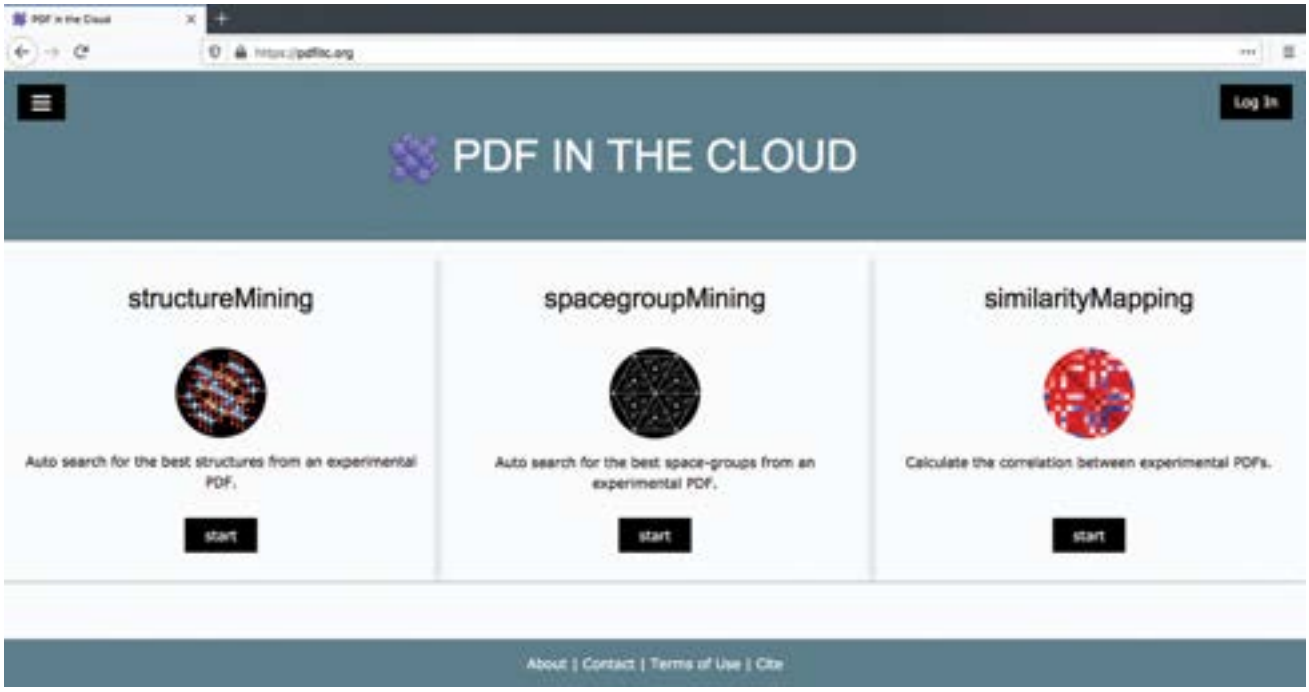


Figure 1. A cloud-based platform for atomic pair distribution analysis (see Yang *et al*., 2021).

Finally, we encourage authors to emphasize the crystallographic context of the work in their article. This is important for maintaining the relevancy, vibrancy and broader impact of the journal. In your view, who in the materials or structural communities will use it, and what will they use it for? We have found that, in these busy times, the more forward facing this information is the better. Can it be hinted at in the title? If not, it should appear in the abstract, or early in the introduction. It should also be captured in any short one- or two-sentence synopsis about the work. In fact, such brief, public facing 'elevator pitches' are enormously valuable to us (and you!) to help promote the work and increase the readership. If you would like guidance in this regard, please feel welcome to contact our editorial team, who can make suggestions.

We thank you for your wonderful contributions and welcome even more in the upcoming years.

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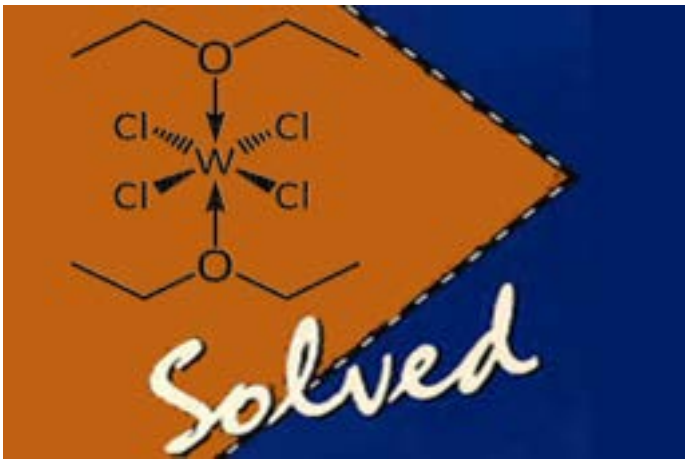
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COMMENTARY

The decades-old mystery of bis(diethyl ether)tungsten(IV) chloride solved



André Schäfer

A hexacoordinated metal centre with an octahedral coordination environment is a very common motif in transition metal chemistry. This can involve neutral, as well as anionic, ligands or a combination of both. The latter can, *inter alia*, be found in many Group 6 complexes, often with donor solvent molecules acting as neutral ligands and saturating the coordination sphere of the metal(IV) centre. In particular, with regard to tungsten, many complexes of the type $WX_4(\text{solvent})_2$ are known in the literature and are even found in textbooks nowadays, as, for instance, $WCl_4(py)_2$ (Brenčič *et al.*, 1979) or $WCl_4(MeCN)_2$ (Manteghetti *et al.*, 1999), which have even been structurally characterized by single-crystal X-ray diffraction. A common, yet ambiguous, example of this is bis(diethyl ether)tungsten(IV) chloride, $WCl_4(Et_2O)_2$. Although this compound has been `floating around' in the literature for many decades, surprisingly little analytical data concerning it have been reported, begging the question if it even truly exists.

Taking a look at the history of the compound, it starts in 1975 when Thiele *et al.* (1975) studied different benzyltungsten compounds, tetrabenzyltungsten amongst others, which they obtained from the reaction of dibenzylmagnesium with tungsten(IV) chloride bis(tetrahydrofuran), $WCl_4(thf)_2$. This, in turn, was synthesized from tungsten(VI) chloride, WCl_6, by treatment with diethylzinc in diethyl ether, whereas the authors proposed that the tungsten(IV) chloride bis(diethyl ether) adduct, $WCl_4(Et_2O)_2$, was formed initially, and was then transformed into the isolatable bis(tetrahydrofuran) adduct. Unfortunately, no analytical data for the bis(diethyl ether) complex was provided. At roughly the same time, Chisholm, Cotton and co-workers investigated the use of $WCl_4(Et_2O)_2$ as a possible precursor in the preparation of tungsten–tungsten triple-bond complexes (Chisholm *et al.*, 1976*a*,*b*). While $WCl_4(Et_2O)_2$ was explicitly mentioned as a bis(diethyl etherate), it is worth pointing out that it was prepared *in situ* (by the same route as described above), with a 100% yield assumed, and was used without characterization. Therefore, although $WCl_4(Et_2O)_x$ had already proven to be an interesting synthon, the exact nature and structure of the complex remained unclear and its composition, suggested to be a bis(diethyl ether) adduct, was based simply upon chemical intuition and the logical assumption of an octahedral complex with hexacoordinated tungsten (Fig. 1).

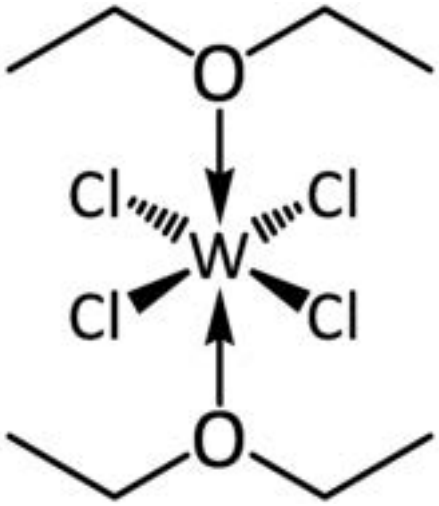


Figure 1: Tungsten tetrachloride bis(diethyl etherate), $WCl_4(Et_2O)_2$.

Almost a decade later, in 1985, Castellani & Gallazzi (1985) revisited the preparation of diethyl ether complexes of molybdenum and tungsten tetrachlorides, and made an attempt to characterize $WCl_4(Et_2O)_x$ by elemental analysis to elucidate its exact composition. In contrast to previous articles, they reported that the mono(diethyl etherate), $WCl_4(Et_2O)$, was obtained from diethyl ether solutions of WCl_6, which was based on elemental analysis suggesting not two but one equivalent of $C_4H_{10}O$ [$WCl_4(Et_2O)_2$: C 20.3, H 4.3%; $WCl_4(Et_2O)$: C 12.0, H 2.5%; reported by Castellani & Gallazzi (1985): C 11.5, H 2.4%]. First, it is worth mentioning that Castellani & Gallazzi seem to be the first to actually attempt to isolate the complex as a pure solid, rather than just synthesize and use it *in situ*. Furthermore, they reported that an orange reaction mixture, along with a yellow solid, formed initially, but that ultimately black crystalline needles were obtained and isolated. It seems odd that a compound could be obtained in the form of black crystals from an orange reaction mixture and, taking into account that a yellow precipitate was observed initially, this might point towards an equilibrium between a mono- and bis(diethyl etherate), due to the relatively weak complexation of the diethyl ether ligands. In fact, Castellani & Gallazzi pointed out correctly that other complexes, such as $WCl_4(thf)_2$ and $WCl_4(py)_2$, always feature two complexed solvent molecules.

It is puzzling that for decades this mystery remained unsolved, even though this complex was frequently used as a starting material in tungsten chemistry. Finally, in 2021, almost half a century after the complex first appeared in the literature, Jurca and co-workers were able to obtain a pure crystalline sample of the bis(diethyl ether) complex, $WCl_4(Et_2O)_2$, and conduct a complete structural characterization by single-crystal X-ray diffraction and NMR spectroscopy (Shaw *et al.*, 2021). Different from previous reports, the authors used tungsten tetrachloride, WCl_4, as the starting material, dissolving it in diethyl ether. In a striking similarity to the report of Castellani & Gallazzi from 1985, they observed a yellow solution and were able to obtain not a black but a yellow crystal from it. Structural characterization of this crystal by X-ray diffraction confirmed it to be tungsten tetrachloride bis(diethyl etherate), $WCl_4(Et_2O)_2$, with *trans*-coordinated diethyl ether molecules in the axial positions (Fig. 1)! With this, the quest for the elucidation and structural characterization of the long-discussed $WCl_4(Et_2O)_2$ finally comes to an end, closing this gap in tungsten tetrachloride bis(solvent) complexes.

The question remains, did Castellani & Gallazzi actually obtain the mono(diethyl etherate), $WCl_4(Et_2O)$, in 1985, as suggested? It seems not unlikely given the fact that diethyl ether is a rather weakly bonded ligand, and they reported black crystals instead of yellow ones and the elemental analysis was very much in line with a mono(diethyl etherate). Two interesting details are given by Jurca and co-workers here as well, namely, that `prolonged exposure to ambient conditions led to the appearance of dark spots on the crystal surface' and that `the compound is unstable under vacuum' (Shaw *et al.*, 2021). This clearly suggests the loss of one equivalent of diethyl ether due to rather weak complexation, which would explain Castellani & Gallazzi's elemental analysis results.

Funding information

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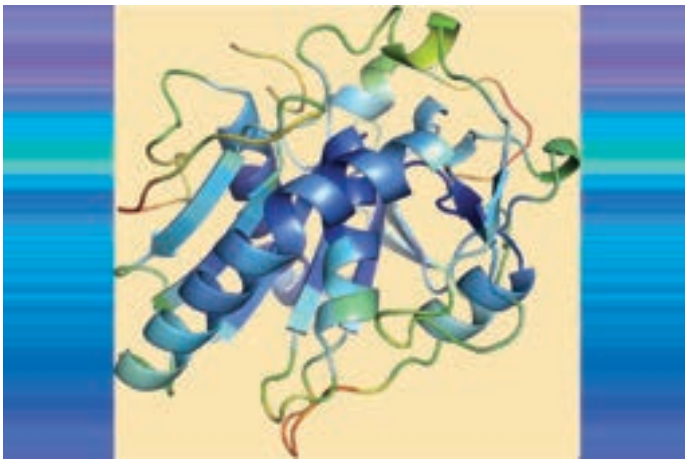
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EDITORIAL

Integrated, rational molecular replacement



Isabel Usón, Charles C. Ballard, Ronan M. Keegan, Randy J. Read

In the past 50 years, molecular replacement (MR) has grown from being a way to shortcut the occasional determination of identical or closely related structures to being the route to the majority of protein crystal structures. The 2019 CCP4 Study Weekend on Molecular Replacement, held on 9th–10th January 2019 in Nottingham, UK, looked briefly at its long history but focused on recent developments that have helped to push its reach to a much greater range of structures. The special issue at https://journals.iucr.org/special_issues/2020/CCP42019/ contains contributions from the majority of the speakers at the meeting.

After an overview of the history of MR by Eleanor Dodson, Airlie McCoy talked about the development of likelihood-based MR and how the use of graph databases will allow even more sophisticated branched searches testing different structural hypotheses. The likelihood approach benefits from accounting for the effects of errors, which must be estimated in advance for structural models. Björn Wallner discussed methods to accurately estimate the local errors in computational models, which can be used to weight the relative contributions of different parts of these models. Kaushik Hatti focused on global errors, discussing how these can be estimated from a combination of factors including sequence similarity scores, model size and model quality scores. Randy Read examined the connection between likelihood scores and measures of information gain, showing that information gain can be used to choose the data that will contribute usefully to MR calculations.

The application of MR can be hindered by problems with the crystals, so it helps to diagnose and understand crystal pathologies. Regine Herbst-Irmer discussed the case of non-merohedral twinning and how this can be dealt with in a variety of circumstances. Iracema Caballero examined issues raised by translational non-crystallographic symmetry: how it can be detected, characterized and accommodated in structure solution. Another surprisingly common problem is for crystals to grow from the wrong component from the protein purification; Adam Simpkin discussed an approach using a database of ensembles of folds to solve such structures, by detecting which contaminant actually crystallized.

Some of the most exciting advances in the past few years have come from the development of methods to solve structures starting from much smaller fragments, including generic fragments such as helices. Several talks focused on new developments on this front that build on better understanding of structural patterns and integration with other computational methods. Dan Rigden showed that success in using *ab initio* computational models can be improved by testing a variety of pruned models. Ana Medina discussed the detection and preparation of generic compact folds and their use for fragment-based MR. Claudia Millán addressed a complementary problem: how to integrate a number of partial

fragment-based solutions to build up a more complete picture. Coiled coils represent a particularly difficult case for MR and Owen Davies described new improvements in how they can be modelled. Electron diffraction is emerging as a promising alternative to X-ray diffraction for microcrystals but it depends heavily on MR because conventional experimental phasing methods do not apply. Jennifer Miao discussed some of the issues with micro-electron diffraction and demonstrated that MR can succeed with fragments generated from distant homologues because local structure is preserved better than global structure.

Even if generic fragments or compact folds can be placed correctly, expanding an incomplete starting model to a good final structure can be extremely difficult. Rafael Borges described a new algorithm to test a large variety of hypotheses for how the protein sequence can be assigned to the fragments, significantly extending model completeness. Grzegorz Chojnowski discussed new methods to detect and exploit local structural similarity between the target structure and distant homologues when rebuilding structures solved by MR. Carmelo Giacovazzo presented results from a new MR pipeline, which follows the MR placement with density modification and automated rebuilding.

The meeting ended with case studies describing the approaches used in some particularly difficult structure solutions. Paula Salgado outlined the path to the solution of a type IV pilin, pilA1. This started with attempts to solve the structure using models and ensembles derived from homologues, an approach that frequently succeeds even if not in this case; the structure eventually yielded to *ab initio* fragment-based phasing, aided by the insight that pilins typically possess a long helix. Montserrat Fàbrega-Ferrer discussed two ways in which low-resolution cryo-EM reconstructions can be used to solve a crystal structure, either by using the cryo-EM map as a model directly or (the approach used in practice in their work) using a partial atomic model built into that map.

One talk (not represented by a paper in this issue) foreshadowed a major recent development with enormous implications for the future of MR in protein crystallography. Andrew Senior presented striking *ab initio* modelling results achieved by deep learning algorithms in *AlphaFold*, which had been tested in the 13th edition of the Critical Assessment of Structure Prediction (CASP) experiment. In CASP14 late last year, its successor *AlphaFold*2 achieved even more astonishing results in predicting the structures of a wide variety of targets, in many cases achieving the levels of accuracy needed for successful MR.

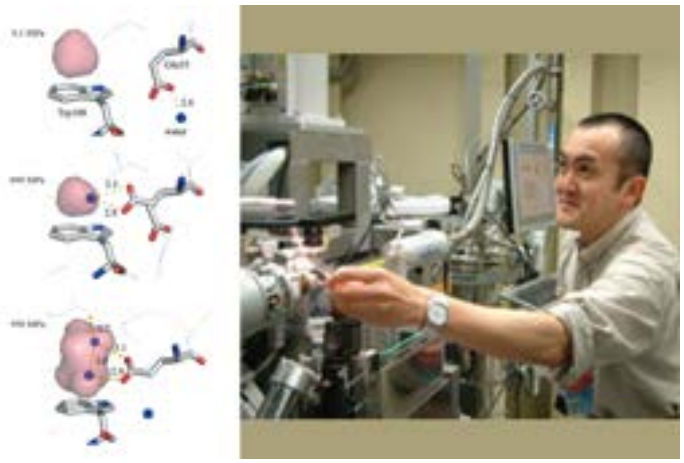
We would like to thank the speakers for their excellent contributions to both the meeting and this collection of papers, and the CCP4 staff who did a great job of looking after the organizational details (Karen McIntyre, Helen Walker, Esme Williams and India Reeves) and audiovisual facilities (Stuart Eyres and Laura Bennett).

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Acta Cryst. D has been home to the proceedings of the CCP4 Study Weekend since 1998. All the proceedings special issues are open access and the one described above is the latest in the series. To find out more visit https://journals.iucr.org/d

EDITORIAL

Diffraction structural biology – an introductory overview



Atsushi Nakagawa, John R. Helliwell, Yuriko Yamagata

The virtual special issue now available at https://journals.iucr.org/special_issues/2021/ISDSB2019 collects together articles published in *Acta Crystallographica Section D* and *Acta Crystallographica Section F* submitted in the context of the 6th International Symposium on Diffraction Structural Biology (ISDSB) 2019, which was held at the Osaka University Hall in Osaka, Japan on 17–19 October 2019. The ISDSB series of symposia was initiated in 2003 by the Japan Society for the Promotion of Science (JSPS) and specifically by the University–Industry Cooperative Research Committee (#169) (169th Committee) chaired by Professor Noriyoshi Sakabe. The phrase `diffraction structural biology' was proposed by the 169th Committee and has shown to the world the importance of research on structural biology mainly by X-ray, neutron, electron and other diffraction techniques. In 2003 the 1st International Symposium on Diffraction Structural Biology (ISDSB2003) was held in Tsukuba hosted by the 169th Committee, followed by the 2nd international symposium (ISDSB2007) in Tokyo in 2007, ISDSB2010 in Paris and ISDSB2013 in Nagoya. The previous conference was held in Knoxville, Tennessee, USA, close to the Oak Ridge National Laboratory (ORNL) neutron user facilities, the High Flux Isotope Reactor (HFIR) and Spallation Neutron Source (SNS) in 2016. The special issue of *Acta Crystallographica Section D*, Volume 74, Part 8 (2018) presented the articles submitted in the context of the ISDSB2016.

The central theme of the series of ISDSB conferences is to `bring structural biologists using diffraction, and the scientists using a wide range of other technologies, closer together as well as stimulate the interface of basic research and industrial applications'. Structural biology has clarified, even exposed, the mechanisms of action of molecular machines responsible for life phenomena through the three-dimensional structures of biological macromolecules. In order to recognize the specificity found in biological macromolecules, which are essential for life, related to disease and drug discovery, it is also necessary to embrace other techniques complementary to the diffraction method. Both domains have advanced enormously. In recent years, diffraction capabilities have advanced greatly – the X-ray free-electron laser facility SACLA and powerful pulse neutron facility J-PARC have been in operation in Japan, and similar facilities are being constructed all over the world. There are also massive advances in synchrotron X-ray sources in achieving extreme levels of brightness. Also, in the complementary domain of microscopy a big breakthrough has been achieved in electron microscopy in recent years. Indeed the Nobel Prize for Chemistry was awarded in 2017 to Jacques Dubochet, Joachim Frank and Richard Henderson for cryo-electron microscopy developments. The ISDSB2019 symposium played an important role based on this new era, and in addition to structural analysis based on diffraction phenomena as a core technology, other scattering, dynamics and computational science developments were presented at the Symposium. A total of 126 participants, with many young scientists and PhD students, from 12

countries took part. The speakers included one Nobel Lecture by Joachim Frank, three Plenary Lecturers (Ian Wilson, Yoshinori Fujiyoshi and Stephen K. Burley), 19 invited speakers, 13 selected oral speakers, 1 sponsored session speaker and 49 poster presentations. Scientific session topics included MX facilities, macromolecular crystallography, cryo-TEM (including single-particle analysis and microED), software and databases, and drug discovery research. High-school students also attended the Nobel Lecture session and gave poster presentations in the symposium, which were of a delightful high quality and with the presenters asking probing questions of the visitors to their posters. Three lunchtime seminars were held and sponsored by JEOL, Bruker and Thermo Fisher Scientific.

A very sad context to the meeting was the death of our close colleague Professor Nobuhisa Watanabe, who died from leukemia on 26 March 2019 at the age of 57. The opening session of ISDSB2019 was dedicated to him and we highlighted his scientific achievements in protein crystallography and beamline instrumentation. An image of him and his work has been chosen to illustrate this special issue. Marking Nobuhisa's memory stimulated us all to focus on the natural living organism and its preferred temperature and pressure.

The symposium was supported jointly by the 169th Committee of the JSPS and by many industrial companies as well as generous individuals. We also wish to express our sincere thanks to the University–Industry Cooperation and Research Program Division of the JSPS, to Osaka University, and to all companies and persons who contributed their donations and cooperation.

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COMMENTARY

Deep neural networks in real-time coherent diffraction imaging



Figure 1. A machine inspects a coherent diffraction pattern and directly forms an image of the sample in its mind. Adapted from Shutterstock image 732725557 by Phonlamai. https://www.shutterstock.com/image-illustration/3d-rendering-artificial-intelligence-brain-ai-732725557

Ross Harder

X-ray imaging methods have progressed rapidly at modern synchrotron light sources owing to the highly collimated, bright, tunable X-ray beams available at them. Included in these advances are high-speed micro-tomography and nanoscale three-dimensional imaging with computed tomography (Maire & Withers, 2014).

In parallel, coherent imaging methods have become a powerful tool for nanoscale imaging of material and biological structure. When combined with tomography and scanning techniques they can achieve quantitative determination of density (Diaz *et al.*, 2015). When used in conjunction with Bragg diffraction one gains sensitivity to crystalline structure, including strain and deformations due to external stimuli (Pfeifer *et al.*, 2006).

In the Bragg diffraction case, the technique can struggle to be effective in some cases. As pointed out by Wu and coworkers in this issue of IUCrJ (Wu *et al.*, 2021), highly strained crystals and samples composed of many interfering domains can produce coherent diffraction patterns that are difficult to invert. In addition to this occasional struggle when implementing the method, fourth generation X-ray facilities such as X-ray free electron lasers (XFELs) and diffraction-limited storage rings can generate a flood of coherent imaging data (Sobolev *et al*., 2020).

Coherent imaging methods use measurements in reciprocal space, where coherently interfering beams produce an interference pattern on the detector. In the case of Bragg coherent imaging the data are acquired in the vicinity of a Bragg peak of the lattice, where typically a volume of reciprocal space is recorded to enable 3D imaging in real space, though 2D imaging from just a single slice through reciprocal space is also possible.

Central to the success of coherent imaging has been the development of iterative phase retrieval algorithms (Fienup, 1982). These computational tools invert the reciprocal space interference patterns, or diffraction patterns, to an image of the sample in real space. Generally based on both forward and inverse discrete Fourier transforms and iterated in both directions, these algorithms see varied success at converging to a reliable solution to the phase problem, sometimes depending on many algorithmic parameters and expert methods (Clark *et al*., 2015). They also rely heavily on a fine sampling of the

interference pattern in reciprocal space. As a result, the computational arrays can be large, both due to high sampling requirements in the data and the resulting over-determination of real space extents (finite support) of the object where it will be surrounded by zeros in the computational array. Since the computational cost of discrete Fourier transforms scales as the logarithm of the size of the array, one quickly reaches relatively long computational times and extensive memory requirements to retrieve an image. These computational requirements are daunting, particularly in the face of the current and future fourth generation X-ray sources like free electron lasers and diffraction-limited storage rings. At these facilities one can produce 2D coherent diffraction data at kilohertz rates or sample large 3D volumes of reciprocal space in tens of seconds.

The current computational requirements of coherent imaging, and other imaging methods, have led scientists to explore the use of modern data analytical techniques to solve problems in image analysis and reconstruction. Machine Learning (ML) methods and in particular the Convolutional Neural Network (CNN), are being used to tackle diverse challenges in X-ray data analysis, including limited angle and streaming tomography (Huang *et al.*, 2020; Liu, Z. *et al.*, 2019), and determination of space groups directly from pair distribution function data (Liu, C.-H. *et al.*, 2019). For coherent diffraction imaging, the idea (see Fig. 1) is quite simple, can a machine be trained to simply look at a coherent diffraction pattern and create, in its synthetic mind, an image of the sample? While using only modest ML tools, Wu *et al.* have shown that the answer to this question may be ‘Yes’. The key to the success of using CNNs to invert coherent diffraction patterns lies in the extent of the training data used to form the neural network. Effectively, the use of a CNN moves the bulk of the computational cost far ahead of the experiment. Using an extensive set of images and corresponding simulated diffraction patterns, the neural network is trained to build the connection between reciprocal and real space into the neural encoding.

Working in 2D with the goal to provide real-time inversion in XFEL ultrafast time resolved imaging experiments, Wu *et al*. have trained a so-called encoder–decoder CNN. Here a set of diffraction patterns have been used to develop a single encoding which is then decoded to produce both the shape and inherent deformation (encoded as phase of input complex density input into the training) of the crystal lattice (Fig. 2). Using additional simulated data to test the trained CNN they report 0.5 ms inversion time! For experimental data they found that a small number of iterations of traditional phase retrieval algorithms were required to converge to a reliable image. This was done, however, with expert-free requirements and found to be highly robust. The result of this work, and other ongoing research in the field, is that the throughput of CDI phase retrieval could keep pace with flood of data at modern instruments (Cherukara *et al*., 2018, 2020; Scheinker & Pokharel, 2020). These advances also enable the expansion coherent imaging applications into scientific realms where current inversion methods either fail or require extensive expertise.

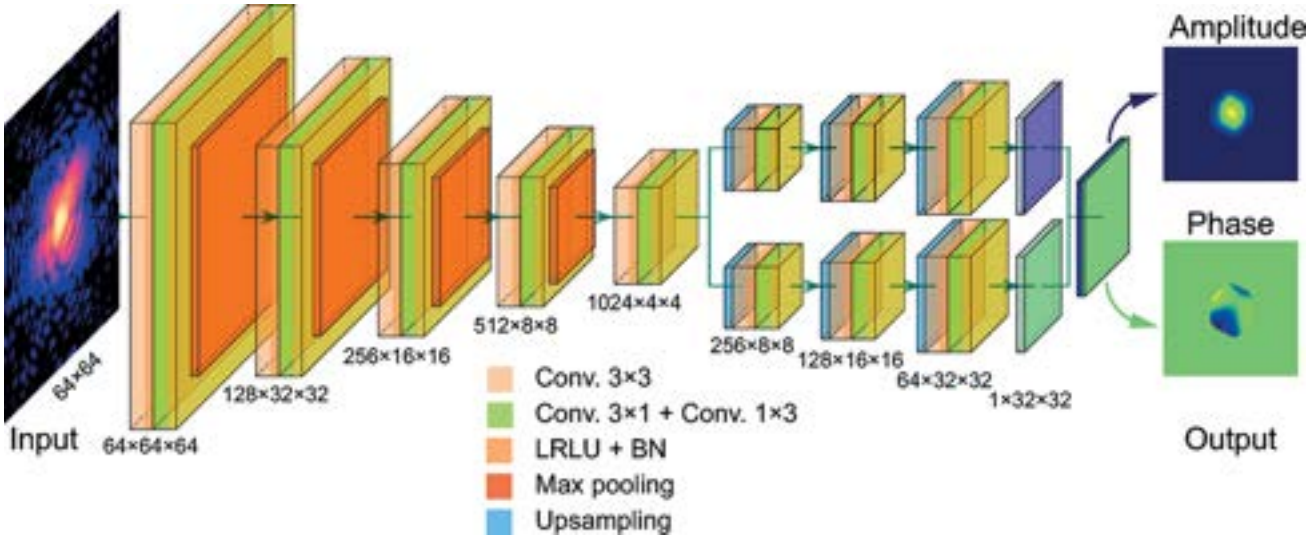


Figure 2. A schematic visualization of the deep neural network for single-particle-imaging inversion used by Wu *et al.* (2021). The neural network is implemented using an architecture composed entirely of convolutional, maximum pooling and upsampling layers. In the network, Conv. refers to convolution, LRLU refers to the leaky rectified linear unit and BN

refers to batch normalization.

With single-particle coherent scattering experiments at XFELs starting to reach significant hit rates for MHz X-ray pulse frequencies, the potential for CNNs to provide real-time imaging capabilities is just being touched. As researchers continue to expand and improve on the ML implementations, we can expect the impact of work like that of Wu and coworkers to bear significant fruit for high-resolution X-ray imaging.

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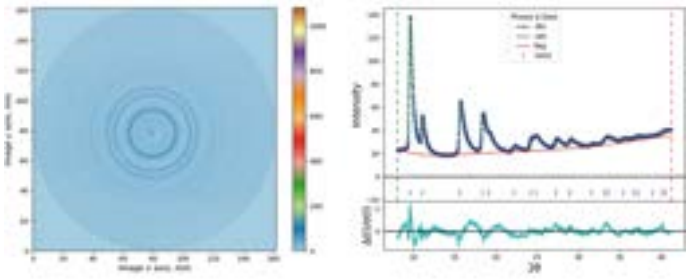
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COMMENTARY

Rietveld in 100 picoseconds



Brian H. Toby

For those of us of a certain age, collection of a data set for a crystal structure represents a major undertaking. With a single crystal and a laboratory instrument, this now requires hours, rather than days or even the weeks of my youth, and is even slightly faster with a synchrotron. From a powder sample, a diffraction data set now typically requires at least minutes and perhaps hours in the laboratory, but can be completed in a second with an area detector at a synchrotron. The structure determined is an average over the measurement duration. But an entirely new paradigm in structure determination, where a complete structural measurement is made in a tenth of a nanosecond, is demonstrated in the February 2021 issue of the *Journal of Applied Crystallography* by Robert B. Von Dreele, Samantha Clarke and James Walsh in their article *'Pink'-beam X-ray powder diffraction profile and its use in Rietveld refinement*. This is truly a new age.

To understand how this works, one must know a bit about the functioning of a synchrotron. Diffractionists tend to think of a synchrotron as a constant source of X-rays, but just as the screen you are reading this on is actually flashing at something like 60 or 120 images each second – faster than our eyes can recognize – the X-rays generated from a synchrotron flash on only while a packet of electrons travels past a bending magnet or insertion device at 99.99... % of the speed of light. The X-rays from this pulse illuminate the sample for only *ca* 0.1 ns. The synchrotron storage ring is filled with a relatively small number of electron packets, so there is a delay of 10–200 ns before the next pulse arrives. The electron pulses circulate around the storage ring and return to the same location in a few microseconds so the flashes repeat in a regular pattern. For most experiments, the on/mostly-off flashing of the synchrotron X-rays is not perceptible, no more than the much slower blinking of our room lights and computer screens. However, it is possible to use high-speed choppers and detector gating to isolate the X-rays scattered from a single electron pulse as an image on an area detector. In a normal synchrotron diffraction instrument, a perfect-crystal monochromator allows only an extremely narrow band of X-ray wavelengths to reach the sample, so few X-rays arrive at the sample and thus far too few are scattered from that pulse to be useful in a single measurement. However, at a small number of beamlines, such as the APS Dynamic Compression Sector (DCS; https://dcs-aps.wsu.edu) beamlines, the wavelength band is greatly expanded to produce what is called a pink beam, and this allows for a much larger number of photons to be measured from the diffraction of a single synchrotron pulse.

The X-ray spectrum from the DCS pink-beam monochromator is somewhat complex and one might expect this would limit the analysis of diffraction data sets only to a qualitative level of analysis. However, Von Dreele *et al.* (2021) show that quantitative Rietveld (1969) fitting to these data is possible, allowing full structural determination up to the limits allowed by the relatively poor peak resolution and signal-to-noise ratio offered by the technique. Since the X-rays are of fairly high energy, the spatial

resolution can be atomistic. Peak resolution and sensitivity will tend to limit the complexity of models that can be developed, but working around this is not a new problem in powder diffraction (*International Tables for Crystallography*, 2019).

Note that this work was greatly facilitated by one author's pioneering experience in developing analysis software for pulsed (time-of-flight, TOF) neutron diffraction (Von Dreele *et al*., 1982), which he noticed offers a similar energy spectrum, even though it arises from a completely different physical process. This demonstrates the value of scientific breadth. No one could have expected that TOF peak shapes would ever be needed at a synchrotron.

While I am far from impartial on this subject, I would also comment that this work points to the value of modern software projects such as *GSAS-II* (Toby & Von Dreele, 2013) that encompass an extended scope and are written in modern languages. While I am certain that analysis of pink-beam diffraction data was not contemplated in the initial design of the package (Toby & Von Dreele, 2007), the flexible data structures provided by Python and the open framework of the project made it a relatively easy task to support a new experiment type and its associated peak shape, despite not being part of the initial project design. This probably would have been a much more difficult task in an old-style Fortran project, such as *GSAS* (Larson & Von Dreele, 2004).

From a diffraction pattern of a state that exists for only 0.1 ns, one can imagine probing the atomistic structure of many exotic transitory chemical and physical states that might be produced in a bulk material. The synchrotron then becomes a stroboscope that freezes ultrafast motion. The interests that prompted construction of the DCS beamlines via funding from the US National Nuclear Security Administration are largely associated with the science of transient pressure spikes in a wide variety of materials, but one can also imagine a range of chemical and physical probes that will produce a rapid structural response. The work of Von Dreele *et al.* here shows that it is now possible to determine structures quantitatively under these conditions. This truly opens new frontiers for structural science. Even faster sampling is possible with free-electron X-ray lasers (FELs), but in more than a decade of FEL sources, there have been very few powder diffraction structural studies (Blome *et al.*, 2005; Freyer *et al.*, 2013; Wehrenberg *et al*., 2017). Perhaps this work will encourage more.

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COMMENTARY

Another step of the APXPS evolution taken at MAX IV synchrotron

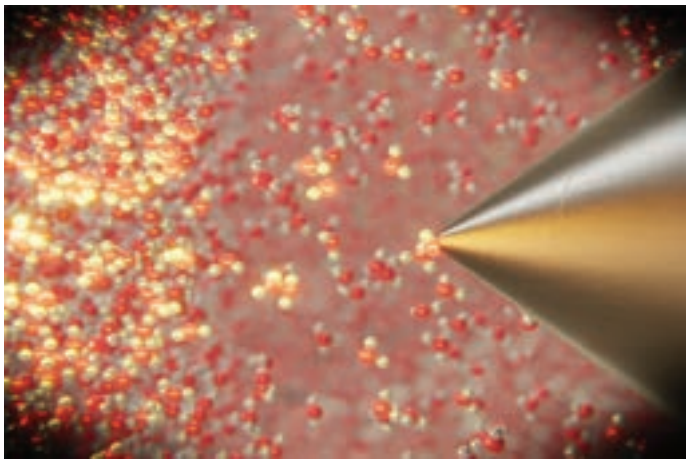


Figure 1. An artistic view of the ambient-pressure hemispherical analyzer entrance aperture in a gaseous and liquid environment. Credit: Tomas Duchon, https://micronano.net/.

Slavomir Nemšák

In the past several decades, X-ray photoelectron spectroscopy (XPS) has been established as a versatile tool to investigate chemical and electronic properties of materials. Its principle is based on a photoelectric effect, which was discovered by Hertz (1887) and explained later by Einstein (1905). However, a practical technical implementation of the technique had to wait until the 1940s, when Siegbahn *et al.* carried out their first pioneering experiments (Siegbahn & Svartholm, 1946).

XPS uses X-ray photon beams, which excite photoelectrons that are emitted from a material. Due to a strong interaction of electrons with solids, liquids and also gases, the technique was initially designed to work with solid samples under ultra-high vacuum only. Even though the early experiments on liquids performed by Siegbahn *et al.* were carried out in the 1970s (Siegbahn & Siegbahn, 1973), it was the development of modern differentially pumped hemispherical analyzers with focusing pre-lens (Figure 1) in the early 2000s that paved the way to widespread deployment of XPS systems capable of measurement under ambient pressure (typically tens of mbar) around the world (Salmeron & Schlögl, 2008).

In the paper by Zhu *et al.* (2021), a new ambient-pressure XPS (APXPS) setup installed at the HIPPIE beamline in MAX IV laboratory in Lund, Sweden, is introduced. It is a state-of-the-art system that was designed to be both modern and versatile to serve a wide scientific community. HIPPIE is an undulator beamline, which covers energies ranging from 250 to 2200 eV and provides high flux ($>10^{12}$ photons s^{-1}) even at high energy resolving powers (~10000). The upper boundary of this energy range is especially important due to the fact that it is the higher kinetic energy of photoelectrons that is needed to overcome attenuation of the electron signal in the gas or liquid environments. Simply speaking, the ability to perform XPS experiments at higher pressures relies on using higher photon excitation energies, pushing the boundaries from soft to hard X-ray excitation.

In order to cover a variety of scientific disciplines, a modular setup allows switching between two concepts: a cell-in-cell design and a backfill ambient-pressure chamber. The first focuses on solid/gas interface studies, catalysis and rapid gas reactions analysis. The second specializes in liquid chemistry and *operando* electrochemistry.

Another highlight of the instrument is the multimodal approach that includes infrared reflection absorption spectroscopy (IRRAS), which has been demonstrated earlier (Head *et al.*, 2017), but at HIPPIE is now an integral part of the experiment. The combination of the high photon flux of the HIPPIE beamline and the fast collection of the electron signal using a CMOS camera enables high-rate spectra acquisition in approximately millisecond time-scales. Apart from static-solid and liquid samples, the setup can also make use of a microjet liquid delivery. Last, but not least, the gas handling system provides automatic mixing of up to eight gases in pressures ranging from ultra-high vacuum to 30 mbar. A small volume of the cell-in-cell design allows a rapid gas exchange in a matter of seconds.

The authors demonstrate the capabilities of the newly built instrument using several scientific examples. The first is monitoring hydrogen gas intercalation under graphene flakes in real time. These time-resolved experiments show how the gas delivery system, providing a train of pressure pulses of hydrogen and oxygen gases, works together with the high spectra acquisition rate. Spectral signatures of graphene with and without intercalated hydrogen are successfully time-correlated with the arrival of hydrogen gas pulses.

Another demonstration uses a lithium/lithium cobalt oxide battery in an *in situ* electrochemical cell. The lithium cobalt oxide electrode was monitored during charging/discharging of the battery. Thanks to the chemical specificity of the APXPS, the team of authors observed a change in the oxidation state as well as electronic structure of the cobalt present in the electrode as lithium was extracted/incorporated into the electrode.

The last scientific example presented in the paper is relevant to catalytic studies. Adsorption of carbon monoxide on a platinum single crystal is studied both by APXPS and IRRAS. Combination of these two methods permitted unambiguous identification of carbon monoxide occupying bridge and top adsorption sites of Pt(111) and their population under changing carbon monoxide background pressure.

These three scientific demonstrations showcase the versatility and strengths of this newly built experimental setup at MAX IV synchrotron. The field of APXPS has undergone dramatic developments in the last two decades. Faster acquisitions, a use of multiple complementary probes and a high level of automation makes the HIPPIE facility another successful iteration in this highly evolving field and a significant achievement, which will benefit all prospective users and the scientific community as a whole.

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IUCR CONGRESS

25th IUCr Congress and its background



A pre-pandemic meeting of the local organisers of the 25th IUCr Congress at the Prague Congress Centre.

Radomír Kužel

History

Czechoslovakia was accepted into the IUCr immediately after the first IUCr Congress in Boston, MA, USA, in 1948 as the fifth member together with USA, UK, Norway and Canada. The membership of the Czechoslovak National Committee in the IUCr was guaranteed originally by Charles University; later this was taken over by the Academy of Sciences and then the Czech and Slovak Crystallographic Association (CSCA) in 2017. A “meeting of crystallographers on special topics in structure analysis” was started by A. Kochanovská in 1954 at the headquarters of the Academy of Sciences and a long series of these traditional one-day seminars was established. Originally, the meetings, called “Discussions”, were organized under the head of the Institute of Technical Physics of the Academy of Sciences, later under the head of the Czechoslovak Society for Science and Technology and finally the CSCA. In 2016, the anniversary 300th Discussions Meeting on Recent Advances in Structure Analysis was organized in Prague.

The formal recognition of the Crystallographic Association – Krystalografická společnost as a stand-alone society was achieved on 6 February 1991. The logo of the association was designed by Z. Zikmund, and variations of it have been used as logos for different meetings including the 25th IUCr Congress. The Executive Committee, headed by the president and secretary, is responsible to the Scientific Board for all activities. All bodies and officers are now elected for a five-year period. See www.xray.cz for current officers and a full list of members of the Scientific Board.

A continuous series of Annual CSCA Conferences began in 1980. At these meetings, people interested in crystallography can meet for four days and discuss informally all scientific problems and directions of future activities of the CSCA. The conference is devoted to diffraction and non-diffraction techniques and methods for structural studies of compounds, applications of diffraction methods in practice, and the use of techniques in materials science, physics, chemistry and biology. The meetings are organized in different places in Bohemia and Moravia. Besides general and broad crystallographic topics, several focused meetings are organized. Recently, these have included Experimental methods in X-ray and neutron analysis, Computational methods, Small-angle scattering and Non-diffraction techniques for structural studies. Nowadays, the conference is named Struktura xxxx including the year. The usual participation at these annual meetings is 70–100 people.

A biennial student symposium is organized as part of the annual conference. The session contains student works – BSc, MSc and PhD theses in the field of crystallography, study of structures and

microstructures mainly by X-ray and neutron techniques. Students from different universities in the Czech and Slovak Republics take part at this meeting. The presentations are evaluated by a wide committee and finally the best students are awarded.

In addition to general plenary lectures and other common contributions, sessions and highly specialized courses are usually organized in parallel for bio-crystallographers (course on protein crystallography – general, preparation of measurements and data collection, macromolecular structure refinement, precision and reliability) and people more directed to powder diffraction and materials science (course on the study of the real structure of materials, phase analysis). Courses on software are organized as well (structure databases, programs *Jana*, *Maud*, *Mstruct*, *etc*.). A course on the use of groups in crystallography was well attended, in particular.

IUCr2020

After several attempts, in 2014 we won the bid for the 25th IUCr Congress. We were looking forward to it and working hard for its preparation. We organized the workshop Current trends and future of crystallography in May 2019, connected with the meeting of the International Programme Committee. Both appeared to be very useful and we recommended such meetings also to future organizers of IUCr Congresses. Everything was going well till March 2020 when COVID-19 appeared. We found it was basically impossible to organize a classical congress in August 2020, and a quick virtual meeting of the IUCr Executive Committee unanimously decided to postpone the Congress to August 2021. This decision was accepted basically by all already registered people and companies with frequent comments that in 2021 people may be even more eager to attend the congress. However, at that time I was already thinking that we may only be postponing the problem.

Struktura 2020

Because we were organizing such a big congress in 2020, we did not plan to hold Struktura 2020. However, when the Congress was postponed we returned to it and decided to prepare Struktura 2020 for the end of November, when, we all hoped, the situation with COVID should have stabilized. Moreover, we did not expect a participation of over 100. The limit for indoor events was varying over time but in summer was as high as 500 so we did not expect problems. We agreed on the venue – a hotel in Tabor, a beautiful historical town about an hour's drive south of Prague – for two reasons. Struktura 2016 was held there, where we had a very good experience with the hotel and location, and the venue was also that planned for the largest pre-IUCr Congress workshop on electron crystallography.

Unfortunately, by the time we reached September, the pandemic was not decelerating but *vice versa*. At that time, it was decided to organize a hybrid congress from the hotel with the possibility for remote participants. We purchased better equipment such as cameras and sound systems and started preparation. We kept that idea till the beginning of November when it became clear that no real meeting would be allowed and possible and the only way was to prepare for a purely virtual conference. Before that point, we had already asked participants for their opinion. Most of them approved both real and virtual participation. Some of them said "No, I am only interested in a real meeting, not a virtual one“ and cancelled their participation. A few cancelled their lectures but approved their virtual passive participation. Others decided not to come to Tabor but were able to give a virtual lecture. In the end, we had about the same number of people as expected for a real conference (about 70).

We decided to host the virtual meeting on the Zoom platform as this was widely used and well known. We prepared a small TV-like studio center in one seminar room of Charles University, where a few presentations were given. The conference (25–27 November) had a few sessions as planned, for example on the use of synchrotron radiation, and it also included the first virtual student symposium and competition. In this competition, the main evaluation takes in a complex picture (scientific significance, contribution of the student, presentation quality, impression given by the speaker); however, just for interest, we evaluated the presentation skills of the speaker separately, *i.e.* how he/she is able to sell their work, almost regardless of the content. It was expected that in virtual form, these features would be

suppressed. However, just the opposite was found, surprisingly. It seems that these skills are also important for virtual presentations. At the end of each day, the Zoom meeting remained open for 1–2 hours for free discussion.



So, our first virtual conference went very well, even though the participants expressed their hope to meet in person next time. The organization was quite easy and low cost. There were no technical problems. All the lectures were available from recordings in the Zoom cloud for registered participants for two months and then they were downloaded to our local storage media.

IUCr2021

In January 2021, we resumed communication with the IPC, keynote speakers, co-chairs and invited speakers in sessions to find out their plans.

The overall situation with COVID is very complicated. At the moment nobody knows anything definite about this summer. Currently, we cannot guarantee whether we will be allowed to organize the Congress in the Congress Centre or, if so, under which specific regulations. People don't know if they will be able to come. Therefore, we have started to prepare the Congress as primarily a virtual one but we would like to keep open the possibility of a real part till the last possible moment, *i.e.* we are retaining the idea of hybrid congress. The time when, I think, we can know more should be in June but not much earlier.

Up to now, we have received answers from about two thirds of the people mentioned above with the following statistics:

About 40% of people are still going to travel to Prague, if possible.

About 15% of people plan to do the same, but they see more problems.

About 15% of people would also like to come but think that it is not very likely.

About 25% cannot come but approved virtual participation.

Actually all the above approved virtual participation.

About 5% had to cancel their participation.

Hybrid system

Recently, we revisited the Prague Congress Centre, mainly to see their registration and presentation system for real/hybrid/virtual events and we were all quite happy with its flexibility. The local Czech company has been developing it for more than 10 years, has used it for even larger conferences than the IUCr Congress and during the last year, has focused on improving and extending the features for virtual or hybrid types of events and used it for such meetings. Over time, they have removed some things/features that had the potential to cause technical and/or quality problems. The system offers several types of virtual rooms (sessions, workshops, meetings) and a wide range of "poster" presentations, which can include videos, *etc*. Companies can have space on the website in the form of a 2D or 3D virtual booth, which allows the inclusion of descriptions, photos and videos and the possibility of multiple chats with individual customers. Every visit to the booth is recorded, with the list of visitors being sent to the exhibitor immediately after the event. Nothing anonymous is allowed.

Sessions

In principle, there is not much difference if the speakers or chairs are on-site or remote. The system does not require any installation of special software by the participants. Several browsers are supported. Two weeks before the lecture, registered participants can post questions in the lecture's Discussion window, which the speaker can answer there at any time. As a typical example, a participant can ask if some problem will be discussed in the lecture.

Individual speakers can communicate with technicians and must upload either a full pre-recorded presentation including sound (this could be useful, for instance, when there is a time difference; these types of presentations are now easy to prepare, *e.g.* in PowerPoint) or just a pure presentation. Everything can be tested.

A short time before the session all speakers and co-chairs of the session can communicate live in real time.

The session is streamed for remote participants. The presentations are always run from the local server in Prague. This is to avoid the possibility of a lower quality connection from the speaker. However, if the speaker is online, he/she has full control of the presentation. During the lecture any participant can type questions into the corresponding Chat window, which is visible by all participants (which helps to avoid duplicate questions). The moderator/co-chair selects questions from the Chat and asks the speaker in the discussion. This discussion is also recorded. No anonymous comments are possible.

Any remaining questions can be moved by the speaker from Chat to Discussion and answered any time later. Both Discussion and Chat windows are accessible all the time but the Chat window is only active during the session. The lectures can be made available for registered participants for two months without extra cost. Different kinds of "rooms" are possible. For workshops, the set-up is similar to Zoom. Anybody can share screens, all participants can be seen.

All the tools for a hybrid congress have been prepared. However, now we can only wait and hope for a successful vaccination program to suppress the spread of the virus.

Radomír Kužel is CSCA Secretary and IUCr25 Chair.

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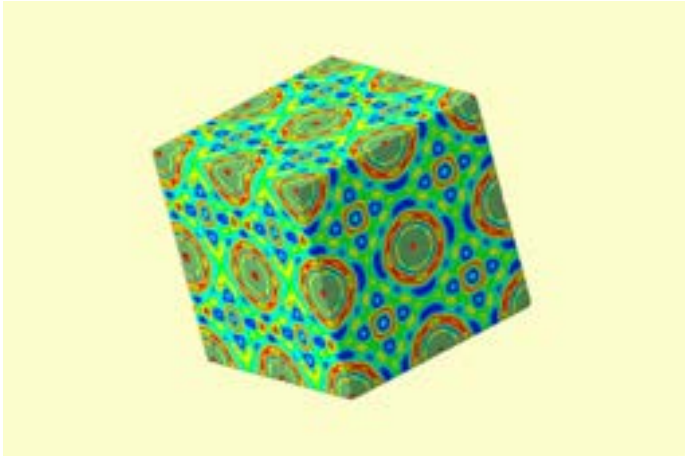


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FEATURE ARTICLE

Quantum mechanics and crystallography: inextricably linked in quantum crystallography



Piero Macchi

In recent years, the name *quantum crystallography* has suddenly entered the scientific jargon. It primarily deals with the application of quantum theory in crystallography, a connection that requires a historical review to be fully appreciated. In fact, the symbiosis between quantum physics and crystallography should not surprise us because the two fields have been tightly entangled since the first applications of X-ray diffraction from crystals that were contemporary with the coming of the quantum age.

Many crystallographers probably ignore the fact that W. L. Bragg gave the inaugural talk at what is remembered as the most famous conference in the history of science, the Solvay Conference on Electrons and Photons (1927), a meeting where the theoretical framework of quantum mechanics was eventually established, merging points of view from different schools of thought. Bragg attended the congress because the development of the X-ray diffraction technique had attracted the particular attention of the quantum physicists, eager to find experimental evidence for the electronic structures of atoms. As a reminder, in 1913, the atomic model in vogue was the incorrect Bohr atom, while physicists were in search for an advanced model complying with the growing complexity of quantum theory. Soon after the first X-ray diffraction experiments were reported, P. Debye wrote: "It seems to me that the experimental study of the scattered radiation, in particular from light atoms, should get more attention, since along this way it should be possible to determine the arrangement of the electrons in the atoms" (Debye, 1915). At the same time, Compton (1915) wrote that "It is hoped that it will be possible in this manner [through X-ray diffraction] to obtain more definite information concerning the distribution of the electrons in the atoms." Thus, it was not unexpected that, close to the fathers of quantum theory (like Bohr, Born, Curie, Dirac, Einstein, Heisenberg, Pauli, Planck and Schrödinger), at the Solvay Conference sat a number of crystallographers, like Bragg, Brillouin, Compton, Debye and de Broglie. The last was sceptical in defining himself as a crystallographer. Still, he actually used crystals to prove the wave nature of electrons, although crystallographers normally use radiation to reveal the inner nature of crystals. Thus, de Broglie definitely deserves to be considered as a crystallographer and indeed a quantum crystallographer. I take the occasion in this article to request that also Compton be included in the IUCr website list of crystallographers who won the Nobel Prize, because he is, surprisingly, excluded. [Note from the IUCr: we thank the author for bringing this omission to our attention; this has now been rectified: https://www.iucr.org/people/nobel-prize.] Compton contributed enormously to the Solvay Conference's success and was probably the most representative scientist linking the worlds of quantum

mechanics and crystallography. In his book *X-Rays and Electrons*, Compton (1926) proposed the first comprehensive quantum theory of X-ray scattering, and Compton scattering is at the heart of electron-density determination in momentum space.



Participants at the 1927 Solvay Conference. Photo: Wikimedia Commons.

Conversely, the *new* crystallography (the one born after the development and application of the X-ray diffraction technique) took enormous advantage of the models derived from quantum mechanics. The above-mentioned quantum theory of scattering is the paradigm to interpret the X-ray intensities and provides the key to opening the lock of crystal-structure solution. In fact, once the correct atomic model was eventually developed, quantum chemical calculations provided accurate atomic form factors, those that are used daily for crystal-structure determinations and refinements.

The period 1913–1930 witnessed the beginning of what I called the *connubium* between crystallography and quantum mechanics in a recent review article (Macchi, 2020). The empathy between scientists of the two communities is the beginning of a huge array of fundamental studies. In fact, Debye and Compton's premonitory statements implied that through X-ray diffraction, we could detail electrons' behaviour in matter, not just the electronic structure of atoms. This means revealing the electron distribution in molecules, polymers, salts, *etc.* However, a realization of this purpose was not possible, at least until accurate data and appropriate models became available. In the early days of X-ray crystallography, one seminal exception was the study by W. H. Bragg on diamond (Bragg, 1921), who revealed the occurrence of scattered intensity for a symmetry-forbidden reflection, the famous 222 reflection. Although it is likely that Bragg mainly measured multiple scattering intensity (Coppens, 1997), his observation was anyway correct. It proved that atoms are not spherical inside a crystal, especially if linked to other atoms through covalent bonds. This was probably the first example of a crystallographic investigation on the nature of a chemical bond.

For many years, however, it was impossible to go much beyond this empirical evidence that chemical bonds, which are *not* quantum mechanical observables, leave measurable fingerprints in the electron-density distribution and, correspondingly, in X-ray diffraction. A breakthrough occurred in the late 1950s, when R. J. Weiss determined the electronic configuration of some metals through X-ray diffraction (Weiss & De Marco, 1958), a quite complicated task and challenging still today. In fact, the deviations from the conditions of validity of the kinematic approximation of X-ray diffraction (quite common for almost perfect crystals) were a significant issue, as admitted by Weiss in his autobiography (Weiss, 2007). Nevertheless, the attempt to break down the atomic scattering into orbital contributions and test different electronic populations for each shell was a terrific breakthrough that eventually gave rise to the field of X-ray charge-density analysis (for a comprehensive review, see Tsirelson & Ozerov, 1996; Coppens, 1997).

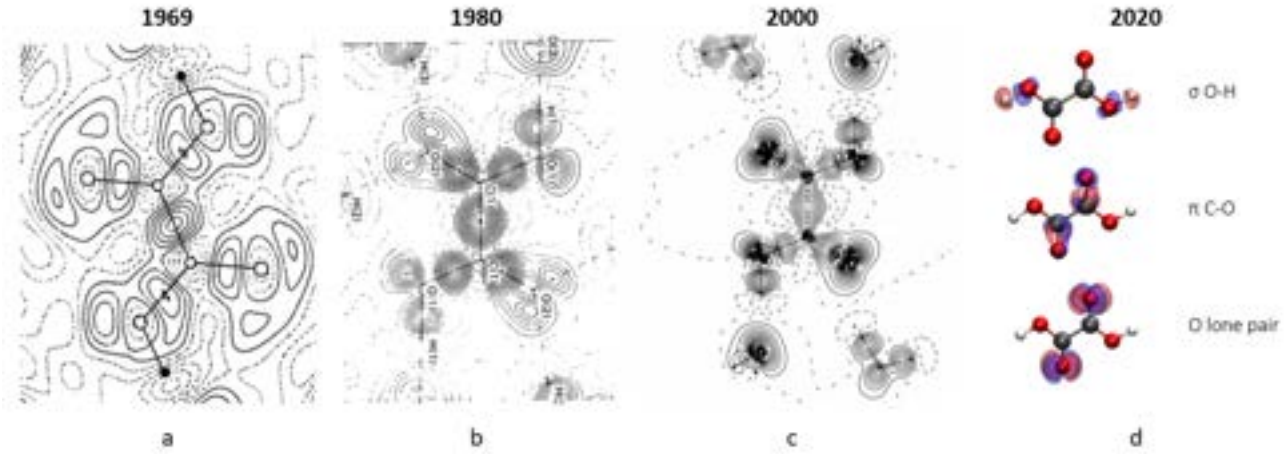


Figure 1. Oxalic acid dihydrate in quantum crystallographic studies over the years. (*a*) The experimental *X–N* deformation density map obtained by using the X-ray diffraction structure factors and subtracting the structure factors computed with the independent-atom model from the geometry determined by neutron diffraction (plot modified from Coppens & Sabine, 1969); (*b*) the deformation density map obtained with a multipolar model (from Stevens & Coppens, 1980); (*c*) the deformation density map obtained from the X-ray restrained Hartree–Fock calculation (Grimwood & Jayatilaka, 2001); (*d*) the main molecular orbitals calculated with X-ray restrained extremely localized molecular orbitals (modified from Ernst *et al.*, 2020).

An even bigger challenge launched by Weiss was the possibility to calculate a wavefunction using X-ray diffraction, combining the elastic Bragg and the inelastic Compton scattering. In his book *X-ray Determination of Electron Density Distributions*, Weiss (1966) proposed to use X-ray diffraction to correct wavefunctions calculated at the Hartree–Fock level, a method that ignores the correlation between electrons. The intuition by Weiss corresponds to a kind of perturbative method, where the wavefunction, calculated from first principles, is a zero-order approximation. In contrast, the X-ray diffraction measurement is the perturbation that enables corrections for the electron-correlation effects. Weiss's suggestion stimulated the work of many scientists in the following decade. However, a determination of the wavefunction coefficients directly from X-ray intensities was very complicated (Coppens *et al.*, 1970; Bentley & Stewart, 1973; Stewart *et al.*, 1975). Even more complicated was the determination of the electron-density matrix elements, as attempted by Clinton and coworkers (Clinton *et al.*, 1969; Clinton & Massa, 1972; Clinton *et al.*, 1973).

Instead, Stewart, Coppens, Hirshfeld, Kurki-Suonio and their co-workers tackled the difficult task of refining wavefunction coefficients from X-ray diffraction and developed simplified models, like the popular *multipolar model* (Hansen & Coppens, 1978), which followed from the original work by a famous quantum chemist, Roy McWeeny (1951, 1952, 1953, 1954) who first proposed aspherical atomic scattering factors. The multipolar model maintains some features of the *independent atom model*, which is the standard model adopted for conventional crystal-structure solutions and refinements. These

common characteristics are as follows: the electron density is expanded as a sum of atomic terms; the thermal motion is simulated with independent atomic oscillators; the atomic electron densities are assigned to the atomic thermal parameters and are constant along with the nuclear displacements. However, the multipolar model introduces important corrections and extensions: the atomic electron densities are no longer spherical; the atoms are not necessarily neutral; the atomic electron density shells are free to expand or contract. The conceptual similarity with the traditional model attracted the interest of many crystallographers, who established a lively charge-density community, closely related to the community interested in spin electron-density distribution (typically obtained with polarized neutron-scattering experiments) and electron density in momentum space (obtained from Compton scattering experiments).

The idea to calculate a wavefunction based on X-ray diffraction intensities was not abandoned and significant research involved J. Karle (Nobel Prize for the introduction of direct methods into crystallography) and L. J. Massa (Massa *et al*., 1995). In this respect, another important breakthrough occurred when Jayatilaka (1998) proposed a method to restrain the theoretical wavefunction, calculated with traditional quantum-mechanical methods, to the measured X-ray diffraction intensities. Jayatilaka's approach followed a prescription by Mukherji and Karplus (1963), who proposed to calculate molecular wavefunctions constrained to some experimental data like the dipole moment measured in some spectroscopic experiments. This strategy was perfect for testing the validity of the earlier proposal by Weiss if the observations to use as constraints or restraints for the calculations are the X-ray diffracted intensities. Several emerging methods were proposed after this significant breakthrough, like the X-ray restrained extremely localized molecular orbital method (Genoni, 2013) or the relativistic X-ray restrained wavefunction approach (Bučinský *et al*., 2019). The quite popular Hirshfeld atom refinement (HAR; Jayatilaka & Dittrich, 2008) also derives from this stream of research, although there is no direct restraint on the theoretically calculated wavefunction to the measured X-ray diffraction intensities. HAR is also an extension of another branch of research that uses predetermined aspherical form factors, stored in databanks from experimental measurements (Domagala *et al.*, 2012), from theoretical calculations (Dominiak *et al*., 2007; Kumar *et al*., 2014) or calculated *ad hoc* (Dittrich *et al*., 2006). In HAR, the main improvement with respect to database approaches is the recursive nature of the calculation, which is reiterated at each cycle of the structural refinement.

Despite the growing interest in wavefunction-based approaches, the multipolar model has not lost its appeal and was recently used for the combined refinement of charge and spin electron densities, a work pioneered by Becker & Coppens (1985) and improved by Deutsche *et al.* (2012, 2014), or to describe core deformations (Fischer *et al*., 2011).

Quantum crystallographic approaches develop at a rapid pace and one can envisage progresses correlated with electron diffraction (Gruza *et al*., 2020), with spectroscopic techniques (like NMR, see for example Macchi *et al*., 2017) and with surface microscopies (Welker & Giessibl, 2012). The applications to solve chemical problems, and especially the chemical bonding puzzle, play a central role in the current literature (Gatti, 2005; Stalke, 2011, 2016). More applications and detailed background will be described in upcoming books and pamphlets (Macchi, 2021; Massa & Matta, 2021; Macchi, 2022).

This field will always follow the roadmap traced by W. L. Bragg (1922): "Finally, there is a still deeper application of the X-ray analysis, to the structure of the atom itself. Since the wavelength of the X-rays is less than the "atomic diameter," as it is somewhat vaguely termed, and since the rays are presumably diffracted by the electrons in the atom, we ought to be able to get some idea of the distribution of these electrons in the same way that we draw conclusions as to the grouping of the atoms. […] The whole subject bristles with difficulties, and the assumptions on which the theory of reflexion rests have not been exhaustively proved. On the other hand there seems to be a prospect that the method will prove a valid way of testing various models proposed for the atom, since the way, in which these models should diffract the rays, can be calculated, and compared with that which is actually observed."

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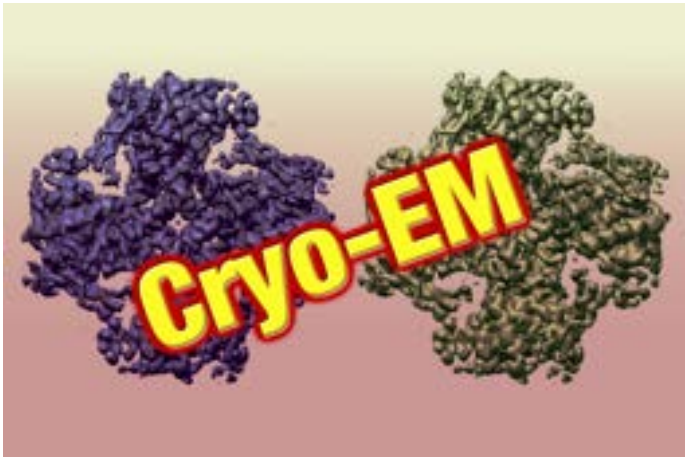
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FEATURE ARTICLE

Cryo-EM: expanding the reach of structural biology



Catherine L. Lawson

Electron cryo-microscopy (cryo-EM) is rapidly becoming the method of choice to elucidate many important 3D structures in molecular and cellular biology, expanding the reach of structural biology well beyond materials that can be crystallized. I provide below a very brief summary of how we arrived at this point. The timeline described here follows in part a more extensive review that will shortly be published as part of a special collection celebrating the 50th anniversary of the Protein Data Bank (PDB) (Chiu *et al.*, 2021).

EM scientists began investigating the overall shapes of biological materials in the mid-20th century. Early successes involved specimens with high internal symmetries – 2D periodicities, icosahedral viruses and helical assemblies. Symmetry enables averaging over many individual imaged subunits to obtain a final 3D reconstruction (density map). Experimental measurements typically include both electron diffraction (spots or layer lines) and direct images (for phasing). The 1982 Nobel Prize in Chemistry recognized the development of electron crystallography (Klug, 2010).

Minimizing radiation damage of biological materials on exposure to high-energy electrons was a major technological challenge. Early strategies involved low-dose exposure procedures and chemical embedding. Methods to vitrify and maintain specimens at cryogenic temperatures began to be developed in the mid-1970s, leading to substantial improvements in the collected data quality (Baker & Rubinstein, 2010).

The first 3DEM Gordon Research Conference was held in 1985 (see photo archived at https://www.ebi.ac.uk/pdbe/emdb/genealogy.html). The inaugural meeting, chaired by Wah Chiu, firmly established cryo-EM as a serious endeavor with a dedicated community of research scientists. The 3DEM GRC continues to play a critical role in sharing recent developments in the field. Meetings are held annually (outside of pandemics) with venues alternating between the US, Europe and Asia.

The 1990s and 2000s yielded many technological innovations, gradually increasing cryo-EM's overall impact (Henderson, 2004). Microscopes with field electron gun sources became common in academic laboratories, yielding improved image signal-to-noise and spatial resolution. Keen interest in asymmetric (*e.g.* ribosomes) and lower-symmetry complexes (*e.g.* chaperonins) sparked the intensive development of single-particle reconstruction methods. Tomographic and sub-tomogram averaging methods were developed, enabling investigations of *in situ* materials in cellular and tissue samples such as muscle fibers. Software developers created packages that automated data collection, image classification and reconstruction. Some embraced electronic CCD detectors for their ability to automate data collection, but

film still continued to be prized for its high sensitivity.

Crystallography and cryo-EM studies started to be combined in complementary ways. A common approach was to fit high-resolution crystal structures into low-resolution maps of large macromolecular complexes. Alternatively, low-resolution cryo-EM maps could provide critical phasing information for crystal-structure determination.

In this period, cryo-EM results were appearing with increasing regularity in the scientific literature. The community recognized a need to archive 3D reconstructions (density maps) and make them publicly accessible. The Electron Microscopy Data Bank (EMDB) was established in 2002 by Kim Henrick at the European Bioinformatics Institute (EBI) for this purpose. Soon after, and with input from many cryo-EM experts, Henrick and Helen Berman (Research Collaboratory for Structural Bioinformatics; RCSB PDB) spearheaded the development of a dictionary of data terms for cryo-EM experiments that could be utilized by both the EMDB and the PDB. In 2006, an NIH-funded international project was founded by Chiu, Henrick and Berman to provide a one-stop-shop for deposition and access to cryo-EM data and to serve as a community resource for news, events, software tools, data standards, challenges and validation methods [*EMDataResource* (Lawson *et al*., 2020)].

Seven years ago, cryo-EM had its famous “resolution revolution” (Kuhlbrandt, 2014). A key innovation was the introduction of new direct electron detectors with improved sensitivity and high speed, permitting the collection of movies. Post-imaging alignment of movie frames enabled researchers to overcome the previous limitations arising from specimen drift, yielding maps with much higher levels of structural detail (Fig. 1). Cryo-EM scientists have also learned how to computationally separate different classes of particles measured within the same set of images, yielding multiple reconstructions that can differ in composition and/or conformation. These innovations have substantially extended the reach of cryo-EM across a wide variety of specimens that are not readily crystallized (Fig. 2). The rapidly rising profile of cryo-EM in structural biology was internationally recognized by the 2017 Nobel Prize in Chemistry.

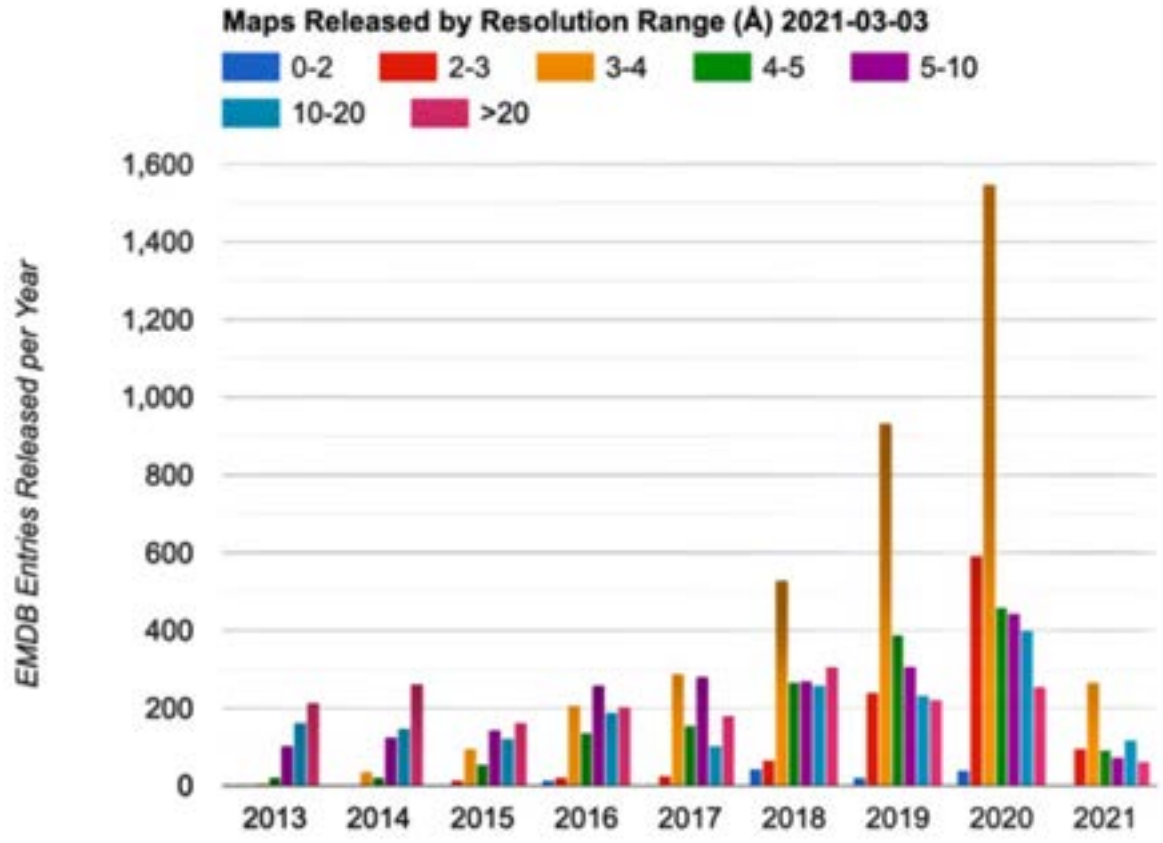


Figure 1. Shifting resolution profiles for cryo-EM maps archived in EMDB, plotted by map release year. The 2021 data are through 3 February. Source: https://www.emdataresource.org/statistics.html

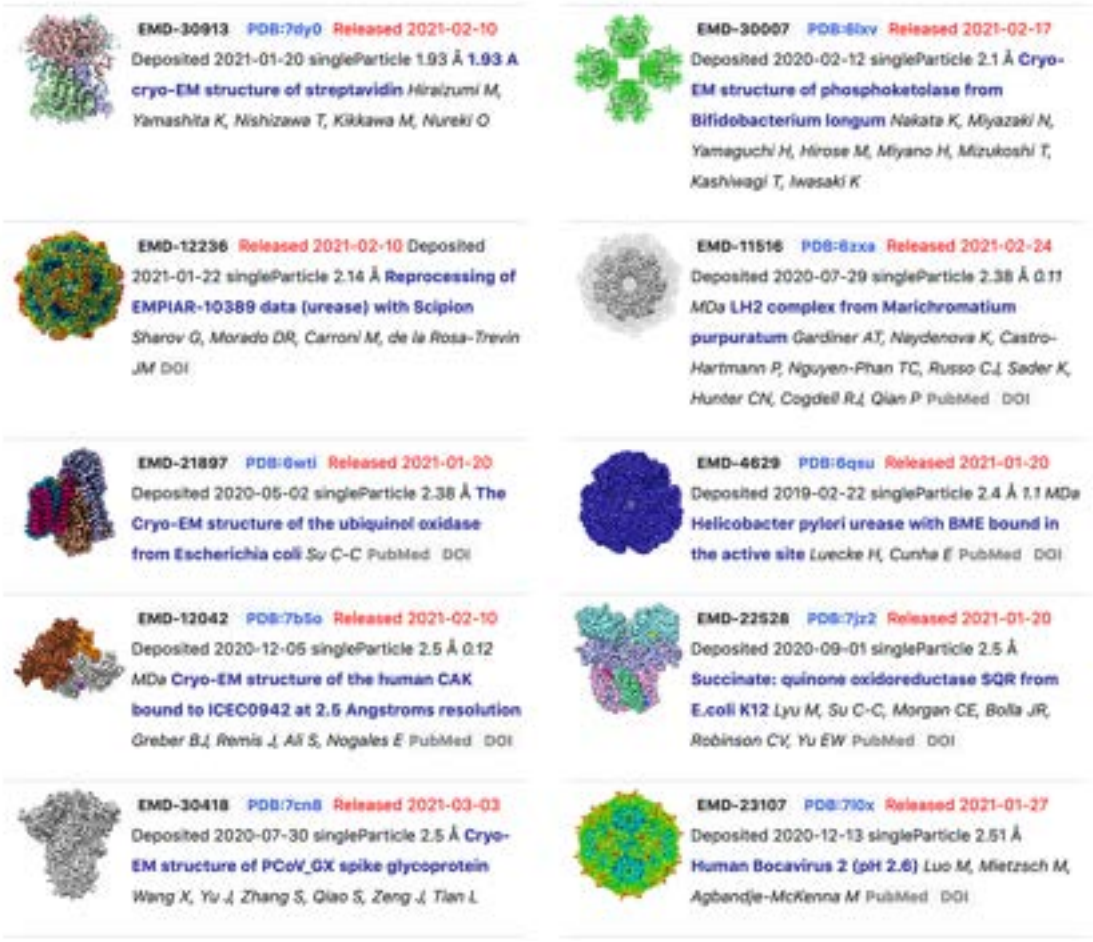


Figure 2. Sampling of cryo-EM maps recently released in EMDB. Maps include several membrane-bound and soluble enzymes, a light-harvesting complex, a coronavirus spike glycoprotein and an icosahedral virus. Source: https://www.emdataresource.org/emdlist=released:2021

The recent pandemic has demonstrated the growing utility of cryo-EM. Important structural data about the circulating virus was produced very early on, with the first SARS-CoV-2 spike glycoprotein structure released on 26 February 2020 (Wrapp *et al.*, 2020). A year later, more than 270 spike-containing map entries have been archived in the EMDB, representing the trimer, either alone or in complexes with antibody or receptor fragments. More than 60 maps are also available for other SARS-CoV-2 virus components such as polymerase and ribonucleoprotein.

In this rapid growth phase of cryo-EM, it is necessary to establish rigorous methods to validate the maps and associated models. *EMDataResource* promotes public awareness of this necessary step in structure determination, as is done in crystallography by sponsoring regular community Challenge activities and organizing and participating in community Task Forces (Lawson *et al.*, 2020, 2021; Chiu *et al.*, 2021).

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Catherine L. Lawson is at the EMDataResource Project, Institute for Quantitative Biomedicine, Rutgers, The State University of New Jersey, USA; cathy.lawson@rutgers.edu.

IUCr Journals have long championed the inclusion of research using techniques that complement crystallography, and recognised the spectacular growth in the adoption of cryo-EM by launching a new section of IUCrJ in 2016. *Acta Cryst. D* regularly publishes the proceedings of the Collaborative Computational Project for electron cryo-microscopy (CCP-EM) Spring Symposium, and together with *Acta Cryst. F* welcomes articles on cryo-EM as well as studies using other structural biology techniques.

SPECIAL REPORT

The ESRF-EBS (Extremely Brilliant Source) is online!



Harald Reichert

After installing the first fourth-generation high-energy synchrotron radiation source in 2019 and commissioning in 2020, significantly shortened by the effects of the COVID-19 pandemic, the ESRF is now back with its new Extremely Brilliant Source (EBS) serving the international community of crystallographers with a performance exceeding expectations right from the start. The goal in terms of injection efficiency, emittance, beam current, lifetime and mean-time-between-failures have all been reached or surpassed. A recent example is shown in the synopsis in Fig. 1.

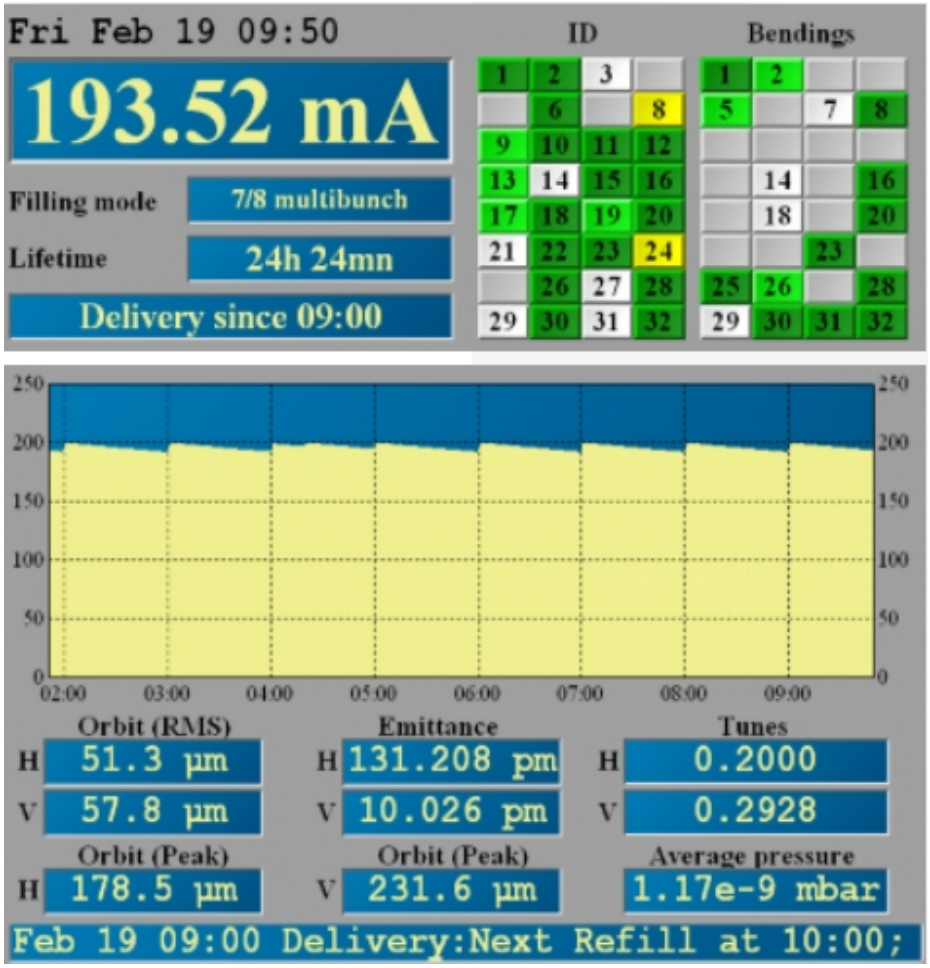


Figure 1. Synopsis of EBS operation.

Core techniques for the crystallography community, such as macromolecular crystallography (MX) for structural biology or powder diffraction, are strongly benefitting from both the dramatically improved source performance as well as numerous upgrades in beamline instrumentation (optics, sample manipulation, detectors). New and previously more exotic techniques, such as crystallography employing the full 3D reciprocal space or spatially resolved crystallography (XRD-CT, PDF-CT), should become routine with this largely improved set of tools for the X-ray crystallographer.

Structural biology

The smaller, much brighter X-ray beams provided by ESRF-EBS are a double-edged sword as far as MX experiments are concerned. Coupled with appropriate detector technology, robotics and automation, the EBS X-ray beams of the six ESRF MX beamlines provide much faster ‘routine’ oscillation data from smaller single crystals and, at the same time, allow a finer sampling when searching for the diffraction ‘sweet spots’ of larger crystals. Both aspects improve signal-to-noise ratios and throughput for a wide range of projects, including those aimed at structure-based drug design. Conversely, increased flux densities call for proper experiment design to deal with radiation damage in single-crystal MX, which is now becoming even more critical than it was before.

For very small crystals, even proper experiment design does not allow for the collection of complete diffraction data sets of a sufficient resolution for meaningful structure analysis. Here, serial crystallography is the saviour. Synchrotron serial crystallography (SSX) experiments – inspired by serial femtosecond crystallography (SFX) developed at X-FEL sources – will become increasingly common, as will multi-crystal data collection (MXD) techniques. For the latter, small, partial oscillation-based data sets collected from 10s to 100s of crystals are combined to produce the final data set.

ESRF-EBS will also help to nurture and develop the current renaissance in time-resolved MX, which aims at the structural analysis of biological macromolecules while they are in action. While much of this will be based on SSX techniques (TR-SSX), studies exploiting serial oscillation crystallography (TR-SOX, see Fig. 2) will also become more prevalent, building on recent advances made at the ESRF. TR-SSX, TR-SOX and even TR-MXD experiments are the domain of a new beamline under construction as part of the EBS upgrade project. This new MX beamline, coming online in 2022, will provide up to 10^{16} photons/second in a spot of approximately 1µm diameter. This will be (by far) the most brilliant resource for MX at a synchrotron source, both complementing and exceeding the capabilities available at ID09.

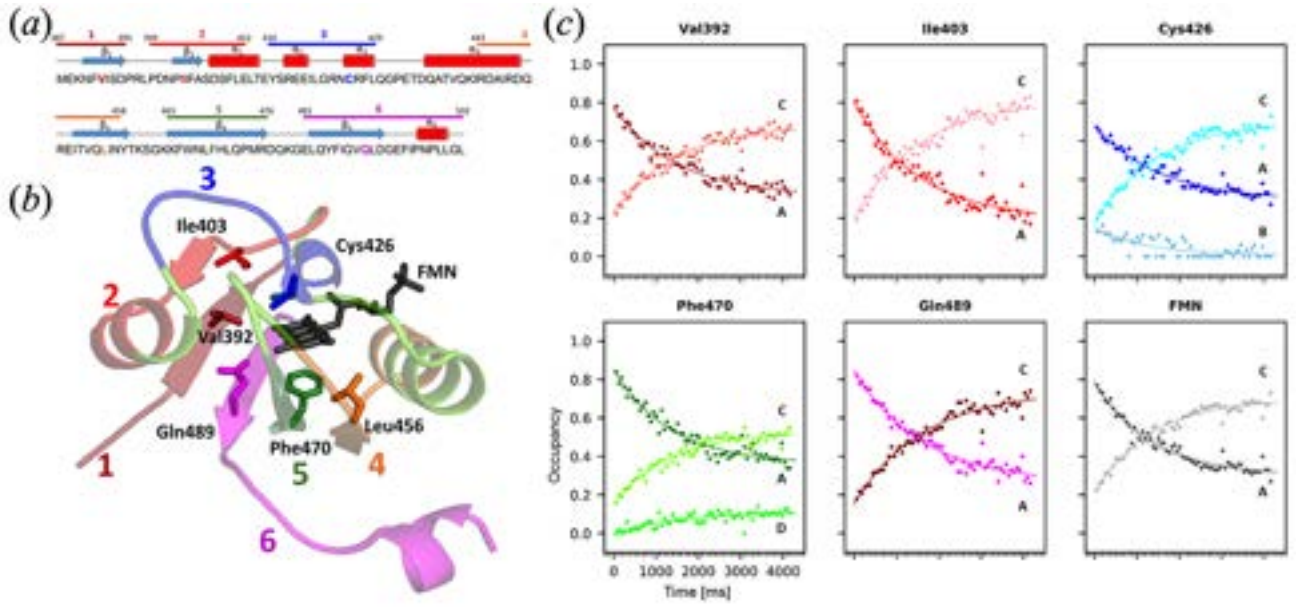


Figure 2. Results from a TR-SOX study of the activation mechanism of *At*Phot2LOV2: time evolution of the relative occupancies of key residues upon blue-light illumination. For more information, see Figure 5 by Aumonier *et al.* (2020).

Powder diffraction

Beamline ID22, the ESRF's flagship for high-resolution powder diffraction, benefits from a strongly increased incident flux from its new in-vacuum undulator, especially at higher energies, and the upgrade of the detector system. A new set of 13 analyser crystals coupled with a spatially-resolving pixel array detector (DECTRIS Eiger2 X CdTe 2M-W) provides increased resolution and counting statistics by controlling the horizontal dimension of the signal integration box from each of the 13 crystal analysers. This leads to a more symmetric peak shape and improvement in overall angular resolution while exploiting at the same time a wider integration box at higher angles for improved counting statistics and reduced data acquisition time. Other advantages include the reduction in parasitic scattering or the filtering of very bright pixels produced by large grains or single crystals in the sample, thus improving the powder average. In the future, one might even exploit the single-crystal signals for further refinement of structural models or reach a high degree of depth resolution through the sample. Upon removal of the analyser crystals, the detector also enables highly efficient collection of high-quality, lower-resolution data for techniques such as PDF analysis. Overall, an increase of an order of magnitude in performance is calling for exploitation by the community of X-ray crystallographers.

Structure refinement from 3D reciprocal space data

Much information on the detailed atomic structure of materials, including their defects and local static and dynamic variations, is encoded in the scattering in 3D reciprocal space between the reciprocal lattice nodes employed in single crystal or powder diffraction. The ESRF operates a dedicated endstation on beamline ID28 optimized to study diffuse scattering (DS) throughout the entire reciprocal space, which is coupled to a high-resolution inelastic scattering instrument for the study of thermal excitations. The analysis of DS in 3D reciprocal space provides information on both static (elastic scattering) or dynamic deviations (inelastic or quasielastic scattering) from the long-range-ordered average structure (see Fig. 3). DS studies are particularly efficient when coupled with spectroscopic investigations and theoretical models. Specifically, a fast mapping of reciprocal space prior to an inelastic X-ray scattering (IXS) experiment allows the identification of regions of interest, which can then be explored in more detail by energy-resolved measurements. This concept can be successfully applied to a large range of materials ranging from soft organic crystals to strongly correlated systems.

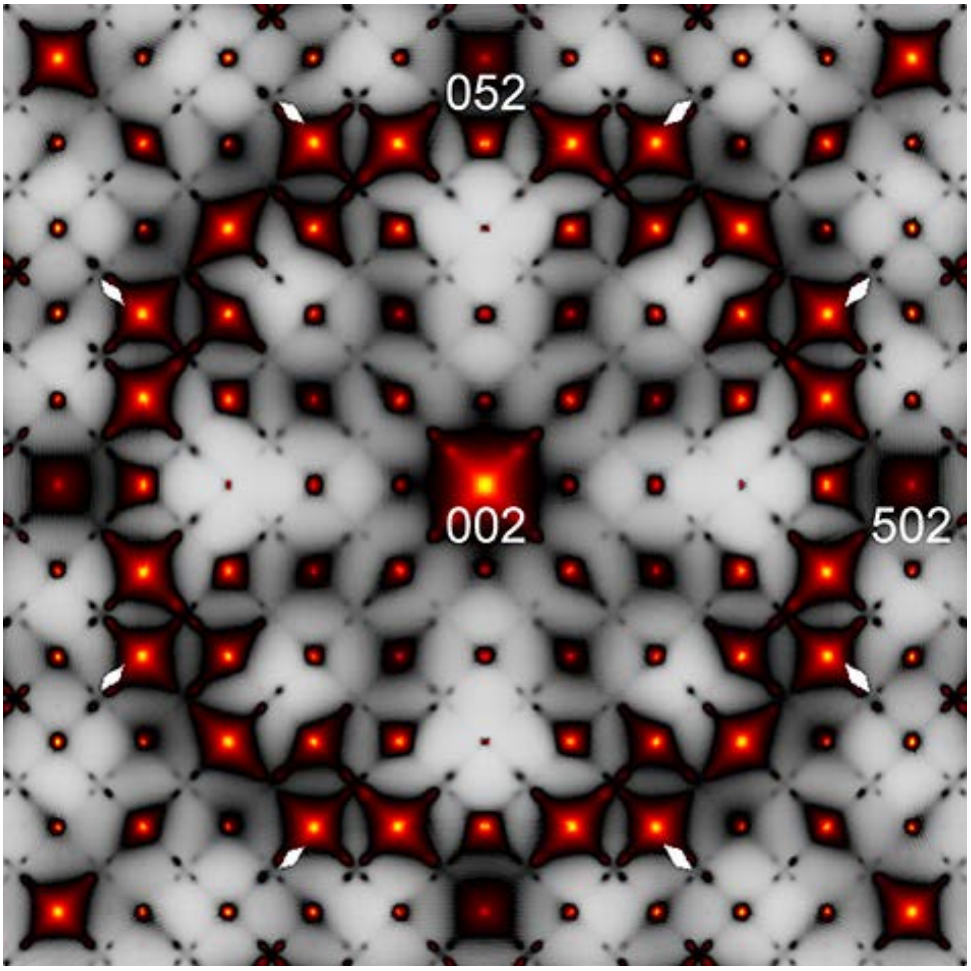


Figure 3. Distribution of the scattered intensity in the *hk*2 plane of $Sr_{0.75}Ba_{0.25}Nb_2O_6$ at ambient temperature. Thermal diffuse scattering, correlated disorder in Nb−O chains and 2D incommensurate modulation with limited correlation length contribute to the diffuse-scattering pattern.

The EBS upgrade enables a reduction in the X-ray beam size down to 5–10 µm for both ID28 branches, enabling data collection from individual grains of polycrystals, including samples under extreme conditions, and the resolution of the individual domains of twinned crystals. From a reverse point of view, for a given focal-spot size, the beam divergence is significantly reduced, thus improving momentum resolution, *e.g.* the investigation of very-long-range modulations or very small structural distortions.

Spatially resolved crystallography

The ESRF-EBS provides the photon flux and fast detectors to collect hundreds of 2D scattering/diffraction patterns per second. A full day of operation sometimes results in tens of millions of 2D images. This presents its own logistical challenges, but such large datasets offer new ways to study materials using X-ray diffraction-based computed tomographic imaging (XRD-CT). By scanning the beam across a sample and rotating it, one can measure projections of the scattering/diffraction in a sufficient number of directions to compute a tomographic image and retrieve diffraction patterns for each of an enormous number of voxels inside a sample. XRD-CT is straightforward to use when the data are isotropic in all directions (powders) but can also be used with single crystals if spots can be indexed. The spatial resolution is generally of the order of the X-ray beam size, which can range from hundreds of microns down to tens of nanometres, depending on the beamline and optics.

One of the most powerful applications of powder XRD-CT is to separate phase-pure materials in a mixture *via* their location inside a working device. Therefore, it is ideal for the study of catalysts or battery materials under realistic operating conditions by obtaining a series of reconstructed volumes to follow chemical reactions in different parts of the sample. The EBS source combined with the latest generation of short-period, small-gap, cryogenically cooled, in-vacuum undulators, *e.g.* at beamlines such as ID15A and ID31, dramatically improves the flux and flux density of high-energy X-rays required to pass through

bulky samples. It also allows an increase of the *Q* range for the application of PDF techniques with 4D resolution. The weak signals at high *Q*, in particular, provide an atomic-resolution picture of the structure for both amorphous and crystalline components of a sample.

The extremely small size of the ESRF-EBS X-ray beams can also convert a typical “powder” sample into a collection of single crystals. Choosing and mounting tiny crystals can be very difficult. Employing high-energy X-rays on solid materials, one can then use XRD-CT techniques to harvest diffraction spots instead of powder patterns. After the spots are indexed, the peak positions can be used to recover internal strain fields within the sample, map spatial variations in the crystal structure, or locate and characterise trace components. For beam-sensitive crystals and phase-pure samples, such data can be used for a “serial crystallography” approach to structure solution and refinement.

In summary, the performance increase enabled by ESRF-EBS represents a big opportunity for major advances in crystallography and an expansion of crystallography into new dimensions in time and space.

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Harald Reichert is Director of Research in Physical Sciences at the ESRF.

OUTREACH

The International Year of Basic Sciences for Sustainable Development 2022: we need it more than ever

Michel Spiro, with a Foreword by Michele Zema

Foreword

"There is nothing basic in basic sciences". This was one of the most compelling take-home messages from HRH Princess Sumaya bint El Hassan's speech at the session on "*Basic Sciences Infrastructures for Ethical and Responsible Collaborative Development*" that Michel Spiro, author of this article, and myself convened at the World Science Forum 2019 (WSF2019) in Budapest, Hungary. That event represented a milestone towards the International Year of Basic Sciences for Sustainable Development (IYBSSD 2022), as it was during that session that the initiative was first announced to the public. Immediate support was granted and explicitly stated in the resolution "Science, Ethics and Responsibility" adopted by the WSF2019.



HRH Princess Sumaya bint El Hassan of Jordan giving her speech at WSF2019. Panellists sitting on stage (left to right): Sekazi K. Mtingwa (former chair, *LAAAMP*), Atish Dabholkar (Director, ICTP), Sanja Damjanovic (Minister of Science, Government of Montenegro), Herwig Schopper (Former Director General, CERN), Michele Zema and Michel Spiro.

I recall it was back in February 2018, when I was a panellist at the UNESCO-Joint Institute for Nuclear Research (JINR) roundtable in Paris, France, that Michel Spiro launched his idea for such an international year. The time was indeed right to build on the successes of recent International Years that had celebrated basic sciences [*e.g.* Chemistry 2011; Crystallography 2014 (IYCr2014); Light 2015; Periodic Table of Chemical Elements 2019]. A strong message to invest more in education and basic science, particularly in small or developing countries, would be sent. The IUCr has supported Michel Spiro's idea since its conception, and I have been honoured to put the expertise I gained from coordinating IYCr2014 at the disposal of his team. We have a new opportunity to celebrate crystallography and, particularly, our relations with all the basic sciences.

Michele Zema, IUCr Executive Outreach Officer, Member (representative for the IUCr) of the Steering Committee for the proclamation of the International Year of Basic Sciences for Sustainable Development in 2022 (IYBSSD 2022)



Michele Zema (left) and Michel Spiro. A full photo gallery of their session at the WSF can be found here.

For more than a year now, the world has been disrupted by the COVID-19 pandemic caused by the SARS-CoV-2 virus. But how much worse could the situation have been without the progress and results produced for decades, even centuries, by curiosity-driven scientific research?

We deplore the many deaths due to COVID-19, and the future is still very uncertain, especially with the detection of new variants, some of which are spreading more quickly. But, in the first place, how could we have known that the infection was caused by a virus, what this virus looks like and what its genetic sequence and variations are without basic research? Viruses were discovered at the beginning of the

20th century, thanks to the work of Frederick Twort, Félix d'Hérelle and many others. The first electron microscope was built in the 1930s by Ernst Ruska and Max Knoll; and DNA sequencing began in the mid-1970s, notably with research by the groups of Frederick Sanger and Walter Gilbert.

We could continue such a list, with basic research at the root of tests, treatments, vaccines, epidemiological modelling, *etc*. We even owe high-speed, long-distance communications, which allow us to coordinate the fight against the pandemic and reduce interruptions in education, economic activities and even the practice of science, to the discovery and study of electromagnetic waves and optic fibers during the 19th century. The COVID-19 pandemic is a reminder (so harsh and brutal that we would have preferred to have been spared) of how much we rely on the continuous development of basic sciences for a balanced, sustainable and inclusive development of the planet.

On many other issues, basic sciences have an important contribution to make to progress towards a sustainable world for all, as outlined in Agenda 2030 and its 17 Sustainable Development Goals, adopted in September 2015 by the United Nations General Assembly. They provide the essential means to address major challenges such as universal access to food, energy and sanitation. They enable us to understand the impacts on the climate, and on life on Earth and in aquatic environments of the nearly 8 billion people currently living on the planet, and to act to limit and reduce these impacts.

Indeed, unlike our use of natural resources, the development of the basic sciences is sustainable *par excellence*. From generation to generation, it builds up a reservoir of knowledge that subsequent generations can use to apply to the problems they will face, which we may not even know about today.

The International Year of Basic Sciences for Sustainable Development (IYBSSD) will focus on these links between basic sciences and the Sustainable Development Goals. It is proposed to be organized in 2022 by a consortium of international scientific unions and scientific organizations led by IUPAP (IUCr, IUPAC, IMU, IUBS, IUGG, IMA, IUHPST, IUVSTA, IAU; IRD, IIASA, EPS, JINR, NuPECC, CERN, ICTP, ISC, SKAO, SESAME, IUMRS, Pierre Auger Observatory, Weizmann Institute of Science), with the recommendation of a resolution voted by the UNESCO General Conference during its 40th session in 2019. Over 50 national and international science academies and learned societies and around 30 Nobel Prize laureates and Fields Medalists also support this initiative. The Dominican Republic agreed to propose a resolution for the promulgation of the International Year during the 76th session of the United Nations General Assembly, beginning in September 2021.

We very much hope that scientists, and all people interested in basic science, will mobilize around the planet and take this opportunity to convince all stakeholders (the general public, teachers, company managers, policymakers, *etc*.) that through a basic understanding of nature, inclusive (especially by empowering more women) and collaborative well-informed actions will be more effective for the global common interest. We especially invite all crystallographers and their organizations to create or join national IYBSSD 2022 committees to organize events and activities during this international year.

More information, as well as communication material, can be found at www.iybssd2022.org. This will also be shared through social media accounts (look for @iybssd2022 on Facebook, Twitter, LinkedIn and Instagram). You are also invited to subscribe to the Newsletter here.

Michel Spiro is President of the International Union of Pure and Applied Physics (IUPAP) and President of the Steering Committee for the proclamation of the International Year of Basic Sciences for Sustainable Development in 2022 (IYBSSD 2022)

SPECIAL REPORT

Slovenian Chemical Society celebrates its 70th anniversary



The Slovenian Chemical Society held an online ceremony on 15 February 2021 to celebrate its 70th anniversary.

Albin Pintar

In 2021, the Slovenian Chemical Society is celebrating the 70th anniversary of its existence. The beginning of the Society dates back to 1951, when Slovenian chemists decided to establish a professional association. The Slovenian Chemical Society was founded on 15 February 1951. The aims and objectives of the Society are set out in its statute, which states its mission to promote the advancement of chemistry, chemical technology and chemical engineering in the broadest sense, to take care about the growth of the expertise of its membership and to work with all organizations involved in the chemical profession, share experiences and provide help. Today, the Slovenian Chemical Society operates locally, nationally and globally in the spirit of the slogan "When chemistry is life".

The Slovenian Chemical Society has developed from a narrow group of experts and around 200 members into an organization that unites over 900 members. Throughout the period, a large number of eminent Slovenian chemists, scientists, professors from academic and research institutions, as well as experts from companies and public organizations worked in the society. It is thanks to them that the Society has been maintained all these years, also through many political and social changes that have always had an impact on the functioning of professional associations.

In order to ensure the progress of the profession, the Slovenian Chemical Society organizes lectures, seminars, congresses, symposia and summer schools, which have developed from local to internationally acclaimed events. The main annual event of the Slovenian Chemical Society is the scientific conference "Slovenian Chemical Days", which the association has traditionally organized as a conference with international participation since 1995. The conference is designed to contribute to the career development of young researchers. It should be emphasized that several members of the Society are also involved in obtaining and organizing international scientific events in Slovenia, with the great help of the Slovenian Convention Bureau.



Slovenian Chemical Days 2018.

As one of its main activities, the Slovenian Chemical Society has been publishing the scientific journal *Acta Chimica Slovenica* throughout its existence, in which domestic and foreign researchers and experts publish their works. Over the years, the journal has developed and gained an international reputation and an exemplary level of citation.



The Slovenian Chemical Society is also active in the field of international cooperation. Special mention should be made of the association's membership in IUPAC, EuChemS, IUCr, ECA, EFCE, EURACHEM, ECTN, EPF and EFCATS.

Although we like to look into the past, evaluate our work and reminisce, it is also important to look to the future, which, in the Slovenian Chemical Society, is full of planned paths, tasks and work enthusiasm.

There is a very active section for crystallography in the Slovenian Chemical Society, which has been headed by Anton Meden. Members of the section participate in activities promoted by the IUCr and ECA, and the main activities are focused on the organization of scientific meetings. Above all, it is worth mentioning the traditional crystallographic conference with international participation that has been organized together with the Croatian Crystallographic Society from Zagreb for almost 30 years.

MEETING REPORT (IUCR SUPPORTED)

4th International Symposium on Halogen Bonding



Oral presenters (from top left) Charles Loh, Martin Breugst, Pierangelo Metrangolo (moderator), Sebastian Hasenstab-Riedel, Marta Mosquera, Stefan Huber, Tatsuo Kaiho and Sekar Govindasamy discussing the theme of 'Applications in synthesis, catalysis and industry'. (Screenshot courtesy of Somananda Sanyal.)

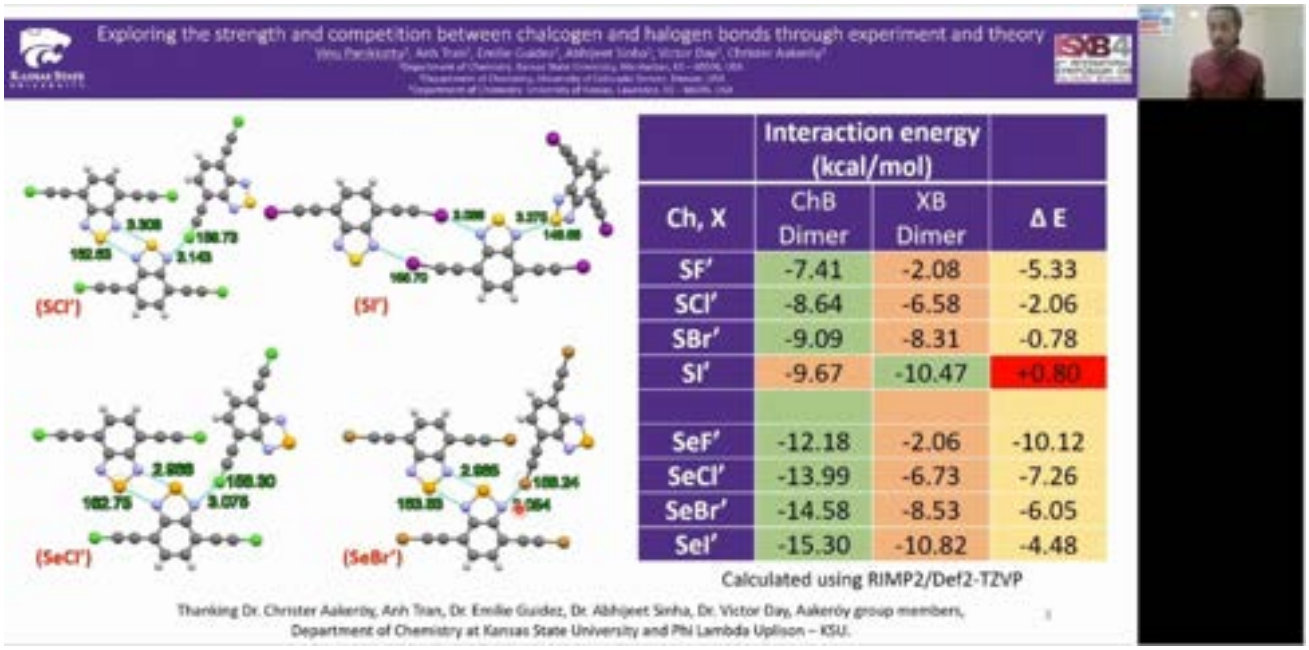
Catharine Esterhuysen

The International Symposium on Halogen Bonding (ISXB-4) was held online from 2 to 5 November 2020 after being postponed from an event scheduled from 22 to 27 March 2020 in Stellenbosch, South Africa, owing to travel restrictions brought about by the COVID-19 pandemic. The ISXB-4 was the latest in the series of ISXB conferences initiated in 2014 by Giuseppe Resnati and Pierangelo Metrangolo. It focused primarily on halogen bonding, but incorporated all forms of σ- and π-hole type bonding, including hydrogen bonding. The symposium aimed to cover both experimental and theoretical aspects of a broad range of fields such as medicinal chemistry, chemical biology, materials science, catalysis, crystal engineering and industrial applications.

When the change to the online format for the conference was announced in July 2020 the response was overwhelmingly positive: where 88 delegates were due to attend the original on-site conference, 220 delegates from 29 different countries joined the online conference with great enthusiasm. This excellent turnout was aided by IUCr funding, thanks to which we were able to support the attendance of 30 young scientists, 13 (43%) of whom were female. The supported scientists represented 14 countries spread over 4 continents. As a result of their generous support, the IUCr was one of the sponsors with a virtual sponsor booth; these booths allowed delegates to get further information about the exhibitor and make contact with a company representative.

The many delegates were not disappointed: the scientific presentations were of an extremely high quality. A total of 25 invited speakers and 45 oral presenters gave live or pre-recorded talks in six sessions: the 'Nature of X-bonding' and 'Supramolecular chemistry and crystal engineering' on 3 November, 'Solid state properties' and 'Understanding X-bonding behaviour' on 4 November, and 'Applications in synthesis, catalysis and industry' and 'Applications in solution chemistry and biology' on 5 November. Within each session, all the oral presenters contributed to a live discussion on the theme, moderated by well-known members of the halogen-bond community. These discussions elicited enthusiastic participation from the audience through a question-and-answer chat function and resulted in some lively debates.

There were also 90 poster presenters divided between two poster sessions on 3 and 4 November. The standard was extremely high, but in the end, Vinu Panikkattu of Kansas State University, USA, was awarded the IUCr journals poster prize for his poster 'Exploring the strength and competition between chalcogen and halogen bonds through experiment and theory'.



Vinu Panikkattu presenting his prize-winning poster.

In addition to the scientific content, the social aspect of the conference was not forgotten: the welcome function included a session of "speed greeting" where delegates were randomly dealt into small groups so that they could greet old friends or get to know new members of the community. Delegates also had the opportunity to meet on an individual basis through the meeting hub, while every day ended with break-away "rooms" to give delegates the opportunity to get together and chat.

These social interactions combined with the live discussions meant that although delegates were sitting in front of computer screens spread over 17 time zones, they still felt a sense of community. ISXB-4 Virtual was, as a result, a resounding success. The organisers would like to thank the sponsors, particularly the IUCr, and all of the delegates for their role in achieving this.

MEETING REPORT (IUCR SUPPORTED)

3rd LACA School on Small Molecule Crystallography - Virtual Edition



Organizing Committee of the 3rd LACA School

The Third School of the Latin American Crystallographic Association (LACA) focusing on Small Molecule Crystallography was originally programmed to be held on 23–29 March 2020 in Mexico City, Mexico. Mexico was selected as the venue because its geographic location permitted coverage of Central American countries that were not covered in the first edition of the School (held in 2018 in Montevideo, Uruguay) owing to the steep travel costs. Thanks to the support of our sponsors (UNAM, IUCr, Bruker, Molecular Dimensions/Anatrace, MiTeGen, MBraun and the CCDC), the organization of the School was complete, including lunch menus (the tacos would have been really delicious), but ten days before the beginning of the School, the University issued a directive canceling all reunions, workshops, schools *etc.* and, shortly after, all presential activities on its campuses. Additionally, the suspension of air travel and the spread of the COVID-19 pandemic in Latin America and the world gave us no other choice than to cancel the School as planned. This was heartbreaking and led to a scramble to cancel hotel reservations, plane tickets and other services; some of these activities have not yet been concluded.

With time, it became apparent that the situation was not improving and that a presential event would not take place soon and certainly not in 2020. Therefore, we decided to hold the School as a virtual event. This decision led to several challenges as the virtual sessions would span over at least four different time zones for the participants. Moreover, the virtual event could not cover the initially planned 60 hours of courses and exercises. Furthermore, the experimental session follow-up would be more difficult without direct access to the participants' computers. Therefore, the School's duration was set for two weeks, with one theoretical lecture (1.5 h) and two practical sessions (1 + 1 h) per day distributed across an eight-hour timeframe. This allowed each lecture to be followed by a practical session the same day and another practical session the next day before a new lecture of a different topic started. The first idea was to have the School in a block of two weeks, but as the second week overlapped with the X Congress of the Mexican Crystallographic Society (SMCr), we decided that the School would flank the week containing the X Congress of the SMCr (2–4 December 2020). Approximately half of the participants initially accepted in the School's March edition preregistered for the virtual edition. Within three days after announcing this virtual edition of the School, we got over 120 applications, far more than we could accept. After a careful selection, 64 participants and 11 instructors from 14 countries (11 countries from Latin America) participated in the School. It is also noteworthy that three instructors, Maria de Jesús Rosales Hoz, Javier Alcidez Ellena and Vojtech Beto Jancik, are Co-editors of *Acta Crystallographica Sections C* and *E*, and the others have ample experience in small-molecule crystallography, frequently acting as reviewers for *Acta Crystallographica* journals. The lectures were hosted on the Zoom platform, and Google Classroom was used for the distribution of class materials. We addressed problem-solving

related questions outside of the School's hours through a WhatsApp group created for this purpose, and last-minute announcements were made through this communication platform. Spanish and English were used as primary languages, although questions asked in Portuguese by students from Brazil were also answered. All lectures were recorded and made available to the participants during the same day of recording.

After a brief inauguration, the School started on 23 November 2020 with a fascinating lecture about the “History of X-Ray Diffraction” presented by María de Jesús Rosales Hoz (Cinvestav, IPN, México) and continued with a talk on “Symmetry” given by Leopoldo Suescun (UdelaR, Uruguay) using the symmetry patterns from IUCr Teaching Pamphlet #14. After that, on consecutive days, lessons on the "Physics of Diffraction" were given by Florencia Di Salvo (INQIMAE-UBA, Argentina), Javier Ellena (IFSC-USP, Brazil) and Leopoldo Suescun, while Hamilton Napolitano (UEG, Brazil) lectured on “Direct and Patterson methods”. Finally, the first week ended with a talk on "Data Collection and processing with *APEX3*" given by Bruce Noll (representing Bruker AXS) and Vojtech Beto Jancik (UNAM, Mexico). The students were given homework for the next week and were encouraged to participate in the X Congress of the SMCr. The week off in between also allowed for a meeting of the organizing committee to assess the School's progress and the teaching methods employed. As a result, the second week's program was amended to operate more efficiently on the lectures' available time.

The second week started on 7 December 2020 with an introduction to *SHELX* and continued with a lecture on “Basic Structure Solution and Refinement”, followed by “Validation” given by Javier and Beto. After a practical session, Diego Martínez (CCIQS UAEM-UNAM, Mexico) gave lectures on the refinement of disorder. Wednesday and Thursday morning were dedicated solely to the practical training of structure solution, refinement, disorder and validation, teaching the students how to use restraints and constraints for the refinement of disorder. Subsequently, Bruce Noll gave a lecture on Daniel Kratzer’s *DSR* plugin, and the course before the final exam was centered on “Data Processing and Refinement of different types of twins”. The last lecture of the School was dedicated to the Cambridge Structural Database (CSD) and was given by Suzanna Ward and Ilaria Gimondi from the CCDC, who showed us, among other great features of the database, how to make a Christmas postcard from a polyoxometalate structure. After the last break and a practical session on the CSD conducted by Natalia Alvarez Failache (UdelaR, Uruguay), only the School's closing ceremony remained on the schedule. Among the School participants and lecturers present at the ceremony were Sven Lidin and Hanna Dabkowska, the President and Vice-President of the IUCr, respectively; Graciela Díaz de Delgado, the IUCr Executive Committee representative for Latin America; and José Reyes Gasga, President of LACA. Following the closing remarks, Javier Ellena paid tribute to Graciela Punte for her life's work in teaching crystallography in Latin America. Finally, Leopoldo shared a virtual toast and the School finished with a short game of Kahoot! in a relaxed mood, as can be seen from the screenshot below.

The organizers of the school would like to thank the IUCr, LACA, SMCr, Associação Brasileira de Cristalografia, Asociación Argentina de Cristalografía, Red Uruguaya de Cristalografía and the UNAM for their support during the organization of the School and to UNAM, IUCr, Bruker, Molecular Dimensions/Anatrace, MiTeGen, MBraun and the CCDC for their sponsorship that made the School possible. Furthermore, they would like to thank the patience, interest and good mood of the students who devoted so many hours of their lives in the very difficult times that the region was living through, and for sharing with all their “zoom-mates” (both students and lecturers) the hope that is embedded in learning as an activity for the future.


Closing Ceremony
and Farewell Toast
Márius Ramírez C...
Cesario Ajpi Cond...
Eduardo L. Gutiérr...

MEETING REPORT

2020 Meeting of the Crystallographic Society of Japan



The Poster Awardees. From upper left: K. Yamashita, N. Toyama, M. Isobe, N. Nakamura and T. Sato.

Kotaro Fujii, Akihiko Nakatsuka

The 70th anniversary Annual Meeting and General Assembly of the Crystallographic Society of Japan (CrSJ2020) and the satellite symposium “The COVID-19 pandemic and the current and future views of crystallography” were held online during 27–29 November 2020. The meeting was initially planned to be held at Tsukuba, Japan, but was switched to an online meeting due to the COVID-19 pandemic. About 200 crystallographers participated in the meeting. There were 109 presentations covering all aspects of crystallography, and five award lectures. In the satellite symposium we had eight invited lectures.

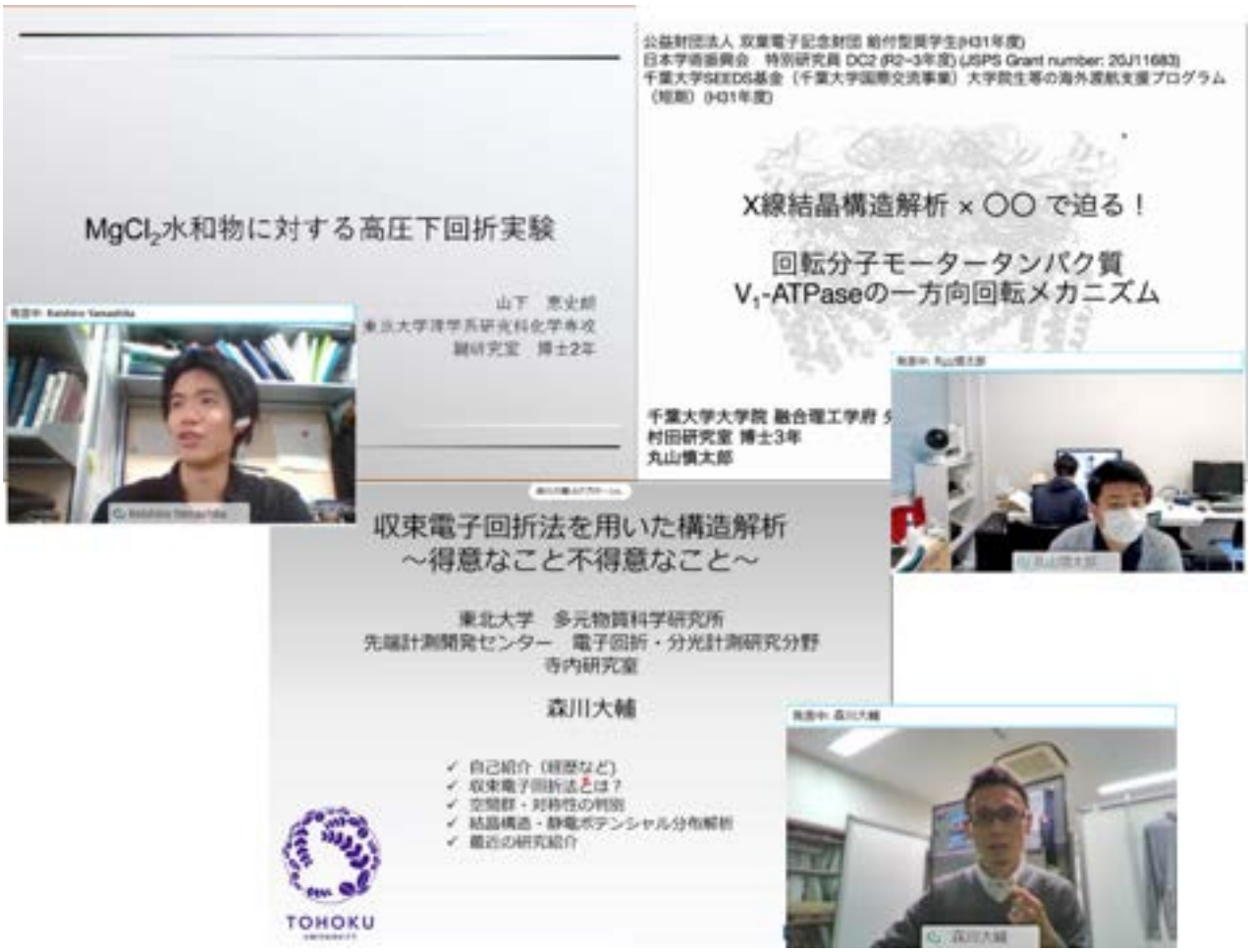


The recipients of the 2020 CrSJ Awards with the President of CrSJ. From upper left: K. Nishikawa, H. Ogata, K. Wada, T. Arimori, S. Kawaguchi and Y. Yamagata (President).

At the CrSJ Awards Ceremony, the S. Nishikawa Award was given to Keiko Nishikawa (Toyota Physical and Chemical Institute) for her research “Pioneering study in structural science of fluctuations for complex condensed systems”; the Research Award was given to Hideaki Ogata (Hokkaido University) for his research “Structural and chemical study of metalloenzymes” and Kei Wada (Miyazaki University) for his research “Study of structural basis for molecular mechanisms of cellular redox control”; and the Young Crystallographer Award was given to Takao Arimori (Osaka University) for his research “Development of a novel antibody fragment format 'Fv-clasp' applicable to protein crystallization” and Shogo Kawaguchi (Japan Synchrotron Radiation Research Institute) for his research “Development of sub-second

synchrotron radiation powder diffraction measurement system under various gas atmospheres”.

Five young scientists were honored with Student Presentation Awards: K. Yamashita (University of Tokyo), N. Toyama (Nagoya Institute of Technology), M. Isobe (Osaka City University), N. Nakamura (Osaka University) and T. Sato (Hokkaido University) (see photo at the top of this page).



Speakers at the Young Crystallographers' Meeting 2020.

The Young Crystallographers' Meeting 2020, a satellite meeting of CrSJ2020, was held online on 13 November, and 50 researchers/students participated. This meeting is held every year to give young researchers and graduate students the opportunity to communicate and network with each other, especially beyond the barriers between physics, mineralogy, chemistry and biology, in an informal environment. This year, three lectures by K. Yamashita (University of Tokyo), S. Maruyama (Chiba University) and D. Morikawa (Tohoku University) were given and the participants engaged in lively discussion.



Group photo of participants in the Young Crystallographers' Meeting 2020.

The full program of the meeting can be viewed here. The chair of the organization committee was E. Nishibori (Tsukuba University) and the program committee was chaired by S. Adachi (KEK).

The next annual meeting will be held during 19–21 November 2021 at Hokkaido University in Sapporo, Japan. The chair of the organization committee is Min Yao (Hokkaido University) and the program committee is chaired by Katsumi Maenaka (Hokkaido University).

MEETING REPORT

Seventh joint Diamond–CCP4 MX workshop



Raquel Costa (NOVA University of Lisbon, Portugal), who won the IUCr-sponsored poster prize at the first online edition of the DLS-CCP4 workshop.

David Waterman

The seventh joint Diamond–CCP4 Data Collection and Structure Solution Workshop was planned, as usual, for early December 2020 at Diamond Light Source. However, it was clear by May 2020 that this would not be possible. The organisers quickly committed to running a virtual workshop instead, even though at that time none of us had much of an idea what would be involved! We went through a number of iterations in our plans, and held a one-day mini-workshop in the Summer to check feasibility and gain experience. In the end, we decided to spread the full programme out over two weeks, but to be merciful regarding the intensity of the daily sessions by restricting to office hours only. This ensured the workshop fit better into the lives of those students and tutors who are sharing their work space with family, and gave everyone a break from the computer each evening.

As ever, we had a day of beamtime at Diamond's MX beamlines, supported by the excellent beamline staff who were on site to run experiments. The other sessions of lectures and tutorials were run over Zoom, with Slack channels for text-based communication. This combination served us very well, and it is likely that some elements of this approach will become the norm in future, even for in-person workshops. Emily and Stefania from the Diamond Events team deserve a special mention for their excellent work hosting the Zoom sessions, setting up breakout rooms, directing students to tutors, and for remaining ever-friendly compères for the full two weeks. Thank you both!

One aspect of the in-person workshops that could not easily be repeated online is the social element. Happily our attendees were a genial group and even self-organised a games evening. Another important social event is the poster session. Unfortunately we couldn't find a virtual equivalent of a poster and drinks soirée that we would normally hold at Diamond House. Nevertheless, we were able to use technology to our advantage by having the attendees upload their posters to Slack and allow conversations to continue around their projects throughout the workshop. This proved extremely useful for tutors trying to keep track of 20 student projects! A team of judges scored the posters based on how informative they were to the tutors as well as on exciting scientific content. There were many good posters but after totting up the scores we found a clear winner, Raquel Costa from UCIBIO in Portugal for the poster "Strategies to solve the 3D structures of two proteins from a prominent human gut commensal".

The 2021 event will hopefully return again live at Diamond Light Source this December, but if we have to make it virtual again, we know we can make it work.

MEETING REPORT (IUCR SUPPORTED)

HPW-21 – A Workshop of the IUCr Commission on High Pressure



Elena Boldyreva

We are all getting used to the new format of international meetings, which has been imposed on us since 2020 by the global pandemic. Despite missing personal contact and in-person communication, we have also learned how to benefit from the new situation. We have made meetings cheaper, enabling the participation of more people independently of their budget, and brought meetings to the individual scientists, targeting those unable to travel because of health, age, visa restrictions or very busy schedules. These benefits are exemplified by a recent Workshop organized by the IUCr Commission on High Pressure. This event was originally planned as a 'regular' event, just like all preceding events in this successful series of workshops organized around the world by the Commission every year, except for the IUCr Congress years. 2021 had been intended to be a non-Congress year, after the Congress in Prague in 2020, before the Corona-crisis arrived. The bid (Fig. 1) was approved by a majority vote of the IUCr Commission on High Pressure in 2019 in Vienna. A warm personal meeting in the cold and snowy, but sunny and shiny, winter of Novosibirsk, Russia, was anticipated for February 2021. The purpose of the Workshop is to bring together scientists working in the field of high-pressure crystallography to discuss the latest achievements in fundamental research, techniques and practical applications.



Figure 1. Preparing the bid for HPW-21 during an HP Commission Workshop in Vienna, Austria, in 2019. Left to right: Boris Zakharov, Elena Boldyreva and Nikita Bogdanov.

As it became clear that no in-person meeting would be possible in 2021, the organizers decided to change gear and opted for an online Workshop. Thus, HPW-21 became a reality and took place from 1 to 6 February. The number of participants (353) significantly exceeded that of all previous Workshops in the series, and so did the breadth of the geographical representation. Moreover, the online format encouraged an unusual, but highly inspiring, number of undergraduate and graduate student participants. The corresponding spread in the time zones challenged scheduling of the sessions; some participants were forced to start their working hours at 4 am, whereas others had to stay awake until 2 am for the evening sessions (Fig. 2).

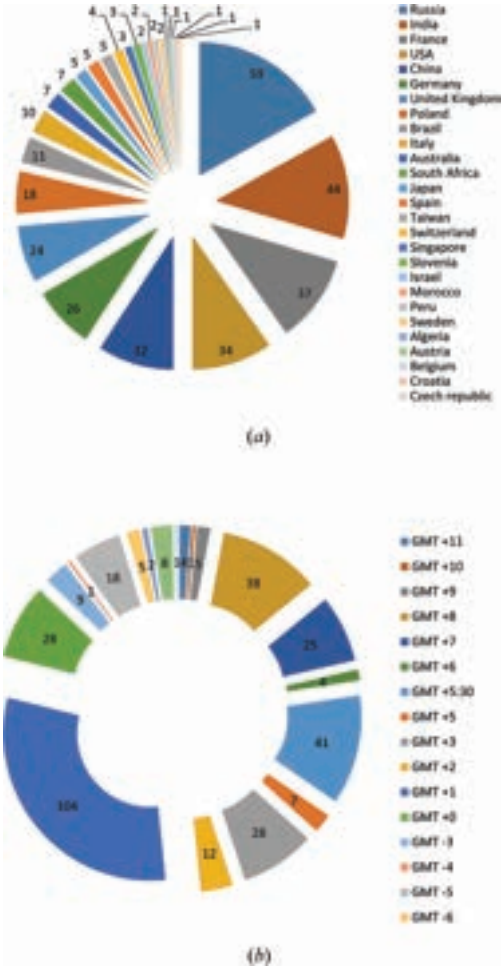


Figure 2. Distribution of participants between (*a*) the countries and (*b*) the time zones.

The program of the Workshop included various activities. The IUCr Commission on High-Pressure Crystallography is celebrating its 25th anniversary in 2021. Therefore, the Workshop started with an introductory lecture dedicated to the history of the Commission presented by the Commission's first secretary, John Parise, on behalf of himself and the first Commission chair, Richard Nelmes. It was a real pleasure to recognize so many young faces of those who are now established researchers (Fig. 3) and to see how the Commission has matured with time.



Figure 3. The historic photos from the presentation by John Parise and Richard Nelmes dedicated to the 25th anniversary of the Commission on High Pressure.

Scientific program

The scientific program included the following sessions: High-pressure research at synchrotron facilities; High-pressure research at neutron facilities; Detectors, sample stages, heating systems, pressure cells; Superconducting and super-hard materials; New approaches to data processing and analysis; Macromolecular crystallography at high pressures; Pressure measurement and pressure scales; and Inorganic, coordination, organic, carbon and hybrid materials. Four Round Tables were organized, which triggered extensive and profound discussions: Data deposition and validation – state of the art (moderated by Kamil Dziubek and Simon Coles), High-pressure for advanced materials (moderated by Haozhe Liu), High-pressure for natural sciences (chemistry, physics, planetary sciences, life sciences) (moderated by Andrzej Katrusiak); and Challenges in instrumentation and techniques (moderated by Elena Boldyreva).

At the end of the Workshop a summary report from the Satellite Meeting "Towards national synchrotron infrastructure for high-pressure crystallography in Russia" was presented by Konstantin Litasov (Troitsk) and Sergey Rashchenko (Novosibirsk) – see the Satellite Meeting summary report below.

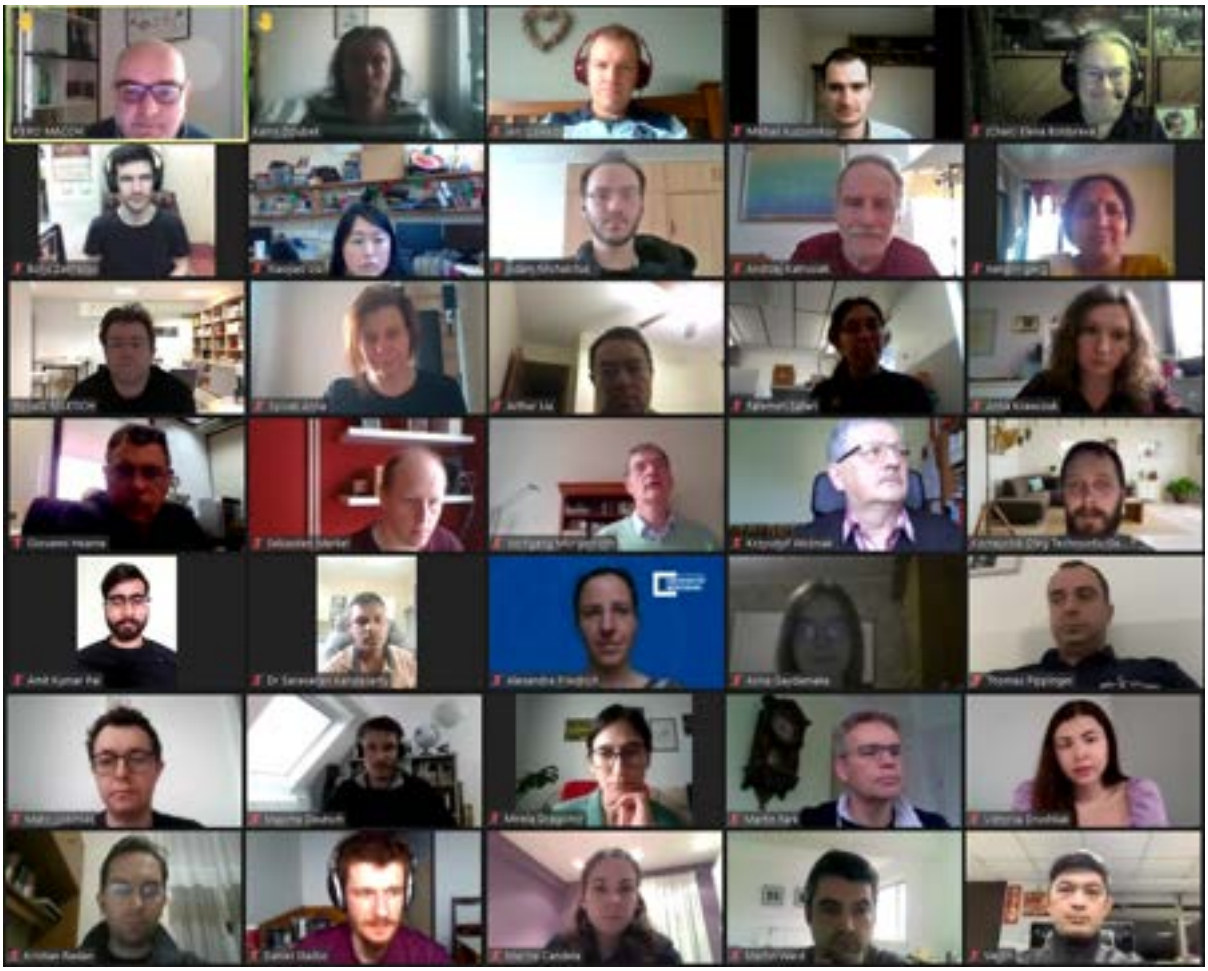
The first day of HPW-21 was dedicated to the instrumental and technical issues of high-pressure research. First, a general overview was given of the studies conducted at synchrotron and neutron sources, as well as those using laboratory instruments, presented by the Chair of the local organizing committee, Elena Boldyreva. Next, Mohamed Mezouar gave a detailed introduction to the new opportunities at the specialized high-pressure stations at the ESRF. This was followed by Frederico Alabarse, who illustrated the status of XPRESS – the dedicated high-pressure diffraction beamline at the ELETTRA synchrotron in Trieste. Nicola Casati presented the new possibilities for high-pressure science, which will be available after the machine upgrade to SLS-2.0 at the Paul Scherrer Institute at the Materials Sciences beamline, which will take place in 2024–2025. Denis Kozlenko gave an overview of the state-of-the-art neutron research at high pressures at the Joint Institute of Nuclear Research in Dubna (Moscow).

Further contributions described the new achievements in developing new detectors, sample holders, pressure cells, laser heating systems and other accessories presented by Almax easyLab (Koen De Hantsetters), DECTRIS Ltd (Tilman Donath, Baden-Dättwil, Switzerland), STOE & Cie GmbH (Thomas Pippinger and Jens Richter, Darmstadt, Germany), the Scientific and Technological Center of Unique Instrumentation (Pavel Zinin, Russian Academy of Sciences, Moscow, Russia) and the Jülich Centre for Neutron Science (Andreas Eich, Jülich, Germany).

During the following days the participants listened to lectures on the synthesis and structural characterization of metal superhydrides that become high-T_c superconductors at megabar pressures (Igor Lyubutin, Moscow, Russia, and Mikhail Kuzovnikov, Chernogolovka, Russia) and on new super-hard boron-rich chalcogenides (Vladimir Solozhenko, Paris, France). Nathalie Colloq'h (Paris, France) gave a general introduction to high-pressure macromolecular crystallography and also presented recent results from the group that was founded by a pioneer in this field, Roger Fourme. The methodology of obtaining high-pressure electron densities was discussed extensively in the contributions by Piero Macchi (Milan, Italy), Krzysztof Woźniak (Warsaw, Poland) and Krešimir Molčanov (Zagreb, Croatia). Matthias Krug (Münster, Germany) gave an overview of the challenges and perspectives in multigrain crystallography in multi-component systems.

A series of oral presentations over three days gave a broad overview of the fascinating high-pressure behavior of various compounds and materials, ranging from intermetallics and simple elements, through complex inorganic and organic synthetic compounds to minerals, materials and pharmaceuticals. The complete list of presentations is available at the HPW-21 site.

Particular attention at HPW-21 was devoted to educational aspects; a series of tutorials was offered alongside a dedicated session for young scientists. The tutorials included DAC handling and loading (Christophe Guillaume and Christophe Thessieu, Almax easyLab), *EoSfit* and data collection for precise lattice parameters (Ross Angel, University of Padova, Italy), High-pressure crystallization (Fatemeh Safari, University of Poznań, Poland), High-pressure data treatment with *APEX* software (by Tobias Stuerzer, Bruker); High-pressure data treatment in *X-Area* (Thomas Pippinger, STOE); and High-pressure data treatment in *CrysAlis Pro* (Fraser White, Rigaku Oxford Diffraction). Young scientists had a chance to present their work at a "Rising Stars" session as flash presentations, as well as during a poster session. Three posters were promoted by the Workshop Scientific Committee to be presented as oral contributions: Shir Ben Shalom (Beer-Sheva, Israel) "Anomalous pressure-dependent phase diagram of liquid Ga-In alloys"; Vishnu Vijayakumar Syamala (Nancy, France) "Evolution of halogen bonding interactions in a co-crystal system: X-ray diffraction under pressure in the lab"; and Anastasiia Iskrina (Moscow, Russia) "P-V equation of state of new phase $Ca(Fe,Al)O_4$ up to 61 GPa".



Two posters received special awards. The "Rising Star Award on Advances in High-Pressure Science" from STOE was given to Viktoriia Drushliak (Poznań, Poland) for her work "Optical and structural high-pressure studies of Cs_4PbBr_6". The "Rising Star Award on Challenging high-pressure experimentation setup," sponsored by TechnoInfo and Rigaku Oxford Diffraction, was given to Amy Lazicki (Livermore, USA) for her work "Pb to 800 GPa using X-ray diffraction and laser ramp compression". Many of the contributors at the 'regular' oral sessions were also young early-career researchers.

Even though the Workshop was online, a virtual exhibition was organized. Manufacturers of high-pressure cells, detectors and modern diffractometers provided links to their sites, presented posters, and organized interactive webinars and user meetings. STOE also ran a quiz, and the winner was announced at the closing ceremony.

Social program

A social program was also provided. The participants were invited to make a virtual journey around Novosibirsk, Akademgorodok and NSU, viewing historical and modern photos of the city, and familiarize themselves with historical facts about the city and its famous people (such as Academician Mikhail Lavrentiev, the founder of Akademgorodok). During this virtual journey, participants were introduced to world-famous symbols of Novosibirsk, including the Trans-Siberian railway, Akademgorodok and the Opera and Ballet Theatre. The participants could then relax in the beautiful botanic gardens, and finished the excursion at the Arnold Katz Concert Hall listening to music or watching a ballet in the Opera and Ballet Theater. The links to the virtual excursions are still to be found at the HPW-21 site. Some movies are in English, some are silent and some are in Russian (with optional English subtitles). Recordings of some concerts, opera and ballet performances are also available at this link.

Acknowledgements

The whole enormous work has been done for free by a small but very efficient team from the Department of Solid State Chemistry at Novosibirsk State University, which included Boris Zakharov, Anna Gaydamaka, Nikita Bogdanov, Ivan Tumanov, Eugene Losev and Alexei Fedorov. Their enthusiasm and dedication made this event a real success. We also acknowledge the assistance of the IUCr Commission on High Pressure and of our industrial partners. Novosibirsk State University provided the access to Zoom for such a large number of participants.

Comments from participants

Comments posted by the participants following the conference were very positive, proving the first virtual HPW to have been a successful meeting. Some comments from participants are shown below:

Krzysztof Woźniak (Poland): "Thank you, Elena, for this excellent conference - really well done. I have enjoyed it very much - plenty of excellent and inspiring talks and discussions".

Nandini Garg (India): "At our place many of us were participating sitting in a conference room. So you can add on an average at least 10 more participants".

Viktoriia Drushliak (Poland): "Thank you all for organizing this Workshop! I learned a lot here, I am also grateful for the comments on my work, I have already found another space group for the second phase, as you suggested. I didn't expect to win the prize, because it is my first conference ever. You really encouraged me to move forward and work even harder! And thank you for making this Workshop free of charge, because probably I wouldn't have had an opportunity to attend it otherwise".

Piero Macchi (Italy): "I agree that online conferences give better opportunities, to present and discuss with a wider audience. Surely we would like to re-activate also the on site meetings, but should not just archive the online meetings. Thank you, Elena and all the co-workers in Novosibirsk and in the rest of the world (like Kamil), for excellent organization and inspiration".

Martin Ward (UK): "A big thank you to the organizers for this Workshop, it has been very enjoyable. Although we may have preferred to have travelled and met in person, the online platform does increase accessibility, and perhaps opens the possibility of having more regular meetings within the community, too?"

Kamil Dziubek (Italy): "Congratulations to Elena and the local committee! Thank you, it was a pleasure to stay with you all together this week. Perhaps we should think about hybrid conferences in the future to allow more people to participate. Even in the post-COVID world, we should also include those scientists who for various reasons cannot or are not allowed to travel".

Anna Krawczuk (Poland): "Thank you for the excellent quality workshop; it was extremely interesting and practical for someone who is just entering the field".

Sébastien Merkel (France): "Thank you everyone. The online workshop was good and allowed more attendance. It worked well for me".

Amy Lazicki (USA): "It has been a pleasure to hear from all of you, and thank you again, Elena, Boris, and the whole team."

Arthur Liu (USA, China): "Thanks, everyone! Congrats to the local organizing committee again for this wonderful Workshop!"

Alejandro Pedro Ayala (Brazil): "Thank you very much, Elena and the organizing committee, for the amazing conference."

Martin Fark (Germany): "Many thanks to all organizers and speakers, very well done!"

Manuel Fernandes (South Africa): "Thanks to everyone and especially to the organizing committee! I really enjoyed the conference".

Further information

A Book of Abstracts is available at the HPW-21 site.

A Virtual Special Issue – a collection of the original research and feature articles – will be published up until the end of 2021 in the IUCr journals **IUCrJ**, *Acta Cryst. B*, *Acta Cryst. C*, *Acta Cryst. D*, *J. Appl. Cryst*. and *J. Synchrotron Rad*.

The location and the terms of the next Workshop of the IUCr High-Pressure Commission will be selected by the High-Pressure Commission and announced later.

Towards national synchrotron infrastructure for high-pressure crystallography in Russia (Satellite Meeting report)

Modern synchrotron infrastructure is a key tool for state-of-the-art high-pressure crystallographic studies. Therefore, the national program for the development of synchrotron and neutron research and infrastructure – approved by the Russian government in 2020 – was met with a lot of enthusiasm in the Russian high-pressure community. The recent IUCr High-Pressure Workshop held online in Novosibirsk from 1 to 6 February 2021 provided us with a brilliant chance to organize a Satellite meeting of Russian groups that actively use synchrotron infrastructure for high-pressure research. The aim of the Satellite was to consolidate the community, discuss demands for high-pressure instrumentation and infrastructure at the future national synchrotron facilities, and coordinate further activities. The following institutions presented a review of their research directions and joined the discussion:

Vereshchagin Institute for High Pressure Physics RAS, Troitsk (Konstantin Litasov)

Shubnikov Institute of Crystallography RAS, Moscow (Igor Lyubutin)

Institute of Earth's Crust SB RAS, Irkutsk (Igor Sharygin)

Institute of Solid State Physics RAS, Chernogolovka (Mikhail Kuzovnikov)

Novosibirsk State University (Elena Boldyreva)

Saint Petersburg State University (Ljudmila Gorelova)

Sobolev Institute of Geology and Mineralogy SB RAS, Novosibirsk (Anna Likhacheva)

Colleagues from the Institute of Experimental Mineralogy RAS (Chernogolovka) and Kirensky Institute of Physics SB RAS (Krasnoyarsk), as well as representatives of the IUCr Commission on High Pressure and the EHPRG Committee (Kamil Dziubek and Boris Zakharov) also participated.

The research fields presented by participants spanned from high-temperature superconductivity, magnetism and high-pressure thermodynamics to phase transitions in planetary interiors and high-pressure crystallography of silicates and organic compounds, including molecular materials and pharmaceuticals; beam times for the corresponding experiments were provided by the most advanced high-pressure beamlines at SPring-8, ESRF, PETRA-III, APS, SLS, *etc*. After the presentations from the research groups, a report on the high-pressure X-ray diffraction opportunities at the future fourth-generation synchrotron source, SKIF (to be built in Novosibirsk, Russia), was presented by Sergey Rahchenko, a member of the SKIF Project Office. After discussion, a résumé was proposed as a result of the Satellite Meeting:

Consider high-pressure community among key user groups for future national synchrotron sources

Support the launch of high-pressure X-ray diffraction end-stations among first-stage beamlines of the future SKIF synchrotron source (Novosibirsk, Russia)

Pay particular attention to user-friendly infrastructure for high-pressure research (DAC access, loading, heating, cryogenic and spectroscopic options, *etc.*) at SKIF

Continue discussion on the development of large-volume press and nuclear resonant scattering (including high-pressure and low-temperature techniques) at SKIF at the future meetings

Develop and promote university programs for future (high-pressure) synchrotron users.

Konstantin Litasov, Sergey Rashchenko (Co-chairs of Satellite Meeting); Elena Boldyreva (Chair of Local Organizing Committee of the IUCr HPW-21); Kamil Dziubek and Boris Zakharov (IUCr High-Pressure Commission and EHPRG Committee)

NOTICE

CCDC 2021 User Group Meetings



This year the CCDC will be hosting User Group Meetings (UGMs) virtually. We have followed the amazing feedback received from the 2020 Global UGM and chosen to break up the day, so we can focus on one topic per meeting. We are happy to announce the dates of the events below:

Science Day, on 26 May – hear from the CCDC PhD Students

Discovery Science, on 9 and 10 June

Material Science, on 7 and 8 September

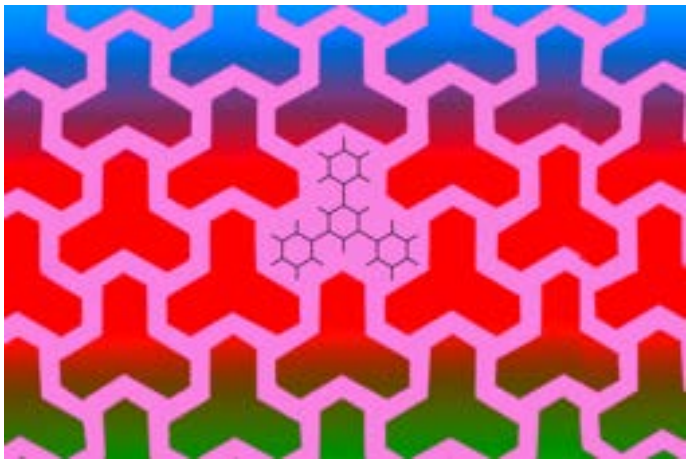
All the UGMs are open to everyone that wishes to join. You can find more details about each meeting and register to attend by visiting our events webpage here.

If you would be interested in presenting your work that uses the CSD or CCDC tools in any of the above areas, we invite you to send a brief 150-word abstract to hello@ccdc.cam.ac.uk.

We look forward to seeing you all there.

HISTORY OF CRYSTALLOGRAPHY

MacGillavry–Escher–Mamedov and periodic patterns



Istvan Hargittai

In my mind, Caroline H. MacGillavry (1904–1993) and the expansion of my interest toward crystallography have blended. I first met her when I attended my first ever scientific meeting, the 7th Congress and General Assembly of the IUCr in 1966 in Moscow, Russia. She was the coordinator of the session in which I gave a talk. Prior to the meeting, we corresponded. She was gently helpful. It was shortly after the IUCr had published the first edition of C. H. MacGillavry, *Symmetry Aspects of M. C. Escher's Periodic Drawings* (A. Oosthoek's Uitgeversmaatschappij). That edition is now a collector's item. My copy appeared in 1976. She worked with the artist on this book, who created a set of beautiful periodic drawings to fill the plane without gaps and overlaps. She discussed the symmetry aspects of these drawings making the book an outstanding tool in teaching crystallography. For me, it served as inspiration when in a few years' time I was searching for examples of two-dimensional space groups among Hungarian folk art. By then, the rest of my family and I had been inoculated by the symmetry virus. The logo of the 12th Congress and General Assembly of the IUCr in 1981 in Ottawa, Canada, was a unit of four stylized maple leaves related by fourfold rotation and also by anti-symmetry if considering the red/white color change among the four leaves. François Brisse designed a series of two-dimensional space-group drawings related to Canada's provinces. One of his patterns displayed the periodically appearing maple leaf. I found a tiling in Lisbon, Portugal, which showed another pattern with the maple leaf as its basic motif.



Caroline H. MacGillavry from *Algemeen Handelsblat*, 1952 (courtesy of Henk Schenk); the logo of the 12th IUCr Congress, Ottawa, Canada; and a Portuguese tile decoration (photograph by the author).

However, it was the 11th IUCr Congress and General Assembly in 1978 in Warsaw, Poland, that brought me the most dramatic experience in two-dimensional space-group patterns. Khudu Mamedov (1927–1988) was their author. Mamedov came from the amalgamation of two vastly different backgrounds. His parents were nomads, and he studied at the most prestigious venues. Following graduation in Baku, Azerbaijan, he earned his PhD-equivalent degree at the Institute of Crystallography in Moscow. He founded an institute of crystallography in Baku and spent half a year what we would call today as a post-doctoral assistant at Birkbeck College in London, UK. There, J. Desmond Bernal was his mentor, and Mamedov became good friends with Alan L. Mackay. Mamedov prepared numerous periodic patterns. His goal was not so much to aid education in crystallography; rather, his motivation was to help the preservation of cultural heritage. At the Warsaw Congress, he set up a small desk in one of the busy hallways and spread out his drawings — all originals. He generated a great deal of interest among the attendees of the meeting. From the start, we engaged in conversation and continued on several occasions during the meeting. He loved to talk about his art. His drawings were most original, and many of the visitors to his stand wanted to purchase his drawings. He politely declined. At the conclusion of the Congress, he gave me some of his drawings, and I have cherished having them ever since. We stayed in contact, and I visited him in 1982.



Khudu Mamedov in 1982 in Baku (photograph by the author) and the “Unity” hand drawing (by and courtesy of Khudu Mamedov).

One of my favorites is his drawing called “Unity,” referring to the old and young generations. It is a periodic pattern, though with minute variations. There are some variations due to the hand-drawing, but even more than that. The facial expressions of the young men are more uniform than those of the old. To me, this hinted at the individuality the old men had developed during their long lives. A few years after Mamedov’s death, his devoted disciples published a luxurious volume of the reproductions of his drawings. The reproductions were not facsimile copies of his hand-drawn art; rather, they were computer-generated patterns. For the geometrical topics, this hardly made any difference. Alas, the new version of “Unity” lost much of its originality. In the computer-drawn version, not only the young had uniform facial expressions, but the old did, too.

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

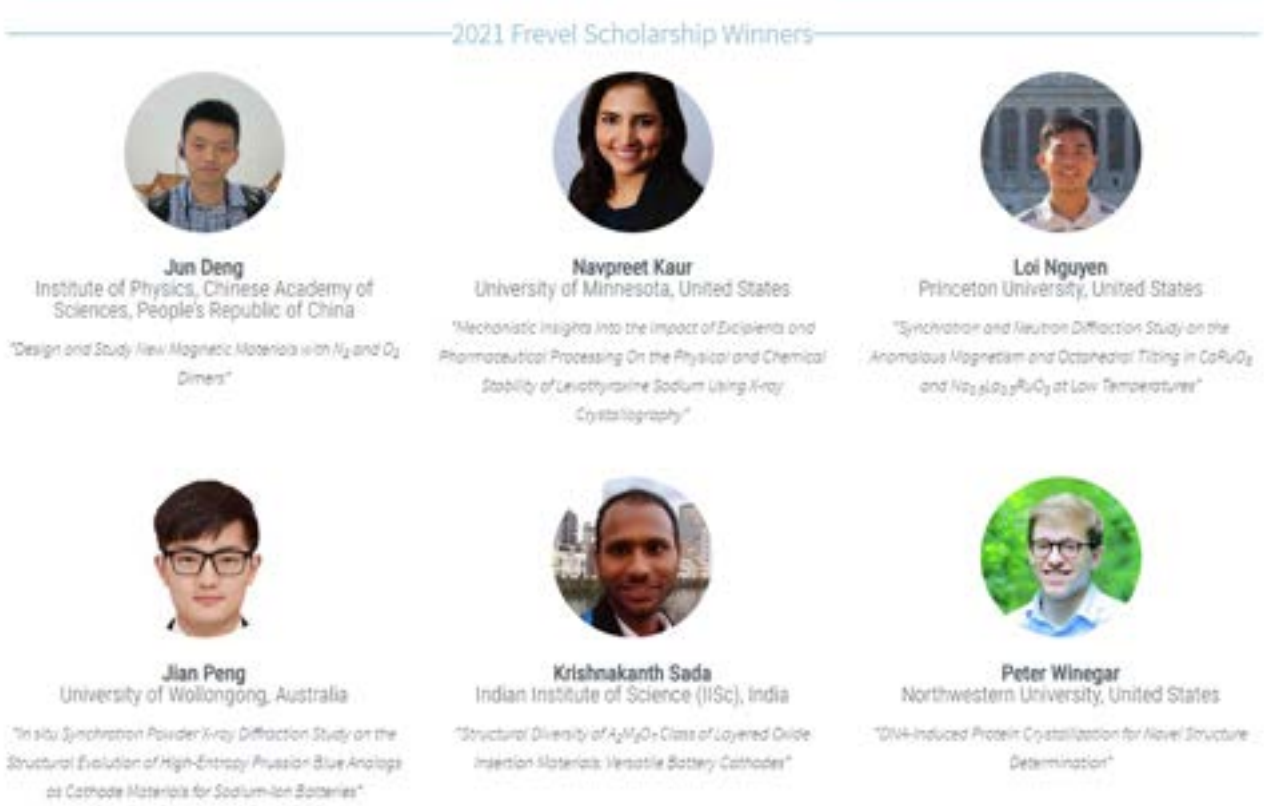
AWARDS AND PRIZES

2021 Ludo Frevel Crystallography Scholarship Awards



To encourage promising graduate students to pursue crystallographically oriented research, the International Centre for Diffraction Data (ICDD) established a Crystallography Scholarship Fund, known as the Ludo Frevel Crystallography Scholarship Fund, in 1991.

The ICDD Ludo Frevel Crystallography Scholarship Committee has selected six recipients for the 2021 Scholarship Program. These recipients were selected on a competitive basis, from 54 applications received by the ICDD Scholarship Committee.



The ICDD will present each of these students with a check in the amount of USD2500 to assist in the continuation of studies in their selected fields of crystallographic research.

Applications for the 2022 Scholarship Awards open in August 2021 at https://www.icdd.com/ludo-frevel-scholarship/.

AWARDS AND PRIZES

Struchkov Prize moves to the IUCr



Yuri T. Struchkov (photo contributed to the IUCr gallery by Leonid Aslanov).

Ilia Guzei, Victor Khrustalev, Tatiana Timofeeva, Alex Yanovsky

The IUCr Executive Committee has just established the Struchkov Prize to promote excellence in structural science and to recognize young talented individuals working in the field of small-molecule crystallography. The Prize honors the memory of the prominent Russian scholar and crystallographer Yuri T. Struchkov. The Prize consists of a certificate and monetary award that will be granted to three individuals on a triennial basis during the IUCr Congress years.

Yuri T. Struchkov (1926–1995) was an outstanding Russian crystallographer who made substantial contributions to the structural chemistry of organic and organometallic compounds. He started his career in the early years of structural studies of organic solids and was perhaps the most vocal champion of this field in the USSR and Russia. He then became the founder and long-time director of the X-Ray Structural Centre of the Russian Academy of Sciences, one of the most productive laboratories in the field of “small molecule” organic crystallography in the world in the last decades of the 20th century. His achievements were highly appreciated by the international crystallographic community: at the XV IUCr Congress and General Assembly in Bordeaux, France, in 1990 he became a member of the IUCr Executive Committee and at the next Congress in Beijing, China, in 1993 he was elected Vice-President of the IUCr. He did not complete his term as Vice-President; his untimely death came as a consequence of an unsuccessful heart surgery in August 1995.

To commemorate Professor Struchkov’s life achievements, his friends and former colleagues established the Struchkov Prize, which has been awarded to young scientists from the former Soviet Union for the best research work in the field of X-ray crystallography every year between 1997 and 2020. Since the inception of the Prize, 24 Struchkov competitions have been held and more than 30 top and 50 secondary prizes have been awarded. The Prize was funded by donations from former colleagues and students of Professor Struchkov, researchers who knew him personally, colleagues closely familiar with his scientific achievements and contributions to the organization and development of chemical crystallography in Russia, as well as by private companies. Over time, the annual prize purse of the Struchkov competition has increased substantially, from USD 500 in 1997 to more than USD 5000 in 2020. Importantly, 100% of all contributions were annually awarded to the laureates of the Struchkov Prize competition.

As the Struchkov Prize gradually became a regular and familiar feature of the Russian crystallographic landscape, it provided name recognition to many young researchers at the beginning of their professional careers. Many winners and laureates of the earlier Struchkov competitions matured to

become prominent scientists and highly regarded members of crystallographic community in their own right. The Prize has been the subject of three *IUCr Newsletter* publications: *IUCr Newsletter* (2000), **8**(4), 18; *IUCr Newsletter* (2007), **15**(3), 17; and *IUCr Newsletter* (2019). **27**(2), 22.

In the spring of 2020, the organizers and supporters of the Struchkov Prize decided to explore the possibility of bringing the Prize to the international stage and reached out to the IUCr President Sven Lidin and the other Executive Committee members, asking if the IUCr would consider incorporating the Struchkov Prize into the growing family of prestigious awards administered by the Union. We were delighted to receive a positive decision and are very thankful to the Union's highest officers' warm and welcoming attitude.

The Struchkov Prize transition from being a Russia-based prize to an international prize is congruent with the international nature of scientific work and multi-national collaborations. While the Prize was established in 1997 to recognize young Russian small-molecule crystallographers and researchers working in related fields, we felt that as a global award the Prize would also reflect Professor Struchkov's life-long conviction that crystallography, just as any other science, should represent joint international effort. Whereas he lived most of his life in a closed and highly prejudiced society, he relentlessly fought for universal integration and openness of the science in the USSR in spite of substantial risks to his career. Therefore, we believe that Professor Struchkov himself would have approved the decision to seek acceptance of the Struchkov Prize as one of the IUCr awards.

Additional information about the Struchkov Prize, including details of the nomination process and how to donate to the funding for the Prize, is available here.

We encourage you to consider nominating your young colleagues (or yourself) for the IUCr Struchkov Prize.

OBITUARY

Judith Milledge (1927–2021)



Judith at Atlantic College, Vale of Glamorgan, UK, in 2011.

Ian Wood, Monica Mendelssohn, Mike Glazer

Older members of the crystallographic and mineralogical communities will remember H. Judith Milledge (née Grenville-Wells) who died in London, UK, on 23 January 2021 aged 94.

Her parents having moved from England in 1923, Judith was born in 1927 in Kokstad, South Africa (a farming community in Kwa-Zulu, Natal, about 300 miles from Kimberley, where diamonds are famously mined), and she attended Rhodes University in the Eastern Cape Province just after the end of World War II. Judith's mother was determined that she should study a science, despite the fact that she had been to a school with no science on the curriculum. Judith said that she took Physics at Rhodes because, when she was discussing the merits of taking either Physics or Chemistry, the professor of Chemistry (probably unwilling to take on a total beginner) was very quick off the mark in assuring her that Physics would be the best for her! It must have been a strange experience, as in those days very few women were admitted to university to study science. Also, the majority of Judith's fellow students were men who had just returned from active war service and who found great amusement in livening up dull classes by discovering ever more spectacular ways of destroying parts of the teaching laboratory. After taking a BSc and an MSc from Rhodes, Judith went straight to work in the new De Beers Diamond Research Laboratory in Johannesburg, but she soon realised that she needed to take a PhD in crystallography. Initially, she approached R. W. James, Chair of Physics at the University of Cape Town, but he was too unwell to take her as a student and so he suggested that she contact Kathleen Lonsdale in London instead.



Judith in the De Beers laboratory, South Africa, *ca* 1948. Photo credit: Robert Caveney, De Beers.

In 1949, Judith left South Africa and moved to London to begin her PhD, working on diamonds at University College with Kathleen Lonsdale, and for some time she lodged with the Lonsdales in return for secretarial help in the preparation of the *International Tables for X-ray Crystallography*. After completion of her PhD, Judith moved to a post-doctoral position at MIT, working with Sidney Abrahams. On her return to UCL, she re-joined Lonsdale's research group in the Department of Chemistry, eventually achieving the position of Reader in Crystallography at the University of London, by which time the University had also awarded her a DSc. Kathleen was one of the most important influences on Judith's life and they became close collaborators. In later years, Judith was very proud of her association with Kathleen, who she clearly held in the highest regard, and she took her role as the executor of Kathleen's literary estate extremely seriously. By the late 1970s, after Kathleen's retirement, the Chemistry Department was going through a protracted phase of transferring to a new building, which did not suit Judith, and so, as her Readership was tenable in any department of the University, she moved to UCL's Department of Geology (now Earth Sciences), which enabled her laboratory to remain in the same location, and where she spent the rest of her career. This proved to be a wise decision, both for Judith and for the Geology Department, as it laid the foundation for the excellence in mineral physics at UCL that continues to this day. Judith continued to work until well after the normal age of retirement; she was still active scientifically until well into her eighties, and co-authored her last paper aged 87.

Judith published well over 100 scientific papers, covering an extremely wide range of topics in crystallography and mineralogy. This tendency to cast her net wide probably resulted in her being somewhat less well known than if she had focused her work more narrowly. Also, although a very intelligent and clever person, she suffered from the problem that once she had an answer to a scientific question she always felt that further work needed to be done before it was ready for publication. On one occasion, relatively recently, an editor of *Nature* was heard to remark to Judith along the lines that "your work on these diamonds looks very interesting, I'm pretty sure that we would like to publish it" only to be

told that “well – maybe – but I don’t think it’s quite finished enough to send to you yet” – a response that was greeted with incredulity by at least one younger colleague. Judith was very aware of Kathleen’s frustration with her; reminiscing after her retirement, she remarked that “Kathleen was always saying to me ‘Judy, you must publish these things’ - but of course I never took a blind bit of notice”.

Crystallographically, Judith had little interest in “routine” structure determination, preferring instead to concentrate on crystals that showed disorder, phase transitions or solid-state reactions. The advent of computers in the 1950s was of great interest to crystallographers and Kathleen observed to Judith that “one of us is going to learn to use a computer and I do not think it is going to be me”. In the earlier part of her career, therefore, Judith became one of the pioneers in crystallographic computing. She was assisted in developing relevant programs, on a Ferranti Pegasus computer, by Derek Milledge from Ferranti, whom she married in 1958. Early in 1964, Kathleen and Judith acquired a Pegasus (now in the Science Museum) for their research group. Judith continued to use Pegasus until 1980 – it had the advantage of giving her full access to what was still a relatively powerful machine (for a single user), but the disadvantage that her codes, written in a very low-level language, could not easily be adopted by others. She did, though, retain an interest in the methods of structure determination, collaborating with colleagues in the Statistics Department at UCL in the use of Bayesian methods in structure refinement. Judith’s interests in crystallographic techniques covered a very wide range, extending from apparatus for calculating Fourier transforms (pre-electronic digital computers) to ingenious devices to improve the methods for collecting data from single crystals. During her time in the Chemistry Department, for single-crystal work, she greatly preferred to use photographic methods, rather than the more fashionable approach that was then extant using four-circle goniometers with single-point counters, arguing that one should always look at the whole of the diffraction pattern, rather than just at the positions where the Bragg reflections were expected, as otherwise X-ray intensity from non-Bragg reflections, such as diffuse scattering, would be missed. She would have been very pleased to see the modern generation of instruments using area detectors.



Judith at the 8th IUCr Congress in Stony Brook, NY, USA, in 1969. Photo contributed to the IUCr gallery by Sidney C. Abrahams. Judith served on the IUCr Commissions on Crystallographic Teaching (1954–1957) and Crystallographic Studies at Controlled Pressures and Temperatures (1968–1969; Chair 1969–1972).

Like Kathleen, Judith took the teaching of crystallography very seriously, considering that it was important to introduce students of many disciplines to crystallographic methods and also that the subject should be taught primarily by means of practical work. For the UCL Chemistry Department, they devised a week-long course during which students mounted and set a single crystal of either urea or hexamine on an oscillation camera, determined its cell parameters, measured a set of intensities and then “solved” the structure (assuming the phase angles were known) by producing an electron-density map using a von Eller “Photosommateur”. After she moved to the Geology Department at UCL, Judith devised a similar set of practical exercises based around mineral samples, where students learned about such things as the determination of crystal morphology, cell parameters, orientation distributions and phase identification from powder data. Sadly, the time taken, level of demonstrating required and expense of running such courses means that they are probably now no longer practicable at universities in the UK; the students are much the poorer for their loss.

After joining the Geology Department at UCL, although Judith continued to collaborate with colleagues in other departments, principally in Engineering, she switched the main focus of her research back to the study of diamonds, the material which, in truth, was her dominant interest throughout all of her career. In collaboration with Monica Mendelssohn at UCL and with colleagues in other universities, she co-authored some highly regarded papers on the formation of diamonds, their isotopic compositions, their micro and macro inclusions and their defects. An obvious necessity for diamond research is that the researcher should have access to diamonds for which the source is accurately recorded, information which, with modern mining practices, can now often be very difficult, or impossible, to obtain. It is probably in this area that Judith’s work will have its most long-lasting legacy as she had very diligently, over many years, accumulated and characterised a very large collection of well-provenanced samples. After Judith retired, she arranged for her collection to be divided between South Africa and the UK where it will provide an invaluable resource for mineralogists for many years to come.

On a personal level, Judith was essentially a rather shy person and quite reluctant to talk about herself too much. She could, though, be an excellent companion over a convivial dinner and she was a loyal friend, adviser and helper to those she enjoyed working with, especially to her former PhD students, several of whom have gone on to distinguished careers as scientists. One of her former students, Josh Thomas (Professor emeritus at Uppsala University) has written of her “She was a unique person – and it was a privilege to have had her ‘pushing me’ as my supervisor. However excited I was to show her some new result – she would always (not listen!) and respond: ‘Now what you should REALLY do is .... ‘! I learnt a lot from that – to never be satisfied with my latest result – it's upset a few of my own students over the years, but it made them, like me, better (true) scientists. I have never forgotten the genius of her studying garnet and olivine inclusions in a diamond – mounted on a thermocouple. A truly inventive “poor man's HT/HP anvil for single-crystal XRD”!!! I'll miss her – but she's always there "in my head"!”

OBITUARY

Stanko Popović (1938–2020)



Dubravka Matković-Čalogović, Marijana Đaković

With great sorrow we inform the crystallographic community that our colleague Academician Stanko Popović, Professor Emeritus, passed away on December 17, 2020 at the age of 83.

Stanko Popović was born in Čitluk, Croatia, in 1938. He graduated in Experimental physics from the Physics Department, Faculty of Science, University of Zagreb (UniZg), Croatia, in 1961, where he obtained an MSc degree in 1965 and a PhD in Physics in 1968. In the period 1961–1987 he worked at the Ruđer Bošković Institute, Zagreb, where he was promoted to Senior Scientist in 1979. At the Ruđer Bošković Institute, he was the Head of the X-ray Laboratory. In 1987 he was elected to the position of Full Professor at the Physics Department, Faculty of Science (UniZg). From 1996 till retirement in 2008 he held a Permanent Full Professor position at the same Faculty. In 2011 he was appointed Professor Emeritus. Since 2004 he was a full member of the Croatian Academy of Sciences and Arts.



Professor Popović specialized at the Metallurgy Department, University of Manchester, UK, and was a visiting professor at the Slovak Academy of Sciences, Bratislava, Slovakia, and at Martin Luther University, Halle, Germany.

Within his long scientific career, his interest was in crystallography, solid-state physics, solid-state chemistry, general physics, powder X-ray diffraction, electron microscopy and spectroscopy. His work resulted in 255 scientific papers and he presented over 250 contributions at scientific meetings, including 35 invited lectures (2nd European Crystallographic Meeting, Keszthely, Hungary, 1974; 1st European Crystallographic School, Pavia, Italy, 2014; 29th European Crystallographic Meeting, Rovinj, Croatia, 2015; and others).

Stanko Popović was a member and a chair of the organizing and scientific committees of many international meetings such as the European Crystallographic Meetings (ECM13 and ECM29) and the European Powder Diffraction Conferences (EPDIC11, EPDIC12). He was a member of the European Powder Diffraction Conferences council (2001–2012).

He put a lot of energy and enthusiasm into international confirmation of the Croatian Crystallographic Association (CCA), where he was Secretary (1992–2006) and President (2006–2017). He was the delegate of CCA during the acceptance of CCA into the IUCr and the ECA in 1992.

Stanko was a scientist with very broad knowledge and a pleasant personality. His friends and colleagues in the crystallographic community will miss him very much.



Stanko Popović with his wife, Božena, on the excursion during the 26th Croatian-Slovenian Crystallographic Meeting in Poreč, Croatia, in June 2018.

This obituary has been republished, with permission, from the ECA website.

BOOK REVIEW

Architects of Structural Biology: Bragg, Perutz, Kendrew, Hodgkin



Helen Maynard-Casely

By John Meurig Thomas. Oxford University Press, 2020. ISBN 978-0-19-885450-0. Reviewer read electronic edition on the Kindle app.

The past year has again highlighted how important structural biology continues to be to the health and wellbeing of the human population. The extraordinary efforts to develop a vaccine to counter the COVID-19 pandemic have been made possible by the body of work that has revealed the structure of coronaviruses, how they interact with our bodies and critically their weaknesses. But how did structural biology come to exist as a field? Where does it have its roots, and how perhaps have these shaped the methodology applied today? This is what the book *Architects of Structural Biology* seeks to address, framing this about the achievements and personalities of some of its pioneers.

The author of the book, John Meurig Thomas, who passed away in November 2020, had a unique perspective on this topic. A celebrated scientist and historian of a number of fields, and though not a structural biologist himself, he views the beginnings of the field through the lens of the Davy-Faraday Research Laboratory and Peterhouse College, University of Cambridge, UK – institutions in which he held leadership positions.

The book is structured as a series of monographs that chart different aspects of the beginnings of structural biology, focusing mostly on activities within first the Davy-Faraday Research Laboratory, which had its home at the Royal Institution in London, and then later the UK Medical Research Council's Laboratory for Molecular Biology, which was founded in Cambridge. The work is framed round four pioneers, named in the title: Laurence Bragg, Max Perutz, John Kendrew and Dorothy Hodgkin. That said, the monographs do in fact reveal a large cast of other personalities who each shaped the field in these early years.

The structuring of the monographs starts from the founding of crystallography and diffraction experiments and charts the application of these from simple salts, to small organic structures, to larger molecular material up to the realisation of the first full protein and enzyme structures. Within each, the achievements of those named in the title are set in the context of their contemporaries and the events surrounding them. The impact of the beginnings of structural biology is brought right up to the present day, through the current research of those now residing at Peterhouse College and the innovations of cryo-electron microscopy in the last two chapters.

From a personal view, I am often uncomfortable with veneration of individuals in the founding of fields of science that have lasted decades and I did find the focus of the book upon four scientists somewhat strange. There is more content written in this work about Aaron Klug and Linus Pauling than there is about Hodgkin and Kendrew, for instance, though the reader is directed to Ferry's 1998 biography of Hodgkin and alludes to Wassarman's now published work on Kendrew. I was left a little puzzled on the framing of Hodgkin as an architect of structural biology. I can see how Thomas applied this moniker to Bragg (in his leadership of the Royal Institution and encouragement of the early years of structural biology), to Perutz (in his role in establishing the Laboratory of Molecular Biology) and to Kendrew (in his inaugural directorship of the European Molecular Biology Laboratory), but I feel that Thomas did not elaborate enough on Hodgkin's role as an architect of the field. This book did also, briefly, draw my attention to a group of still invisible individuals – the human 'computers' that were vital in the early charting of the hundreds of thousands of diffraction spots from the early diffraction patterns; I would like to read more on the contribution of this group.

I do enjoy reading accounts of this rather golden time of science; in particular I find the tales of chance encounters and interdisciplinary meetings that pepper the monographs very enriching. A haunting passage recounts how Max Perutz (who was from an Austrian-Jewish family) hosted Heidelberg for dinner in Cambridge, and later remarked how he was unconvinced that Heidelberg had not assisted the Nazis in their attempts to create an atomic weapon. Though I have previously read much on the life of Dorothy Hodgkin and Laurence Bragg, I admit quite a blind spot as to the writings of Max Perutz, and am now searching for a copy of his *Is Science Necessary?* work.

The book is a fascinating behind-the-scenes journey through the early years of structural biology, though viewed very much from a UK perspective. The real insight of this book is not so much the stories of the four cited pioneers, but their interactions with a wide cast of people who founded the field. The commentary on different leadership styles is very acute, as well as the respectful telling of some of the personality clashes and rivalries that developed. This would be an excellent read for those who are beginning to specialise in structural biology, and those with a love of the history of crystallography.

Helen Maynard-Casely is at the Australian Nuclear Science and Technology Organisation.

BOOK REVIEW

International Tables for Crystallography, Volume H, Powder Diffraction



Leopoldo Suescun

First edition. Edited by Christopher J. Gilmore, James A. Kaduk and Henk Schenk. Wiley, 2019. Pp. xxxiii + 904. Price (hardcover) GBP 320.00. ISBN 978-1-118-41628-0.

Volume H of *International Tables for Crystallography*, a long-expected update and expansion of Chapters 2.3–2.6 and 3.4–3.6 of Volume C of *International Tables for Crystallography* (2011) (ITC-Vol. C), has been published.

This 904-page-long book provides a comprehensive description of the powder diffraction method, aimed at novice users who need to familiarize themselves with the details of the method and related techniques based on polycrystals or multiple-particle systems. Furthermore, it provides a very good compilation of fundamentals, methods and case studies useful for the specialist looking for theoretical details, application notes and up-to-date references. This book will soon become an irreplaceable tool for teachers, researchers and students.

The book is divided into seven parts organized as follows: fundamentals (Part 1); instrumentation requirements, both standard and state of the art, and sample preparation tips and tricks (Part 2); methodologies, ranging from instrument alignment and data collection to the many possible aspects of data analysis (Part 3); applications to structure (Part 4) and microstructure (Part 5) determination and analysis; available software (Part 6); and applications and perspectives of powder diffraction for characterizing different families/classes of materials (Part 7). Although the book is mostly devoted to X-rays, neutron and electron powder diffraction are introduced and discussed in Chapters 2.3 and 2.4, respectively. These techniques are also discussed in many examples throughout the text.

A detailed description of each part, with some highlighted chapters, is given below.

Part 1, the *Introduction*, gives the reader an overview of the concepts required to understand the information contained in a powder diffraction pattern (diffractogram). It follows a logical approach, starting with peak positions, then moving to peak intensities and peak shapes, and finally background, in Sections 1.1.1–1.1.5, respectively. Bragg's law is first introduced, then reciprocal space and Laue equations are covered, and finally the Ewald sphere and Debye rings are described. The nomenclature used for the scattering vector (**h**) and related direct- and reciprocal-space magnitudes is consistent with that used in the *Online Dictionary of Crystallography* (https://dictionary.iucr.org/Main_Page), which is much appreciated. Peak intensities are discussed very briefly. The structure factor is calculated from the

sum of all scattered waves from individual atoms in a crystal [the reader is directed to the discussion of atomic scattering factors (f_j) in ITC-Vol. C], later using the periodicity to restrict the sum to one unit cell. Finally, the scattered intensity from a powder, including all required corrections, is presented. Profile shapes are described using convolution and Fourier transform equations that will later be derived in detail, such as Scherrer's formula and microstrain broadening (Chapters 5.1 and 5.2). A long digression leading to atomic pair distribution function analysis is given when the background is discussed (Section 1.1.5). This finally leads, in Section 1.1.6, to a first mention of Rietveld analysis combined with structure determination, local structure and parametric refinements. The end of the *Introduction* is a one-paragraph *Outlook* section (1.1.7) with a concise discussion on why powder diffraction has been and will continue to be so relevant to the materials community, despite progress in electron diffraction and synchrotron single-crystal instrumentation that has enabled structure solution with samples of the size of one powder grain.

Part 2 is devoted to *Instrumentation and sample preparation* and is the longest (197 pages), thus stressing the experimental nature of this area of crystallography. Experts on experimental techniques and instrumentation take the reader from conventional in-house powder diffractometry to the latest developments in *in situ* multi-technique characterization of polycrystalline materials. Sample preparation advice for each type of experiment is given. Chapter 2.1 explores all aspects of in-house laboratory equipment, focusing on relevant details of the widely used Bragg–Brentano geometry. Frequent alignment errors and corrections are discussed, and geometries for non-routine powder/polycrystalline diffractometry are described. Non-expert users who wish to learn about different options for in-house instrumentation will find this chapter enlightening. Chapter 2.2 focuses on powder diffraction using synchrotron radiation; production of X-rays, monochromatization, instrumentation and details of choice of instrument parameters for specific applications are discussed. This chapter highlights the main advantages of synchrotron radiation relative to in-house instruments, including anomalous/ resonant scattering and specialized fast data collection instruments for *in situ*/*operando* experiments. Chapter 2.3 focuses on neutron powder diffraction. Most of its initial section emphasizes the complementarity of this technique with X-ray diffraction. A detailed section on neutron production follows, covering both reactor and spallation sources. A neutron powder diffraction instrumentation section completes an up-to-date review of the state-of-the-art neutron powder diffraction multi-user facilities. A succinct review of the type of experiments that could be performed to characterize powder and polycrystalline samples concludes the chapter. Although magnetic neutron diffraction is mentioned, no details are given; as a result, Part 6 of ITC-Vol. C remains the only source of magnetic neutron diffraction in the *International Tables* series. Chapter 2.4 gives a brief description of electron powder diffraction. This chapter is too short to provide the reader with an adequate perspective of the technique; references to figures and tables from other books are overabundant. The most interesting parts of the chapter are those devoted to texture, Rietveld and future applications of the pair-distribution-function analysis of electron diffraction data. Chapter 2.5 deals with two-dimensional powder diffractometry and provides extensive geometrical details, as well as a derivation of scattering equations for the purpose of describing each pixel of an area detector used in powder diffraction. It is a very good introduction to the experimental details of texture and microstructure analysis and to the newest trends of powder diffractometers for non-conventional experiments. Chapters 2.6 and 2.7 are devoted to nonambient-temperature and high-pressure powder diffraction, respectively. They are short and well written with enough examples to give the newcomer a good overview of the requirements, difficulties and possibilities of these methods. Chapter 2.8 discusses powder diffraction in external electric and magnetic fields. Although this chapter overlaps significantly with previous ones, the many interesting examples make up for the repetition. Chapter 2.9 describes cells for *in situ* powder diffraction investigation of chemical reactions. A plethora of reaction chambers and setups for X-ray and neutron powder diffraction are illustrated with results obtained using these setups, making this chapter to the point and practical. The final chapter (2.10) covers powder specimen preparation, both for in-house and for user-facility experiments, and focuses on describing deviations from an ideal powder that result from poor sample preparation and how to avoid such issues. It is also an excellent reminder that no data set is better than the sample used to collect it. Again, a plethora of

examples are provided; special sample holders to facilitate proper sample preparation are described, and practical advice is given. This chapter is indispensable for any user of powder diffraction instruments, whether in house or user-facility based.

Part 3 focuses on *Methodology*, giving an in-depth treatment of some of the concepts set out in the *Introduction*. Chapter 3.1 describes all the elements of a conventional diffractometer and the step-by-step alignment process to obtain the best possible powder diffraction pattern. It will be very useful for scientists and technicians who need to take care of an in-house instrument on a daily basis. Chapter 3.2 deals with diffraction physics. All relevant equations to understand the observed powder diffraction intensities are presented. It is the only chapter where some phenomena relevant to quantitative phase analysis such as microabsorption, surface roughness and extinction are discussed. Texture and anisotropic strain broadening are also covered, with a focus on modelling profile widths. Anisotropic strain broadening is again treated in Chapter 3.3, which is devoted to modelling powder diffraction peak profiles for different experimental techniques. These two chapters are particularly relevant for users of the Rietveld method because profile modelling is a common issue for beginners. Chapter 3.4 deals with indexing of powder diffraction patterns from unknown phases. The challenge behind indexing a pattern is described, as well as how the success of the indexing process is assessed; details of the computations performed by the different indexing methods are wisely skipped. The most successful traditional indexing programs and some new approaches developed in the past three decades are discussed, including examples of use of free and commercial programs. Chapter 3.5 deals with intensity extraction and data reduction, *i.e*. how to obtain the observed structure factor modulus from an indexed powder diffractogram. The material presented in this chapter relies heavily on assumptions made in the Rietveld method, which has not been treated extensively at this point. Chapter 3.6 discusses whole powder pattern modelling, aiming to determine particle size, strain defects and other microstructural features of the sample without the use of structure factors. It is a long chapter with a significant number of complex equations that are very well contextualized and illustrated by examples, making this chapter instructive for beginners. Crystallographic databases are discussed in Chapter 3.7, with a very strong focus on the Powder Diffraction File (PDF) from the International Centre for Diffraction Data. This database is the product of extensive international collaboration for the compilation of accurate powder diffraction data from different sources and in different formats with physical and chemical context. Currently, this database provides both calculated and experimental powder diffraction patterns, which makes it a comprehensive tool for users. This chapter also covers other relevant crystallographic databases that contain structural details, such as the Cambridge Structural Database, the Inorganic Crystal Structure Database, the Protein Data Bank, Pearson’s Crystal Data and the Crystallography Open Database. More specific databases devoted to metals, minerals and zeolites are mentioned too. Also discussed in this chapter is the search–match process of identifying phases in a powder diffractogram. This discussion contains a very interesting series of examples using the PDF-2 database. Chapter 3.8 focuses on clustering and visualization of powder diffraction data, with application to sequential or multi-sample studies. This is a new and exciting area of powder diffraction analysis, brought about by the availability of robotic instruments and *in situ* studies at user facilities; as such, it deserved to be included in this part. Correlation coefficients that are used to identify similarities and differences between diffraction patterns (or spectra in general) are described, finally leading to the identification of groups of powder patterns by similarity in composition (cluster analysis). The chapter layout, however, is far from satisfying. The examples presented throughout the chapter are worth reading, including a multi-technique analysis combining powder diffraction and Raman spectroscopy data. This chapter requires significant improvements in future editions. Finally, Chapters 3.9 and 3.10 describe quantitative phase analysis methods based on individual peak intensities and the Rietveld method, respectively. The accuracy of the results obtained with the latter with regards to quantification of phases is also discussed. These two are very well written chapters that present the fundamentals in a didactic manner and discuss several examples from different disciplines, including data that the reader can download and analyse on his/her own.

Part 4 is entirely devoted to structure determination using powder diffraction data. The opening chapter (4.1) begins with a presentation of the problem underpinning structure determination using powder diffraction data and an overview of relevant methods to tackle this challenge. Chapters 4.2 and 4.3 discuss the structure determination of molecular crystal structures by reciprocal-space and direct-space methods, respectively. Both chapters are very didactic; they skip the deep mathematical details yet discuss many methods and programs and use multiple examples to illustrate how structures may be successfully determined. Chapter 4.4 shows how to incorporate supplementary crystallographic information into a structure solution procedure, with examples and test data. Chapter 4.5 is devoted to structure determination and refinement of inorganic structures, where the inclusion of restraints for polyhedral coordination and connectivity is important. Chapter 4.6 introduces the reader to the world of zeolites and their structure determination and refinement. Similarly to other chapters, it provides a good introduction for the beginner and is full of examples. Chapter 4.7 is devoted to the history and working principles underlying Rietveld refinement. This chapter is entirely descriptive, with no figures or examples given, yet very useful for understanding how and why the method works and the details of its implementation in computer programs. Chapter 4.8 introduces and discusses the maximum-entropy method (MEM) for refining structures from powder diffraction data. A number of detailed examples help the reader follow the strategy of refinement programs and MEM-assisted structure determination with the chargeflipping method. Chapter 4.9 discusses the required steps for validation of a structure determined from powder diffraction data. This is a very useful chapter that helps the reader identify key points to assess the quality of the refined structural model and what could reasonably be obtained from a structural Rietveld refinement based on a specific data set. This discussion is mostly based on examples from different types of materials. Part 4 closes with Chapter 4.10, which introduces and discusses reporting of structures, data and fit results using the powder-diffraction-oriented Crystallographic Information File standard (pdCIF) in the broader context of the general CIF. The last two chapters are a must-read for students and researchers who aim to publish in this area.

Part 5 provides an in-depth description of the impact of defects, texture and microstructure on a powder diffraction pattern, expanding on concepts first introduced in Section 1.1.4. None of the relevant equations are skipped and a detailed derivation of each one of them is given. Chapter 5.1 explains the origin of size broadening and derives Scherrer’s formula, emphasizing the limited applicability of its most simplified version. Chapter 5.2 deals with stress and strain. The chapter contains no figures or examples, making it one of the less didactic of the book. Chapter 5.3 discusses quantitative texture analysis, including the study of samples with texture, defects and microstructural effects. The chapter contains many examples, making it very approachable for the beginner as well as useful for the expert looking for more details. Chapter 5.4 introduces thin-film and multilayer analysis by diffraction techniques, including diffraction and reflectivity characterization; this is an important addition to the *International Tables for Crystallography* series. The chapter discusses instrumental requirements and different configurations, and also provides an engaging perspectives section that highlights future challenges in this area. Chapter 5.5 discusses multigrain crystallography and three-dimensional grain mapping. These are also new techniques that were born from modern synchrotron sources with micro/nanometre-focused and coherent beams. The chapter provides examples and experimental details that help the reader understand the basics and results that may be obtained. Chapter 5.6 is devoted to X-ray diffraction from non-crystalline materials and the Debye model. This is an enlightening chapter showing how much information is available in peakless patterns and in the background of partially crystalline samples. It is the perfect transition to Chapter 5.7, which is devoted to total scattering and atomic pair distribution function (PDF) analysis; special emphasis is placed on the nanostructure problem. This is also a very didactic chapter, without skipping the mathematical formulation, and includes plenty of easy-to-follow examples and details. It discusses X-ray, neutron and even electron PDF analysis, including data reduction and processing, structural analysis, and determination using total scattering data. Chapter 5.8 goes one step beyond Chapter 5.7 and discusses the characterization of disordered heterogeneous materials by small-angle scattering techniques. In this chapter, the nanostructure problem is discussed beyond the atomic structure of the nanoparticle, with a focus on the nano- to submicrometric scale.

Small-angle X-ray and neutron scattering are presented, including magnetic small-angle neutron scattering, with a good number of applications and examples and a very inspiring perspectives subsection.

Part 6 contains a table with a survey of 200 computer programs and software packages for powder diffraction data analysis in all of the areas discussed in the book. Although it is not expected that such a complete list of programs will remain accurate for a long time, it is surprising that more than 15% of the programs listed could not be found at the given web addresses, maybe due to the COVID-19 pandemic; furthermore, five of them appear to be permanently unavailable.[1]

Part 7 contains 14 different chapters, unrelated to each other, where applications of powder diffraction are shown. The relevance of the Rietveld method to the analysis of powder diffraction data is highlighted in this part, with 12 of the 14 chapters discussing at least one example of its use. This is the perfect place to find examples for a dissemination lecture or an introductory powder diffraction course. The applications that are discussed are macromolecular crystallography (7.1), forensic science (7.2), materials for energy storage and conversion (mainly Li-ion batteries) (7.3), arts and archaeology (7.4), pharmaceuticals (7.5), and mining and minerals processing (7.7), along with specific chapters on aluminium ores (7.6), the petroleum and petrochemical industries (7.11), and cements (7.12). Ceramic and glassceramic materials are discussed in sections 7.8 and 7.9, respectively, followed by industrial organic pigments (7.10), superconductors (7.13) and finally minerals (7.14). Each reader will find at least one chapter on his/her area of interest, regardless of the area of powder diffraction (or crystallography in general) they come from. Noteworthy is the final chapter of the book, entitled *Powder diffraction by minerals*, which instead of focusing on past achievements highlights the challenges and future developments needed to address the most important questions in the area today; this makes it one of the most inspiring chapters of the book.

As in every first edition of this kind of multi-author book, a number of nomenclature discrepancies and repetitions are found that may be corrected or better addressed in future editions.[1] Use of colour is very uneven through the book: many figures, but especially those in Chapter 4.5, would immensely benefit from it. In many chapters, examples of results obtained with different programs are given, extracted from the literature or from the author’s database. Having more of these data sets available for the reader to reproduce the results given would be a great addition to the book. Finally, an index of phases for which powder patterns are shown would also be a good addition to a second edition of the book, since a search for phases would quickly help the reader identify interesting characteristics or frequent problems of his/her samples and relevant literature.

In summary, *International Tables for Crystallography* Volume H is a book that the community has been long expecting from the IUCr. It will undoubtedly occupy an important place on the shelves or desks of every modern powder diffraction laboratory, especially multi-user laboratories where researchers with different backgrounds could benefit from the fundamentals, multiplicity of practical advice, examples, and up-to-date bibliography presented in each chapter of the book. This book should be celebrated as an achievement of the Editors, the authors, and the well established and broad community of powder diffraction users.

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References

International Tables for Crystallography (2011). Vol. C, *Mathematical, Physical and Chemical Tables*, 3rd ed., edited by E. Prince. Chichester: Wiley.

[1] A list of corrections, including updated addresses for computer programs that have changed sites, has been communicated to the Editors of Volume H, and corrections to be included in the next edition will be

posted on the *International Tables* web site (https://it.iucr.org/H/) in due course.

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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