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LETTER FROM THE PRESIDENT

Positive vibes and reasons for celebration



Hanna Dąbkowska

Many positive things are happening around us now. Countries – and employers – are opening up for international, non-essential travel, and schools are moving back to in-person teaching and laboratory programs. Unfortunately, the situation can change very fast – as it just did since I wrote this Letter in late November.

Many organizers of crystallographic meetings have to decide if their meeting should be virtual, in person or hybrid. What we have all learned is that hybrid meetings can be a great success (for example the Prague Congress) as can virtual meetings (for example both recent ACA meetings). Having said that, we all want to see our friends and get together in person. Meeting organizers must now follow local regulations. It will probably make attending a meeting more difficult for our unvaccinated colleagues. I do not expect there will be many of those – but we all have to respect the rules.

The positive vibe in the IUCr community is that the Commissions (and the IUCr has 24 of these) are getting together, planning future meetings and starting to prepare for the (still hybrid?) International Program Committee (IPC) meeting in 2022 and for the Melbourne Congress in 2023.

I recently received a few questions about the role of Consultants to the Commissions. The Commissions' role is described in the Statutes and By-Laws of the IUCr. Commissions are responsible to the General Assembly (GA). “They shall generally have full freedom in arranging their internal structure and work. They may formulate their own Rules of Procedure within the framework of the Statutes and By-Laws of the Union, and within their terms of reference.” More explanation about the role of Commissions, their Members and Consultants is clearly presented in the General Statement of Principles Regarding Commissions of the IUCr. “Subject to the approval of the President, Consultants may be appointed at any time to strengthen any Commission. The immediate past Chair is automatically appointed as a Consultant. Consultants who have proved active in working for a Commission are good candidates for nomination as full members.” From my own experience, I can say that Consultants are a vibrant and important part of any Commission. They are passionate about the Commission's work and can be great advisers to the Chair. Some of them served as the Commission Members in the past.

On a different note: two important events have happened very recently. I was invited to speak at both of them virtually.

The first one, the Constitution of the African Crystallographic Association (AfCA), took place on 17 November 2021. Representatives from the 17 founder members (Algeria, Benin, Cameroon, Congo, Côte d’Ivoire, Democratic Republic of Congo, Egypt, Gabon, Ghana, Kenya, Nigeria, Morocco, Rwanda, Senegal, South Africa, Tunisia and Zimbabwe) voted to constitute the Association. These representatives also elected AfCA's first Executive Committee. A report from this Committee is included in this issue of

the *Newsletter*.

This is a very important event for the IUCr. Many of our colleagues (Alessia Bacchi, Gautam Desiraju, Bill Duax, Marvin Hackert, Claude Lecomte, Luc Van Meervelt, Andreas Roodt and Michele Zema – to name just a few) worked together with African crystallographers and politicians (like Benin's Minister of Higher Education and Scientific Research, Eléonore Yayi Ladekan) to make the creation of AfCA possible. Since 1990, the Crystallography in Africa initiative (Claude Lecomte's project, financed by the IUCr) nourished the development of crystallographic labs and training local crystallographers on African soil. In 2013 the Moroccan Crystallographic Association (led by President Abdelmalek Thalal) supported the IUCr in its successful application to UNESCO to establish 2014 as the International Year of Crystallography (IYCr). The IUCr Outreach and Education program (led by Michele Zema, IUCr Executive Outreach Officer) provides support to meetings, schools and OpenLabs in Africa. You can read about it all in the *IUCr Newsletter* and in real life. Today we all welcome AfCA to the IUCr family.

The 70th Anniversary of the Crystallographic Society of Japan (CrSJ) is another reason to celebrate. This festive meeting (postponed from 2020) was organized by Genji Kurisu on 20 November 2021 in a hybrid mode. Leading Japanese crystallographers presented talks about their innovative research. Japan is a category IV IUCr member and joined the Union in 1951. Japanese scientists have long been and are very active in the Union. Japan gave the Union two Presidents, N. Kato (1978–1981) and Y. Ohashi (2005–2008), and two Vice-Presidents, I. Nitta (1963–1969) and M. Tanaka (1999–2002), along with Executive Committee (EC) Members K. Kuchitsu, J. Harada and M. Takata. The IUCr representative to COSPAR is now Y. Kimura, while K. Kakimoto serves as the President of the International Organization for Crystal Growth.

I would also like to inform you all that since the Prague Congress I have signed two Memoranda of Understanding (MoU):

#1 is an MoU between the International Union of Pure and Applied Physics (IUPAP), the IUCr and the Abdus Salam International Centre for Theoretical Physics (ICTP) for the Operation of Lightsources for Africa, the Americas, Asia, Middle East and Pacific (*LAAAMP*). Michele Zema, IUCr Executive Outreach Officer (and Chair of the *LAAAMP* Executive Committee) negotiated this MoU.

#2 is an MoU between the IUCr and the Standing Committee for Gender Equality in Science (SCGES). Jenny Martin, the Chair of our Gender Equity and Diversity Committee (GEDC) (and IUCr EC Member), is the IUCr representative, and Sven Lidin, GEDC Member (and IUCr Immediate Past President), will serve as her deputy.

2021 is slowly coming to an end. On the one hand, it was a good year as we had a successful 25th Congress and GA, some very good virtual meetings and IUCr Journals are doing well. On the other hand, we are all tired of pandemic restrictions and hope that with more people vaccinated life will go back to normal, whatever our new normal may be. There will be new rules and expectations, but at least it will be possible to see each other in person and leave behind the Zoom-only life.

An African proverb says that wisdom is like a baobab tree: no individual can embrace it. We need each other to create a brighter future for ourselves and for the next generations. I wish you all a safe and enjoyable holiday season. Please take good care of your loved ones, stay connected with the IUCr and stay safe. Happy 2022!

EDITORIAL

Editorial



Fractal Circle Limit III, by permission of the artist Vladimir Bulatov.

Mike Glazer

We do live in strange times. Just when COVID-19 seemed to be getting under control, along comes Omicron to foul up any arrangements we had planned for the next few weeks. Let’s hope that this variant turns out not to be as harmful as the others.

We have some recent changes to the Editorial Board of the *IUCr Newsletter*. Regional Editors Ted Baker and Serena Chiara Tarantino have both retired from the Board, and I thank them very much for their support. At the same time, we welcome some new members of the Board:

Chris Sumby (Asia including Australia, New Zealand, and Pacific Island Territories)

Anders Madsen (Europe including Russia and the Middle East)

Panče Naumov (Europe including Russia and the Middle East)

The complete list of Editors can be seen at https://www.iucr.org/news/newsletter/editorial-board. Please contact them or any other member of the Editorial Board with news and information that we can publish in the *Newsletter*.

We also bid a fond farewell to Patti Potter, who is standing down from the *Newsletter* after having worked on the publication since its launch in 1993. Originally based in Buffalo, Patti was employed as the Production Manager alongside Editors Bill Duax and Judy Flippen-Anderson, and then, when production moved to Chester in 2018, continued in advertising sales. We thank Patti for her role in disseminating news to the crystallographic community for 28 years, and send our best wishes for the future.

The IUCr, initially proposed by P. P. Ewald in 1944 (see https://www.iucr.org/iucr/history/early-history), has represented the crystallographic community throughout the world since its founding in 1947. In its first international meeting in 1948, participants came from Belgium, Canada, France, Germany, India, Italy, Netherlands, Spain, Sweden, UK and USA. In the intervening years, we have seen the IUCr promote the growth of crystallography further around the world. In most countries, national crystallographic associations were founded, followed by supranational bodies such as the American Crystallographic Association (representing the USA and Canada), the European Crystallographic Association, the Asian Crystallographic Association and then later, the Latin American Crystallographic Association. This left a noticeable gap (are there any crystallographers in Antarctica?), which has been filled, finally, with the foundation of the African Crystallographic Association (AfCA) – read all about the launch from the AfCA Executive Committee here. The African crystallographers are to be applauded for reaching this

momentous step and are welcome members of our community. To reach this point has taken much hard work by stalwarts such as Claude Lecomte and Michele Zema, with support from the IUCr through its various schemes, such as OpenLabs, together with a number of commercial companies who have donated equipment to some African countries.

Also of note is the recent rise of crystallographic research in the Arab world. Panče Naumov, Sharmarke Mohamed, Liang Li and Wael Rabeh tell us about this research here. The Emirates Crystallographic Society was set up and is now an adhering body of the IUCr. Another example of the widespread crystallography community can be seen here, where we have an article about crystallography in Guatemala, which also became a member of the IUCr in 2021.

I am looking forward to the next IUCr Congress, which will be held in Melbourne, Australia, in 2023. I hope that we shall all be able to attend in person by then. Australia is such an exciting country, with strange animals and plants, and I have always enjoyed visiting. Now, how about an Australian walk-about? Chris Sumby suggests a road trip with stops at places that should be of interest to crystallographers. Looks great!

To mark the inauguration of the new Sir William Henry Bragg Building at the University of Leeds, a major exhibition devoted to the work of W. H. Bragg, the father of Sir William Lawrence Bragg, is currently under way. As every crystallographer surely knows, both father and son shared the 1915 Nobel Prize in Physics for their work on crystal structure determination by X-ray diffraction. You can read about the exhibition here.

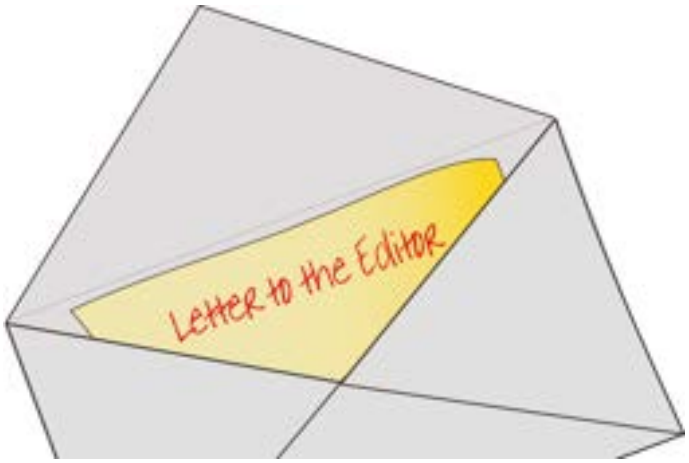
Another of our Nobel Laureates, Herbert Hauptman, is featured in an article by Istvan Hargittai, focussing on his creation of stained glass polyhedral models with close packing of spheres. Istvan includes a brief biographical sketch.

All crystallographers who publish crystal structures, and that is no doubt the majority, are well used to creating the infamous CIF, which I always called the Crystallographic Information File. I now see from the fascinating article by James Hester and Brian McMahon that CIF stands for “Crystallographic Information Framework”! James and Brian relate the history of this all-important development that has become so standard in the lives of most crystallographers. I remember when the CIF all started but had forgotten how many people had involvement in its creation.

Finally, The Royal Society has just published a biographical memoir on Nobel Laureate Tom Steitz here written by Venki Ramakrishnan and Richard Henderson.

LETTER TO THE EDITOR

Equality, equity, diversity, parity and discrimination



Massimo Nespolo

Western societies move every day further in the direction of “equality”, in particular “gender equality”. Quotas are enforced to ensure we move as far as possible towards “parity”: committees, commissions, panels, governing bodies must be composed of the same number of women and men. Decision-makers seem obsessed by the idea of being possibly accused of discrimination.

We face the same move in science, despite the highly different representation of women in different fields. When women are under-represented, enforcing parity means those women have to participate in many more commissions, juries *etc*. than do men; an example where equality contradicts equity. One may wonder if those women are happy to be solicited because of their gender, rather than just because of their skills. The will to enforce parity in science implicitly means to assume we are guilty – of discrimination – until innocence is proved. I grew up believing that scientists are among the most open-minded people: another dream fading away?

Discrimination seems today the worst felony unless it is “positive”, of course. The relentless effort to fight *some* discrimination by fellow scientists in the governing bodies makes an astonishing contrast with the deafening silence against *other* discriminations. The next European Crystallographic Meeting will be held in Versailles, France, and will be *off limits* not only for a number of *bona fide* scientists: the COVID-unvaccinated ones, but also for all those who come from countries where “vaccines” different from those authorized by the European Union are used; Russian scientists and scientists from Northern Africa are just two examples. Neither the ECA nor the IUCr has said a single word against such discrimination. The IUCr Congress and General Assembly of 2023 will be held in Melbourne, where the zero-COVID policy has enforced a severe deprivation of freedom and where freedom of speech is today brutally repressed when it comes to the “vaccines”, as live video recordings continue to show. Who can believe that the participation of *bona fide* scientists will be guaranteed under these circumstances? The Congress website carefully shows compliance with the “gender equality and diversity” policy of the IUCr; not a word, instead, about the restrictions that will prevent the participation of all the *bona fide* scientists who do not comply with the enforcement of periodic injections.

Fully absorbed in the noble task of building a better, equal, diverse world, we are blindly running towards a *Brave New World*. Whistle-blowers are accused of promoting conspiracy theories. Humanity has already seen this in the past, and we know how it ended.

Editor's note: We do not want political correctness to rule science, crystallography or the IUCr but we should be open to change. We (the IUCr) have always led the way in "equal opportunity" and this is what we should still advocate. The IUCr is and wants to be known for building connections between scientists, not for destroying them. We do not want to discriminate.

Disclaimer: The views and opinions expressed are those of the author and do not reflect the official policy or position of the IUCr.

FEATURE ARTICLE

30 years of CIF



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James Hester, Brian McMahon

A new paradigm in data characterization

Thirty years ago, in November 1991, *Acta Crystallographica Section C* published the first of a new category of articles, Regular Structural Papers. At the same time, an article appeared in *Acta Crystallographica Section A* describing a new standard archive file for crystallography. The two, of course, were not unconnected: the *Acta C* article was the first to be submitted using the new file format, CIF, described in the *Acta A* paper. Since that time, CIF has grown to be the accepted standard way to describe crystal and molecular structures derived from single-crystal X-ray diffraction experiments. Many journals will not publish such a structure unless it is accompanied by a CIF; and in many cases, the decision to publish will have included a technical review of the quality of the structure using the IUCr's automated *checkCIF* procedure.

However, CIF has grown far beyond its original design as a standard file format for single-crystal structure reports, and extensions of the original standard are found in an increasing number of crystallographic and other structural science applications. The acronym now stands for 'Crystallographic Information Framework', in recognition of its application across all of these fields, and many of the Commissions of the IUCr are actively engaged in extending its use within their disparate fields. In an age of data-driven science, crystallography has come to be seen as a pioneer in defining experimental and derived data with the precision and scope necessary to achieve the goals of the FAIR data management strategy - namely, to ensure that data are findable, accessible, interoperable and reusable.

Out of the blue?

As with most great ideas, CIF did not spring into the world fully-formed and with no history (Fig. 1). Of course, crystallography is a discipline blessed by an area of study that - to a first approximation - is inherently orderly and well defined (regular three-dimensional packing of atomic or molecular motifs), and that produces copious results from certain reasonably standard types of experiment (diffraction, whether of X-rays, electrons or neutrons). And classification of crystallographic properties, whether of mineral types, crystal habits, or space group symmetries, has been a key activity for decades, if not centuries.

Even so, efforts towards capturing all the information necessary to repeat a crystal structure determination, especially when electronic computers became a significant research tool, go back further than many people realise. Fig. 1 captures some of the steps in the path towards the creation and early

implementation of the CIF standard, based on the current authors' memories. Mario Nardelli, a distinguished and prolific structural chemist, launched the journal *Crystal Structure Communications* (1972-1983) at his home institution at University of Parma, and developed software (*Parma Structural Checking – PARST*) to ease the labour of checking the reported structures. When the journal was taken into the IUCr family of publications as *Acta Crystallographica Section C*, its rigorous standards of checking were adopted by the Editor-in-Chief, Sidney Abrahams, who formalised the requirements for information (what we would now call experimental metadata) needed to check the consistency and reasonableness of the reported structure. Similar requirements were emerging at that time within the relatively new structural databases, such as those developed for inorganic structures (ICSD) and organic/organometallic structures (CSD). Within the Cambridge Crystallographic Data Centre (CCDC), validation software (*UNIMOL*) was developed and subsequently used for the CSD and in early automated structure checking in IUCr journals.



Sir Isaac Newton

Shoulders of Giants

Mario Nardelli *Crystal Structure Communications*, *PARST*

Sidney Abrahams *Acta Crystallographica Section C*

Frank Allen, Peter Murray-Rust, David Watson, Sam Motherwell, Olga Kennard CSD

I. David Brown, Günter Bergerhoff ICSD

Jim Stewart *XRAY76*

Ted Maslen Working Party on Crystallographic Information

Syd Hall *Xtal*, CIF

Eric Gabe *NRCVAX*

George Sheldrick *SHELXL*

David Watkin *CRYSTALS*

Ton Spek *PLATON*

Walter Hamilton, Tom Koetzle, Joel Sussman, Helen Berman PDB, NDB

Paula Fitzgerald, John Westbrook mmCIF

Figure 1. Selection of key contributors to the evolution of 'a new standard archive file for crystallography' that would revolutionize the reporting of crystal structures in databases and journals.

Special mention should be made of David Brown, of McMaster University, who led the IUCr's first initiative towards a computer-readable standard file format - the Standard Crystallographic File Structure (SCFS)[1]. In the 1980s, when Fortran dominated scientific software development, any such standard was inevitably tied to Fortran input/output conventions (80-column records, fixed field lengths for different types of data); and by the late 1980s this was seen as lacking the flexibility to meet the increasingly complex requirements of increasingly capable and ambitious programming projects. Nevertheless, the SCFS project (informed by the requirements of the databases and journals) identified many of the discrete data items that needed to be transferred between different crystallographic programs, work that was to bear fruit in the development of the CIF core dictionary.

Jim Stewart pioneered a type of structured information storage within the crystallographic software package *XRAY* that was further refined by Syd Hall (University of Western Australia) in *Xtal*, an early example of a collaborative project where crystallographic programmers around the world contribute separate modules to a growing library of software. Syd, Frank Allen of the CCDC and David Brown together developed CIF as a standard format in 1991, an outcome of the Working Party on Crystallographic Information that the IUCr had convened in 1987 under the leadership of Ted Maslen. Together with a lightweight extensible free-form structure, CIF was populated by the data items identified as essential to validation and structure characterization in databases and journals. Authors of leading structure refinement software of the time rapidly adopted this standard, giving the impetus for its universal adoption within the small-unit-cell community. Ton Spek developed a very powerful software tool that checked both the internal consistency of the reported structure and its chemical reasonableness, the latter informed by the wealth of data in the structural databases.



Figure 2. David Brown, Syd Hall, Frank Allen: authors of the original CIF specification.

Meanwhile, the Protein Data Bank (PDB), founded in 1971 as a repository for biological macromolecular structures, was also feeling the limitations of the Fortran-style standard that it had adopted. The community embarked upon an extension of CIF – the macromolecular Crystallographic Information File – that could capture all the experimental data associated with a protein structure determination by X-ray diffraction, but that could also adequately describe the complex structure of intricately folded protein and nucleic acid molecules. To meet the needs of the new relational database that was being designed for the PDB, mmCIF imposed more constraints on the relations between the data items that it defined. In a series of workshops[2], the mmCIF standard was refined to become a superset of the core dictionary with the additional attributes that made it formally equivalent to a relational database.

Timeline of Crystallographic Information

This timeline illustrates significant milestones in crystallographic publishing, database development and information management.

Figure 3. Interactive timeline of developments in crystallographic information before and after the publication of the CIF standard. Drag in window to traverse the date line; click on bullets for more information.

CIF and Crystallography

Many young researchers will have grown up with the idea of CIF as the natural way to publish single-crystal structure reports and import structural models; and they will be equally familiar with *checkCIF* as a validation tool and indicator of the completeness and precision of a structure determination.

While many journals require a CIF as supporting information, Fig. 4 shows the particular power of the complete integration of CIF in the publishing process that IUCr journals offers. In this interactive figure, the author has provided some alternative views of the molecule studied, highlighting different areas of interest. However, the reader can right-click into the main image to find a much larger menu of options, permitting visualization of the unit-cell packing, the crystal structure, or individual symmetry operations; and interrogation of the data for arbitrary geometric measurements.

Highlight none

Highlight N4-methyl group

Highlight propeneyl group

Highlight N4-methyl & propeneyl groups

Avoiding steric crowding of N4-methyl and propeneyl groups may be key factor in observed "key torsions".

Figure 4. Slightly modified version of Fig. 2 of Knott *et al*. (2008)[3] demonstrating the ability to visualize and interrogate CIF data sets *in situ* within a research publication. Interactive functionality provided by *Jsmol*[4].

However, researchers may have had fewer opportunities to use the small-unit-cell derivatives of CIF that have been developed during their lifetime, and that are gradually becoming established as ways to describe more complex types of structure. There are now separate extension dictionaries that cover such fields as: powder diffraction (embracing the different measurables of a wider range of instrumentation, the practice of using multiple data sets to fit a single crystallographic model, and the need to characterize different phases); modulated and composite structures (with the ability to assign superspace groups and modulation wave vectors); magnetic structures (describing both commensurate and incommensurate magnetic structures exhibiting long-range three-dimensional magnetic order); and the description of the topology of lattices and their relation to crystal structures (Fig. 5).


CIF
core


CIF
pd


CIF
ms
CIF
rho


CIF
twinning


CIF
mag


CIF
topo


CIF
mm


CIF
sym
CIF
img



Figure 5. Logos of the CIF dictionaries under the curation of the IUCr Committee for the Maintenance of the CIF Standard (COMCIFS) published by 2021.

There are also small extension dictionaries describing aspects of twinning, multipole expansion of electron density, and structure refinement restraints and constraints. These are not very widely used, but are available as starting points for more detailed treatment when required. Many of the IUCr Commissions are also interested in developing CIF dictionaries to provide standard machine representations within their own spheres of interest.

In the area of structural biology, the Worldwide Protein Data Bank curates the mmCIF family of dictionaries, including PDBx (the main extension to mmCIF that tracks the developing field of protein crystallography) and a number of extension dictionaries relevant to NMR structure determinations, small-angle scattering, three-dimensional electron microscopy, integrative/hybrid methods, features of synchrotron radiation facilities and beamlines, and validation reports.

Another important development has been imgCIF, designed to capture diffraction image data and also the necessary experimental metadata allowing proper interpretation of the images captured. Since imgCIF and its binary data representation equivalent CBF (the Crystallographic Binary File) were first developed in the late 1990s, data acquisition volumes and rates have increased so rapidly that this type of file format is no longer suitable for real-time data capture. Nevertheless, the data definitions of imgCIF have partly informed the NeXus macromolecular crystallography application definition (NXmx) that provides full metadata definitions in the HDF5 format increasingly used by beamlines.

This is a significant illustration that the real power of CIF lies in its definitions of concepts and quantities. While the concrete CIF file format is a useful information exchange mechanism, it is relatively easy to translate the format to other common standards, such as XML, the old PDB format, or – increasingly popular – JSON.

A simple catalogue of this plethora of dictionaries and their specific applications perhaps obscures the real importance that CIF has acquired during the course of its evolution. It now touches upon the complete workflow of a structure determination, from the capture of the experimental data, through its interpretation, modelling and publication, to worldwide dissemination in curated databases (Fig. 6). In data science applications, the collection of controlled vocabularies and interrelationships among detailed data definitions has come to be known as an 'ontology', and crystallography now has one of the most completely developed of any science. It is now possible to offer schools and workshops to early-career structural scientists where experimental best practice is developed with the full rigour of data characterization, interpretation and validation[5].

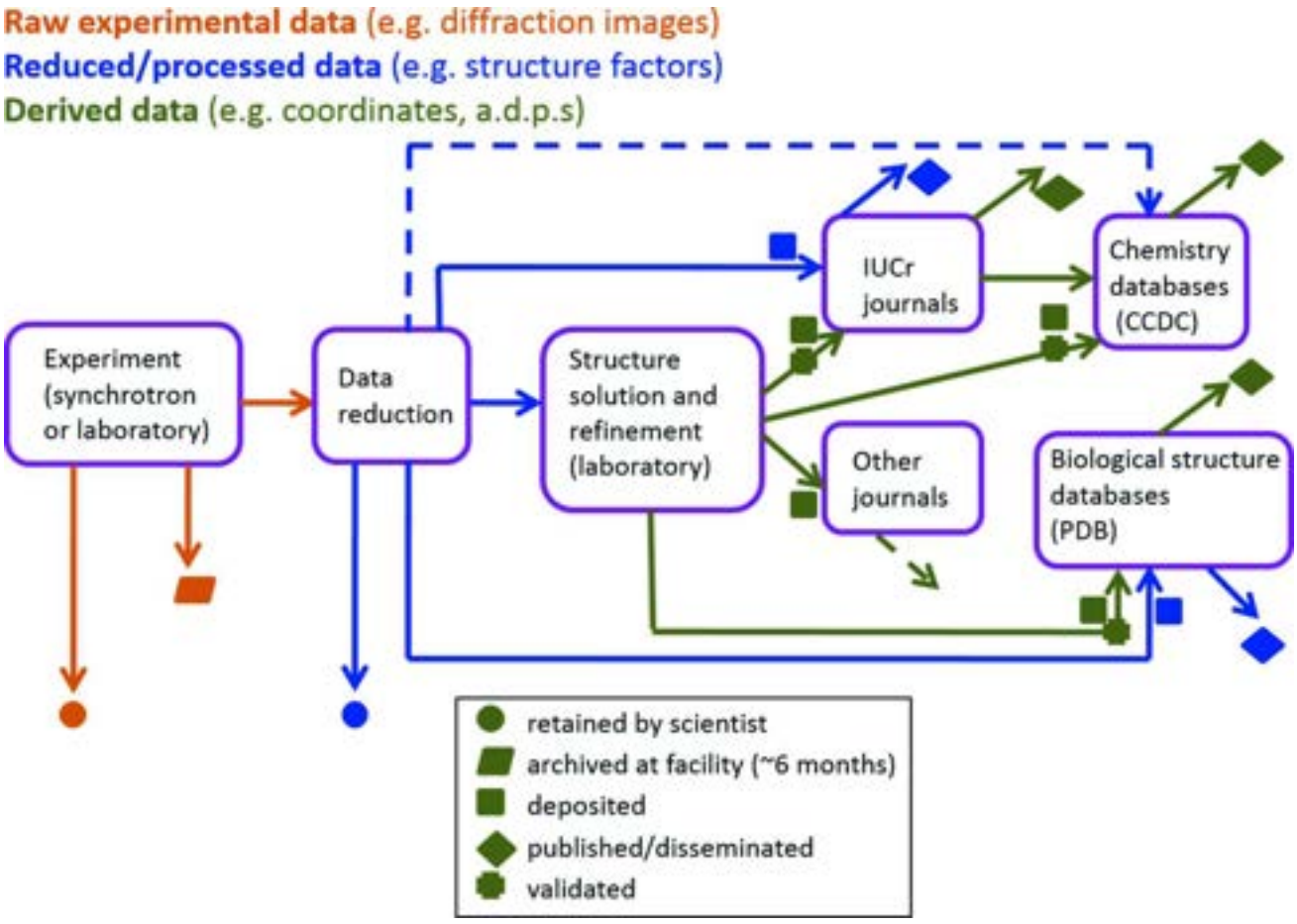


Figure 6. A coherent information flow in crystallography. CIF ontologies characterize data at every stage of the information processing life cycle, from experimental apparatus to published paper and curated database deposit.

Leading the way

The significance of CIF has been recognised in the information and data science communities, in the form of the 2006 Association of Learned and Professional Society Publishers Award for Publishing Innovation and the prestigious 2014 CODATA Prize to Professor Sydney Hall. In both cases the award citations were generous in their acclaim for what the CODATA judges called 'a momentous contribution'.

Yet despite the potential applicability of the approach to any field of science, there has been relatively little penetration in other scientific domains. Syd Hall intended CIF to be just one application of a general approach – 'STAR' (Self-Defining Text Archive and Retrieval) – which has also been used in small-scale pilots in chemistry (MIF, the molecular information file), quantum chemistry, and botany, and most successfully as the basis for the NMR structures database of BioMagResBank, one of the partners of the wwPDB[6].

There are also encouraging signs of novel projects in solid-state science that are inspired by CIF[7]. These are greatly to be welcomed, as a proliferation of domain ontologies in a common format will certainly lead to easier interoperability. It is likely that, despite its success within crystallography, many other disciplines consider the STAR/CIF approach as niche, and not sufficiently supported by the wider information and data science communities. Nevertheless, in our opinion as people who have been involved with CIF for a combined 45 years, STAR and CIF have much to offer, not least in the process of devising new ontologies. The basic file syntax is lightweight and clean, and the dictionary attribute sets (that is, the terms used to express definitions of concepts in machine-readable ways) are not unduly complex, and extensible where needed.

Relationships may be expressed in many different ways – early interest in the STAR File with its nested loops that are absent from CIF explored its suitability for populating object-relational databases. Yet the more natural relational-database type structure that CIF more easily encapsulates is adequate for developing conceptual frameworks of sufficient complexity for most scientific purposes[8]. We respectfully encourage scientists who need to provide machine-readable descriptions of scientific data and metadata within their own discipline to consider the STAR/CIF approach as a useful starting point. Development into more complex web ontology frameworks such as OWL[9], if needed, can be left to a later implementation stage, once the essential definitions and relationships have been expressed in the manner of a CIF dictionary.

Constancy and change

As is apparent from the title of the 1991 CIF paper, one of its primary design goals was to archive data. As such, stability is crucial, both of the file format and of the dictionary definitions. Definitions should not be changed, as that could invalidate archived data sets. On the other hand, concepts do evolve, and the dictionaries will acquire new data names with their associated definitions. Where there is a clear shift in the way an existing concept is realised, there are mechanisms to mark an old data name as deprecated and to express its relationship to a new entry.

In fact, the core dictionary has grown rather little since its original release, reflecting the relative maturity of single-crystal structure determination. In marked contrast, the PDBx extension to the original mmCIF dictionary has raised the number of data names defined for the core biological macromolecular structure determination from around 1670 to over 6400, reflecting both the complexity of the structural description of proteins and nucleic acids and the explosive growth of the subject itself.

To accommodate new requirements in data management the CIF file format itself was revised in 2016[10]. Its main differences from version 1 were the adoption of Unicode as the native character set, the ability to represent all possible text strings, and simpler ways to represent vectors, matrices and other compound data structures. This was coincident with the adoption of a new formalism for dictionary definitions known as DDLm, a methods-capable dictionary definition language. The term 'methods'

indicates that formal relationships between different data items can be expressed, evaluated and validated by machine-executable statements within the dictionary itself. This opens the way to more rigorous validation tools, and in principle brings closer the idea of a universal processing engine that can manipulate scientific entities by inputing a suitable dictionary – no domain-specific coding would be needed within such programs.

Again reflecting the maturity of single-crystal diffraction and the existence of established software that adequately handles the publication requirements of such structures, relatively few 'CIF2' files are yet found in the wild. However, we expect that they will be popular in newer areas of research, and we note, for example, the adoption of CIF2 in a novel Raman spectroscopy database[11].

The image we have chosen to introduce this article is, we feel, an appropriate metaphor for CIF at the end of its first three decades of deployment. From small beginnings, it has grown to a significant size, constantly propelled by a small core of developers and adopters. In the process, it may have acquired some grit and irregularities around the edge, and is now at a stage where even more effort will be needed, especially to gather up more material from the fresh 'snowfields' of new techniques, structural representations, and understanding.

However, most of the pioneers from the early days have now retired or otherwise withdrawn from the scene. If we are not to lose momentum, we need fresh young blood to keep the snowball rolling and growing ever larger. Please join in the fun!

Resources



Find out more about CIF:

The IUCr CIF website

CIF dictionaries maintained by COMCIFS

CIF software for small-unit-cell structures

PDBX/mmCIF dictionary resources maintained by wwPDB

CIF software for macromolecular structures

cif-developers mailing list

Crystallographic Information and Data Management Symposium, U. Warwick, 2013

Crystallographic Information Fiesta School, Naples 2019

International Tables for Crystallography Volume G: Definition and exchange of crystallographic data (1st online edition 2006; a second edition is in preparation)

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[4] *Jsmol* is the HTML5 modality of *Jmol*: an open-source Java viewer for chemical structures in 3D. http://www.jmol.org/ Under continual development by its principal developer, Robert M. Hanson, this tool provides innovative and insightful visualizations of structures described by many flavours of CIF, including macromolecular (mmCIF), incommensurate modulated (msCIF), magnetic (magCIF) and topological (topoCIF) structures.

[5] The pioneering CIFiesta school, hosted by the Italian Crystallographic Association in Naples in 2019, has been described in the *IUCr Newsletter*. Teaching materials from the school are available at: https://www.iucr.org/resources/cif/comcifs/cifiesta-2019

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Appreciation

As we were working on this article, we were saddened to hear of the unexpected passing of John Westbrook (1957–2021), who did so much to develop the mmCIF/PDBx and related extension standards, and whose companionship along almost the entire route of CIF development will be greatly missed.

Brian McMahon is based at the IUCr offices in Chester, UK, and has been COMCIFS Secretary since 1993. James Hester works at ANSTO, Australia, and has been COMCIFS Chair since 2008.

IUCR CONGRESS

Congress reports



The 12th Ewald Prize acceptance Lecture was presented on behalf of Dr Olga Kennard by Dr Suzanna Ward of the CCDC.

The 12th Ewald Prize and Lecture at IUCr25

Report by John R. Helliwell

The 12th Ewald Prize had been awarded in 2020 to Dr Olga Kennard (Cambridge, UK) *for her invaluable pioneering contribution to the development of crystallographic databases, in particular the Cambridge Structural Database (CSD), which as she early foresaw, has led to the discovery of new knowledge which transcends the results of individual experiment. Her own surveys using the CSD were fundamental in the development of crystal engineering, and are outstanding examples of the use of crystallographic databases as an essential tool for analysis and prediction. As founder of the CSD, director of the Cambridge Crystallographic Data Centre (CCDC) over decades, and being involved in the founding of the Protein Data Bank (PDB), Olga Kennard has made a fundamental impact on the development of modern crystallography* (see the report in a previous issue of the *IUCr Newsletter*).

The opening ceremonies of IUCr Congresses traditionally feature a lecture by the Ewald Prize awardee. The IUCr25 ceremony on the evening of Saturday 14 August 2021 was hosted by the IUCr President Professor Sven Lidin. The Lecture was presented on behalf of Dr Olga Kennard by Dr Suzanna Ward of the CCDC (see screenshot above) and can be viewed here.

After the acceptance lecture, it was remarked in the chat by Dr Catherine Lawson, a structural biologist at the Department of Chemistry and Chemical Biology of Rutgers University, USA: “Thank you for this wonderful overview of Olga Kennard’s work.” Suzanna Ward responded “Thank you for listening, such an inspirational lady. I hope I did her justice.” I think that Suzanna Ward truly did do her justice, and, as Suzanna drew attention to it, one can view Olga Kennard’s wonderful lecture looking back, and looking forward, that she presented at the 50th anniversary of the CSD in 2015, at the age of 91. Her lecture can be viewed here, from which Fig. 1 is a screenshot of the opening of her lecture.



Figure 1. Dr Olga Kennard opens the CSD 50th celebration conference entitled “The Cambridge Structural Database at 50: Origins, Influences and Directions” held 1–3 July 2015.

The CCDC published a blog of scientists' reactions to the 12th Ewald Prize award. For example, Senior Scientist-Emerita Dr Biserka Kojić-Prodić, of the Rudjer Bošković Institute, Zagreb, Croatia, said:

“The Croatian Crystallographic Association and I owe a lot to Olga Kennard and F. H. Allen for their strong support and the benefits disseminating and implementing of the Cambridge Structural Database over the territory of South-East Europe. The CSD has been used extensively in teaching and research.”

And Professor Emerita Carolyn P. Brock, Department of Chemistry, University of Kentucky, USA, said:

“Olga had great vision, good business sense, and remarkable tenacity; without those attributes, the CSD would never have survived, never mind become the tremendous resource that it is today.”

We all might wonder, as I did: Why the wait for her to receive an Ewald Prize? Well, I suppose reaching the millionth structure in the CSD does rather make all crystallographers sit up and, quite simply, burst into applause. The heartiest congratulations from all of us to Dr Olga Kennard.

Keynote Lecture: Metadata and *checkCIF* for raw diffraction data in realizing ultimate crystallographic objectivity

Speaker: Loes Kroon-Batenburg

Chair: John R. Helliwell

In my opening introduction to her Keynote Lecture, I summarised Dr Loes Kroon-Batenburg’s extensive research interests and achievements based at the Structural Biochemistry lab of Utrecht University in the Netherlands. She had worked there for 20 years with her husband Jan Kroon on carbohydrate crystal structures and hydrogen bonding. Her scientific interests expanded to include biological crystallography and data science as well as structural studies and fibre diffraction of cellulose and wood fibres. Her interests also cover software development, for example the *EVAL* diffraction data processing method and computer program, and more recently diffuse scattering of protein crystals. Loes has served throughout the six-year term of the IUCr Diffraction Data Deposition Working Group (2010 to 2017) and subsequently the first four years of the IUCr Committee on Data. Loes is leading the IUCr Journals’ initiative launching the *IUCrData* journal’s new section Raw Data Letters.

Her Keynote spanned macromolecular crystallography, chemical crystallography, powder diffraction and diffuse scattering. In several places Loes focussed on macromolecular crystallography with detailed

reuse of raw data examples that she made to illustrate the FAIR data principles in practice as well as some specific, quite serious, problems of raw data reuse that can exist such as totally incorrect beam centre or severely incomplete metadata. FAIR is the acronym used by all science communities these days to measure their progress in organising effective data reuse. This requires that data be findable, accessible, interoperable and reusable in modern science practice. Her conclusions slide is shown in Fig. 2.

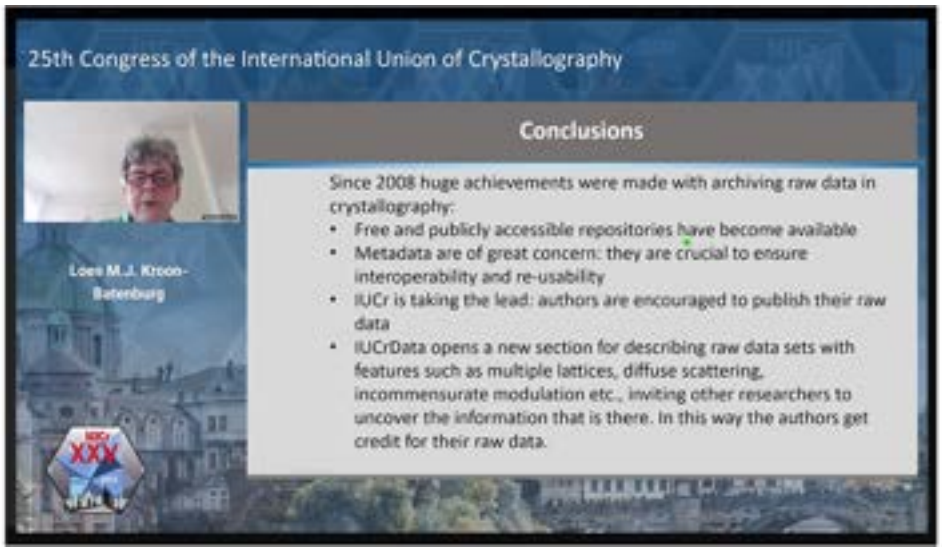


Figure 2. Dr Loes Kroon-Batenburg's conclusions to her Keynote.

There were questions to Loes both from the chat and from the audience present in Prague (Fig. 3). These included recording of a test powder diffraction from Saulius Gražulis and neutron data archiving from Alison Edwards. Time ran out before the intricate question of who owns the raw data (experimenter, the PI, facility, university or funding agency) could be explored, a question that is important for determining release to the public or data deletion rights. These rights may also be different in different countries.



Figure 3. Dr Loes Kroon-Batenburg answers a question from Dr Kamil Dziubek who described the specific challenges associated with high pressure and/or materials science diffraction studies.

IUCR ACTIVITIES

The new IUCr General Secretary and Treasurer visits Chester (twice!)



Bo Brummerstedt Iversen (left) and Luc Van Meervelt outside the IUCr offices in Chester.

Alex Ashcroft

After an unprecedented 10 years in office as General Secretary and Treasurer (GS&T) of the IUCr, Luc Van Meervelt (Katholieke Universiteit Leuven, Belgium) stepped down at the Prague Congress and was replaced by Bo Brummerstedt Iversen (Aarhus University, Denmark). Usually, the outgoing GS&T briefs the incipient GS&T at the Congress, but as Luc was unable to travel to Prague, Bo and Luc visited Chester in September 2021 for the briefing meeting. This allowed the Convenor of the Finance Committee, Malcolm Cooper, and the Executive Managing Editor, Peter Strickland, and me to join in for parts of the meeting to talk about the Union's finances, the Finance Committee and the IUCr journals. With a vacancy on the Finance Committee due to Hanna Dabkowska being elected as President (and so, for two years, becoming an *ex officio* member), Luc agreed to stay on the Finance Committee for two more years to support Bo. The Chester staff have been mostly working from home since March 2020 for safety reasons, and the 2020 and 2021 Finance and Executive Committee meetings had been virtual, so apart from this being the first time that we had met Bo, it was the first time any of us had met each other in person for more than 18 months. The meeting was useful and enjoyable, and covered off one of the main areas of responsibility for the GS&T.

Another main area is the welfare of the Chester staff, and Bo and I were very keen for him to meet with as many staff members as possible. Bo returned to Chester in November 2021 to accomplish this, and despite part of the time being taken up by a visit from the IUCr's new Jersey investment manager, he was able to meet one-to-one with 16 of the IUCr's 25 staff members. I did not attend the meetings, but I saw a lot of smiling faces afterwards, and none of the meetings finished earlier than scheduled. Again, coming into the office was an opportunity to socialise for many staff members who had not seen each other since March 2020. For safety reasons, we asked people not to remain in the offices outside of their meeting with Bo, but there were plenty of socially distanced outdoor meetings in Abbey Square despite the November chill. After his visit, Bo commented "It was wonderful to meet in person and learn about the many aspects of the IUCr. I am amazed at the skills and dedication of the Chester staff, who have been able to run our complex organisation so smoothly, even sitting at home. Let us hope we get past the pandemic, so Abbey Square can again become a lively place full of exciting crystallographic endeavour." Bo is hoping to come back to Chester early in the New Year to meet with any remaining members of staff who want to meet him, but is also happy to meet virtually with anyone who is unable to come to the offices then.

REGIONAL NEWS

It’s official – the African Crystallographic Association is born!



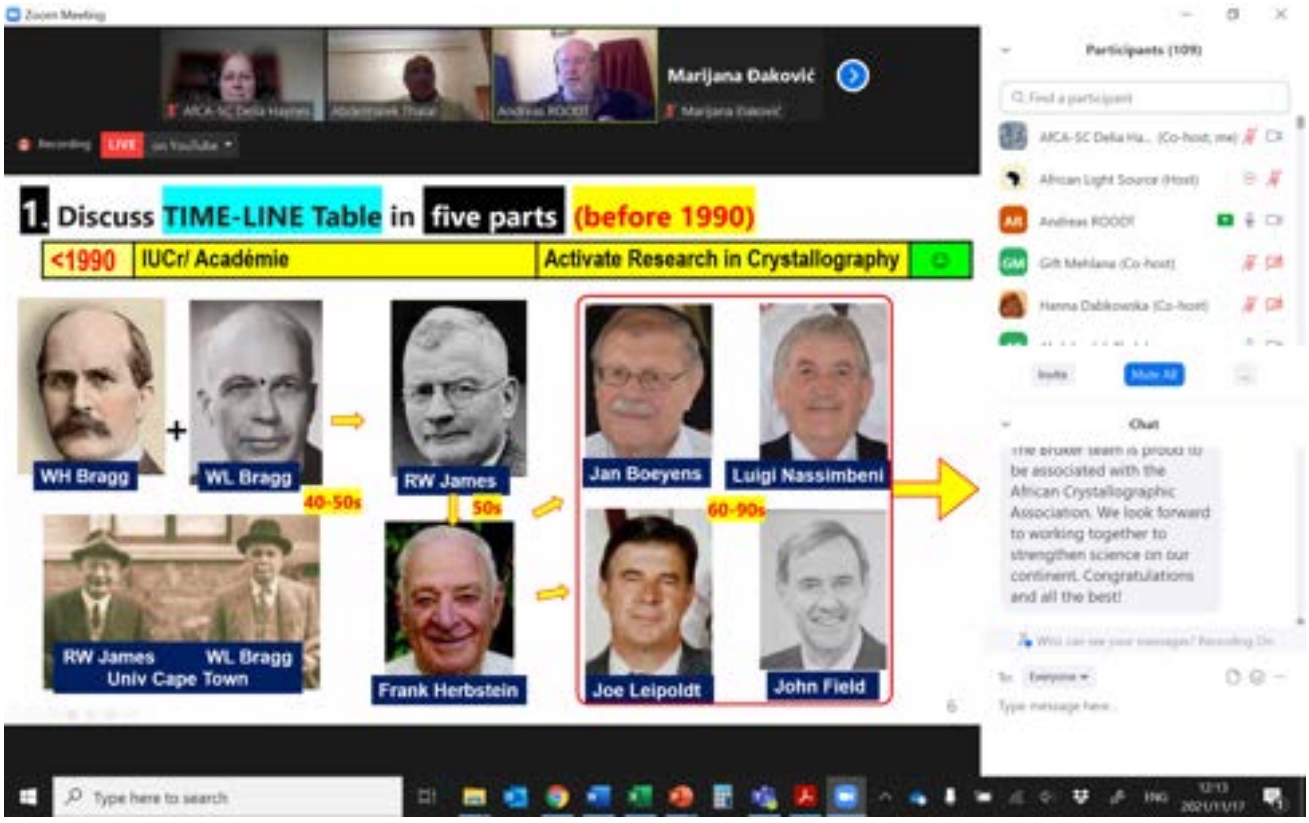
After many years of crystallographic activity on the African continent, on 17 November 2021, we witnessed the birth of the African Crystallographic Association (AfCA). This follows years of work by many groups and individuals, including the IUCr Africa Initiative, the IUCr Outreach Program and the AfCA Steering Committee, with the collaboration of institutions like the United Nations Educational, Scientific and Cultural Organization (UNESCO) and the International Science Council (ISC) and many companies like Bruker and the Cambridge Crystallographic Data Centre (CCDC).

The Association was launched during the online ePCCr meeting, organised as a joint conference with the African Light Source and the African Physical Society. The ePCCr meeting attracted 205 delegates from 37 countries, including 17 African countries. AfCA was officially constituted during a special session at this online meeting, chaired by Delia Haynes, the chair of the Executive Committee of the AfCA Steering Committee.

The session opened with addresses from the IUCr President, Hanna Dabkowska, and the President of the European Crystallographic Association (ECA), Marijana Đaković. Hanna indicated how, since 2011, under the presidencies of Gautam Desiraju (2011–2014), Marvin L. Hackert (2014–2017) and Sven Lidin (2017–2021), the Union has advanced the promotion of crystallography in Africa. She hopes AfCA will apply for regional membership of the IUCr during the 26th IUCr Congress in Australia. In her address, Marijana mentioned that several African countries with active crystallography communities have been members of the ECA, and the ECA has been a strong support on the road to forming AfCA.

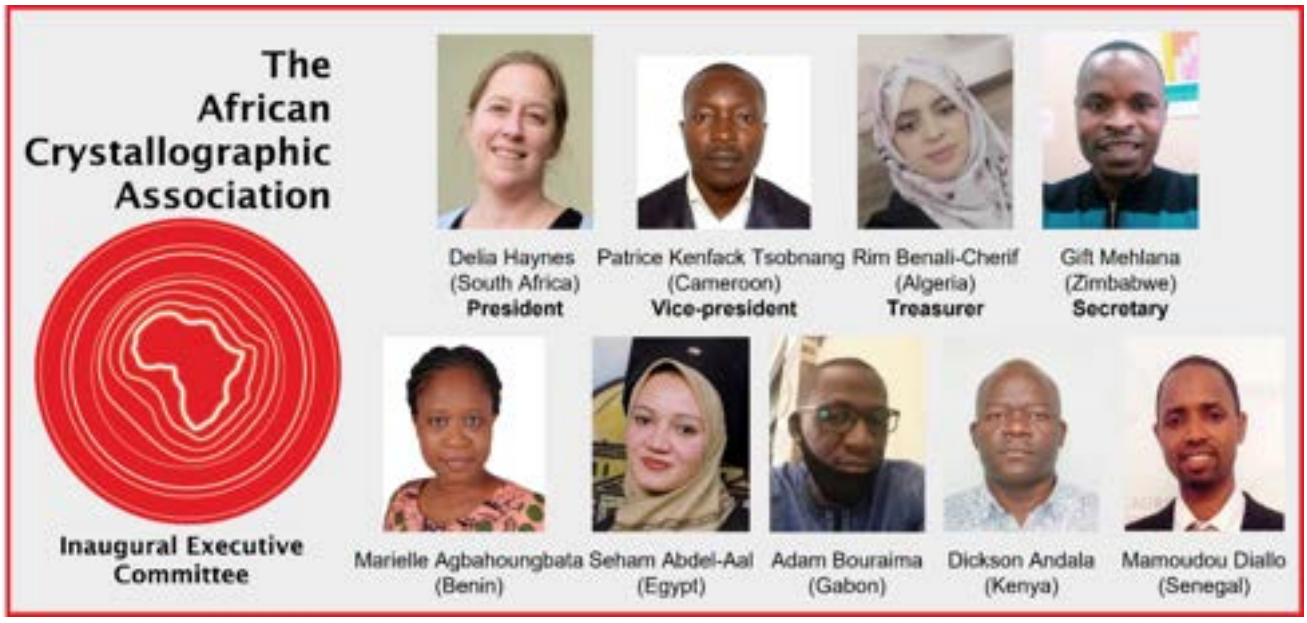
Andreas Roodt (South Africa), Claude Lecomte (France) and Patrice Kenfack Tsobnang (Cameroon) then gave presentations. Andreas Roodt, a past president of the ECA and the first chair of the AfCA Steering Committee, outlined the history and development of crystallography on the African continent. He particularly highlighted the key role played by Claude Lecomte, as well as the importance of meetings held on the African continent, including ECM21 in South Africa and ECM24 in Morocco, as well as the important meetings held during the International Year of Crystallography in 2014. Claude Lecomte then discussed the development of crystallographic activities in Africa, focusing on the installation of diffractometers in several African countries, and well as the highly successful OpenLabs. He finished by presenting a new project involving remote access to diffractometers for the collection of diffraction data. Finally, Patrice Kenfack Tsobnang spoke about the Pan African Conferences on Crystallography, the PCCr series. He mentioned that the idea to launch these conferences arose from the declaration signed during the IYCr2014 Pan African and South African Summit meeting, and how the meetings contribute to growing the African community working in crystallography. PCCr1 and PCCr2 were held in Cameroon in October 2016 and Ghana in January 2019, respectively, and PCCr3 is planned to take place in Kenya in

January 2023.



A slide from the presentation given by Andreas Roodt, outlining the history of crystallography in Africa.

These inspiring presentations were followed by the first AfCA Council meeting. Whilst it would have been fantastic to hold this meeting in person, one advantage of the online meeting format is that representatives of crystallographic societies and groups from across the continent were easily able to participate in the meeting. Representatives from the founder members in Algeria, Benin, Cameroon, Congo, Côte d'Ivoire, Democratic Republic of Congo, Egypt, Gabon, Ghana, Kenya, Nigeria, Morocco, Rwanda, Senegal, South Africa, Tunisia and Zimbabwe were present. These representatives voted first to approve the constitution and by-laws of AfCA and to officially constitute the Association. This was followed by a vote to approve the proposed AfCA Executive Committee. Both votes were unanimous.



The inaugural AfCA Executive Committee. The committee of nine includes members from the five regions of Africa as defined in the constitution.

The session closed with presentations from Professor Walter Oyawa from the International Science Council, and Dr Jean-Paul Ngome Abiaga from UNESCO. The event was attended by representatives from the European, American, Asian and Latin American Crystallographic Associations, as well as the African Light Source, the African Physical Society and the African Academy of Sciences. Many crystallographers from the African continent and across the globe, also joined this important occasion, as well as representatives from *CrystEngComm*, *Crystal Growth & Design*, CCDC, ICDD, Bruker and Rigaku.



Attendees at the AfCA session at ePCCr.

The birth of the African Crystallographic Association was a significant and historic moment, both for science in Africa and for crystallography worldwide. In the words of the ePCCr chair, Gift Mehlana, which he shared at the conference closing ceremony:

"*Just like a baby, the AfCA will learn to sit, crawl, stand up, walk and run. During all these stages, AfCA will need maximum support from the crystallographic community, African governments and the world at large. African governments must support science and, in particular, crystallography through the provision of infrastructure and equipment that is needed to carry out meaningful research. Crystallography has the power to change people's lives.*"

We hope to see AfCA go from strength to strength as it aims to fulfill its objectives. These are to

contribute to the advancement of crystallography and structural science in all its aspects, including related topics concerning non-crystalline states

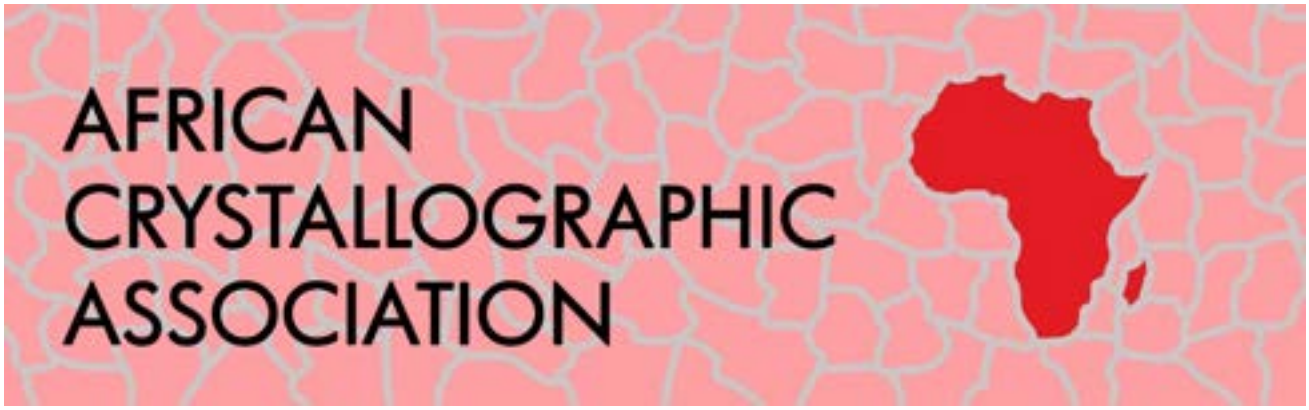
promote African cooperation in crystallography and related areas

contribute to the development of education and research in crystallography and structural sciences in Africa.

The new AfCA Executive Committee would like to extend particular thanks to the three *ex officio* members of the AfCA Steering Committee, Alessia Bacchi, Claude Lecomte and Michele Zema. They have been incredibly generous with their time and their considerable experience, and this point would not have been reached without their help.

Thank you to all those who contributed to this great event to enable this continent, with abundant resources in minerals and mining, materials science, green chemistry, biotechnology and archaeology, to have its crystallography association.

Good luck to AfCA!


AFRICAN
CRYSTALLOGRAPHIC
ASSOCIATION

SPECIAL REPORT

Crystallography in Guatemala



Foundation of the Guatemalan Crystallographic Association (ACriGUA) on 14 August 2019.

Ingrid Benítez, Ricardo Posadas, Omar Velásquez-González

In May 2018 the first crystallography seminar was realized in Guatemala with the visit of Professors Miguel Delgado and Diego Lamas. With the support of visiting professors at the assembly, a crystallography association was formed in Guatemala (ACriGUA), which was founded on 14 August 2019 according to the Guatemalan Civil Associations book. It currently has 10 founding members.





CRYSTALLOGRAPHY AND X-RAY DIFFRACTION SEMINAR
for use in the Characterization of Materials.
Guatemala, 7-9 May 2018

The research and development center – CI+D (for its acronym in Spanish) – of Cementos Progreso, S.A. has been an important pillar in the development of powder crystallography in Guatemala, having been pioneers in having an X-ray diffraction instrument for research (PANalytical Empyrean Series II) and a

scanning electron microscope (JEOL JSM-IT500LV), which have been put at the service of researchers, professors and students through public–private alliances with university educational centers, archaeological sites *etc*.

Contributions to the conservation of Mayan archaeology in Guatemala, listed according to the archaeological site, include the following:

- La Corona: analysis of dental pieces with inlays and different types of fibers, characterization of the composition of soils and artifacts of different kinds
- Cuenca El Mirador: analysis of stuccoes from different structures for their reconstruction and conservation
- Piedras Negras: analysis of construction material for possible restorations
- El Sotz: analysis of the composition of soils and stuccoes of ornamental pieces for their reconstruction and conservation
- Waka Perú: analysis of pigments from different types of ceramics
- Takalik Abaj: characterization of metal pieces and soil
- Kaminaljuyu: analysis of Mayan jewelry, composition of stuccoes for their reconstruction and conservation and analysis of pyrite mirrors.

The public–private alliance reached with academia has led to fruitful collaborations. Senior students of the bachelor’s degree in Chemistry and Chemical Engineering of the San Carlos de Guatemala University and Del Valle University of Guatemala have been trained year by year. Research in materials science has been the greatest force, going through to the study of nanoparticles, such as the addition of carbon nanotubes and their functionalization with different functional groups in cement mortars. Other studies include the addition of organic molecules, such as chitosan, to mortar; the bioremediation of mortars through the addition of microorganisms to cementitious mixtures; and the characterization of modified clays.

CI+D of Cementos Progreso has its own research lines, such as the development of environmentally friendly products, new additions from waste materials, pure phases of cementitious materials, microstructural characterization and hydration of different types of cement and carbonation of cementitious materials.

We should also mention that we have started to participate in the activities of the Latin American Crystallographic Association (LACA) as our Regional Associate. SENACYT, the National Office of Science and Technology of Guatemala, has supported our membership in LACA and supports our membership in the IUCr, which was formalized during the first General Assembly session on 15 August 2021 during the 25th IUCr Congress in Prague, Czech Republic.

In addition, students have shown enthusiasm for crystallography. Guatemala had students attending the lectures in the 1st and 3rd LACA Schools on Small Molecule Crystallography. The first event was held in Montevideo, Uruguay. The 3rd school was scheduled to take place in Mexico City but because of the COVID-19 pandemic, the course was redesigned into a virtual edition. 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.

In the divulgation of crystallographic sciences, a short lecture was held in the II National Congress of Biotechnology. The chemist Jorge Solis-Portillo presented an Introduction to single-crystal X-ray crystallography for small molecules of biological interest. This event was organized by the inter-sectoral technical commission on biotechnology of the CONCYT (National Council for Science and Technology in Guatemala). This event was used as a platform to increase the interest among the Guatemalan population of the potential applications of crystallography in industry and academia. Leaders of industry,

students and entrepreneurs in the biotechnology sector attended this online event.

Since its creation, ACriGUA has organized several events, with the purpose of disseminating crystallography in Guatemala, with the support of national and international speakers.

The activities that ACriGUA has carried out have been announced on local Facebook and YouTube networks, and have been seen by the public in Guatemala and countries such as Costa Rica, Colombia, Brazil, Peru and Uruguay. We plan several virtual events for this year and hope we will be able to have in-person activities in Guatemala, once the global health situation caused by COVID-19 improves.



The authors of this article from left to right: Ingrid Benítez, Ricardo Posadas and Omar Velásquez-González.

Recently, Professor Omar Velásquez-González (San Carlos University) obtained a grant for Structural Biology Research. A lectin from an endemic sea cucumber (Holothuroidea class) is the main object of the study. Professor Veláquez-González was a student of Professor Abel Moreno, studying crystallography and crystallogenesis.

Ingrid Benitez is a Professor in the Engineering Faculty and Omar Velásquez-González is a Professor in the Chemistry and Pharmacy Faculty, both at San Carlos University. Ricardo Posadas is a researcher at Cementos Progreso.

SPECIAL REPORT

Crystallography in the United Arab Emirates



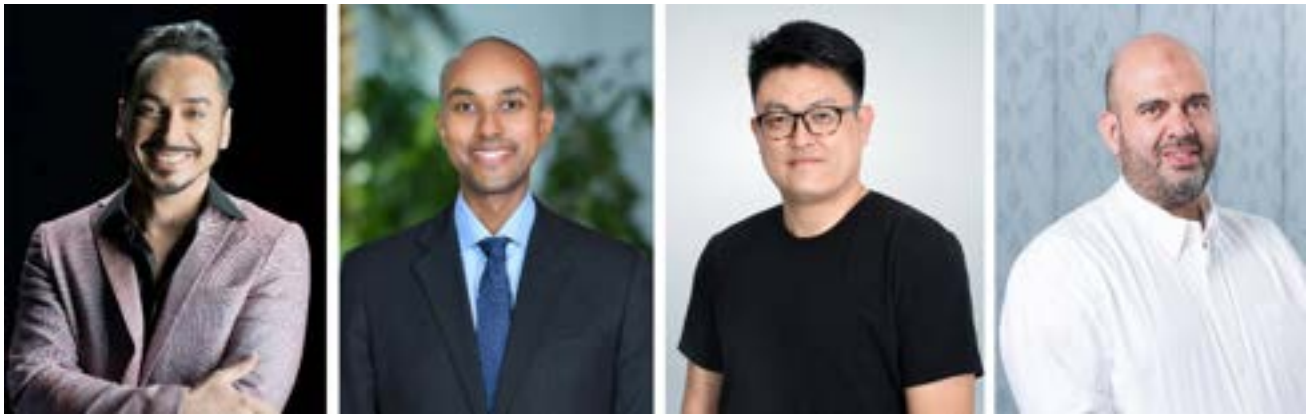
Students on the NYUAD campus.

Panče Naumov, Sharmarke Mohamed, Liang Li, Wael Rabeh

On 20 September 2020, researchers from academia and industry in the United Arab Emirates (UAE) established the Emirates Crystallographic Society (ECS). The ECS is the culmination of years of work and represents the only internationally recognized professional body to represent UAE researchers who use diffraction methods. For a country that is only 50 years old, the UAE has made significant investments in scientific research over a short period of time. The establishment of the ECS is another milestone for the growing research community in the UAE.

Since its founding in 2020, the ECS has gained a string of admittances to a number of international crystallographic bodies. With each admittance to an international body, the ECS and its representatives are working hard to bring better visibility and resources to the growing community of researchers in the UAE that use diffraction methods. On 28 April 2021, the council of the European Crystallographic Association (ECA) voted to admit the ECS as a full national member. On 13 August 2021, the ECS was also admitted to the Asian Crystallographic Association (AsCA). Most recently, on 15 August 2021, the ECS was admitted to the International Union of Crystallography (IUCr) as a Category 1 adhering body, which was formalized at the 25th Congress of the IUCr, which took place in Prague.

The World Database of Crystallographers (WDC) currently has 15 entries from the UAE. However, the ECS currently has over 100 members from across industry and academia in the UAE. Until about 10 years ago, most diffraction experiments conducted in the UAE were limited to powder X-ray diffraction (PXRD) methods. Such PXRD methods were typically used for phase identification. In 2013, the first two single-crystal X-ray diffractometers were procured by the newly established New York University Abu Dhabi (NYUAD) in Abu Dhabi, the capital of the UAE. The commissioning of these instruments was initially supervised by Professor Panče Naumov and the late Professor Joel Bernstein of NYUAD. The instruments are now supervised by Dr Liang Li, a member of the Core Technology Platforms (CTPs) at NYUAD. These instruments supported the establishment of several local and international collaborations with leading researchers. Within the UAE, strong collaborative ties were established with Khalifa University (Professor Sharmarke Mohamed), United Arab Emirates University (UAEU) and other institutions. In 2018, the first protein crystal structures were determined entirely at NYUAD with high-resolution data collected at the Swiss Light Source (SLS) at the Paul Scherrer Institute as part of work that was published by Professor Wael Rabeh and Professor Naumov. The protein crystal structures represent an important hallmark for the initiation of structural biology research in the UAE.



The authors of this article from left to right: Panče Naumov, Sharmarke Mohamed, Liang Li and Wael Rabeh.

Single-crystal diffractometers are also now starting to be procured and used by national universities in the UAE. With the merger of the Petroleum Institute, Masdar Institute and Khalifa University of Science Technology and Research in 2017, a new national university was created in Khalifa University (KU), bringing together existing strengths in engineering and earth sciences but also adding new research and teaching focus with the opening of a College of Arts and Sciences as well as a College of Medicine and Health Sciences. These changes have attracted new faculty and research staff working at the interface of materials science and crystallography. KU currently has five PXRD instruments and three single-crystal diffractometers. Professor Mohamed's research group is currently applying both small-molecule crystallography and computational modelling techniques to design, synthesize and characterize new solid-state architectures of organic crystalline materials with useful properties. Two new single-crystal diffractometers were also recently procured by UAEU and Sharjah University. A search of the Cambridge Structural Database and other databases indicates that as of September 2021, over 400 crystal structures had been deposited by researchers from the UAE. We anticipate that this will increase over the coming decades as more researchers use the growing research capabilities of UAE institutions in the area of X-ray crystallography.

Over the past decade, crystallographers from the UAE have actively participated and presented their research in crystallographic conferences, notably those organized by the ECA, AsCA and IUCr. Since 2012, researchers from NYUAD were also involved in the academic activities of the SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East) synchrotron in Jordan. Professor Naumov gave a number of invited lectures at SESAME’s annual user meetings. In 2016 and 2018, NYUAD hosted two materials science conferences – the First and the Second Middle-Eastern Materials Science Conferences – where crystallographic research featured prominently in the conference program. In 2017, KU also hosted the first Environmental and Materials Science Symposium (EMSS’17), bringing together industrial and academic researchers working in these disciplines.



Participants at EMSS'17.

Looking forward, the UAE has set an ambitious target of transitioning to a knowledge-based economy by 2030. As a consequence of this ambition, the UAE has invested significant resources in education and research within the natural sciences. Given that crystallographic methods are important to advances in a number of sectors that are critical to the UAE economy, the establishment of the ECS and its membership of a number of regional and international bodies will support the work of researchers and the transition of the UAE to a knowledge-based economy.



Scenes from the UAE.

Professor Panče Naumov, Dr Liang Li and Professor Wael Rabeh are at New York University Abu Dhabi, Abu Dhabi, United Arab Emirates, and Professor Sharmarke Mohamed is at Khalifa University, Abu Dhabi, United Arab Emirates.

REGIONAL NEWS

Recent news from the European Crystallographic Association



Anticlockwise from top: ECA President Marijana Đaković and Past President Udo Heinemann (photo contributed to the IUCr gallery by M. Jaskólski) with Grygoriy Dmytriv, Chair of ECM35, which will be held in Lviv, Ukraine, in August 2025.

Arie van der Lee

During the COVID-19 pandemic the European Crystallographic Association (ECA) had, as all scientific organisations, its activities reduced to a strict minimum, especially in 2020. The most important decision to be taken was to postpone the 33rd European Crystallographic Association (ECM33) from August 2021 to August 2022 in order to avoid a clash with the 25th Congress and General Assembly of the IUCr that needed to be deferred from August 2020 to August 2021. The ECA Executive Committee is grateful to the local ECM33 organisers for their proven flexibility.

In 2021 two ECA Council meetings took place, the first one virtually in April and the second one in August in hybrid mode during the IUCr25 Congress in Prague. These meetings, attended by the ECA Executive Committee, the ECA national member representatives, the individual member representatives, the corporate affiliate member representative and a number of invited attendees, are an opportunity to discuss business pertinent to crystallography throughout the ECA region, which currently covers Europe, the Middle East and Africa. The most important decision taken during the April meeting was to welcome the United Arab Emirates as the 35th National Member of the ECA.



An exciting new project was born between the April and August Council Meetings: the virtual monthly ECA lunchtime webinars. This webinar series, which is organised by the young crystallographers gathered in the ECA General Interest Group No. 1, aims to strengthen and vitalise the European

crystallographic community by proposing educational or scientific webinars along the crystallographic areas of ECA's Special Interest Groups. Until now (November 2021) five well attended webinars have taken place. Stay tuned!

The Council Meeting in Prague saw the completion of several ECA Executive Committee members' three-year terms in office, and consequently ballots were held to elect candidates to a number of official positions. Marijana Đaković (Zagreb, Croatia) was elected President, succeeding Udo Heinemann (Berlin, Germany) who takes up the position of Past President. Arie van der Lee (Montpellier, France) was elected Vice-President, while Andy Maloney (Cambridge, UK) was elected Secretary. This year saw Alessia Bacchi (Parma, Italy) and Carl Henrik Gørbitz (Oslo, Norway) complete their respective terms as Past President and Officer for Grants. Klaudia Hradil (Vienna, Austria) was elected to the latter position. The remaining members of the Executive Committee remain in their previous offices: Jacob Overgaard (Aarhus, Denmark), Treasurer; Jan Dohnálek (Prague, Czech Republic), Officer for Interest Groups; Delia Haynes (Stellenbosch, South Africa), Officer for National Members; and Consiglia Tedesco (Salerno, Italy), Officer for Education.

ECA Council Meetings are also an opportunity to hear about the progress towards the planning of future ECMs and to receive and vote for bids for prospective meetings. The 33rd European Crystallographic Meeting, ECM33, will take place in Versailles, France, from 23 to 27 August 2022. Planning is well underway for this meeting set to take place in a magnificent venue, and the organisers are optimistic that a full programme can be delivered in person. Further information can be found on the conference website: https://www.ecm33.fr/. This congress will see as well the celebration of the 25th anniversary of the ECA.* ECM34 is scheduled to take place in Padova, Italy, from 20 to 24 August 2024, and a successful bid from Lviv will take ECM35 to Ukraine in 2025.

Of particular interest to younger members of the crystallographic community, the ECA Council heard a report on the 6th European Crystallographic School (ECS6), which took place virtually from Budapest, Hungary, in July 2021. European Crystallographic Schools combine lectures and hands-on tutorials to provide attendees with a fundamental understanding of the principles underpinning crystallography. Each school is unique, however, and offers a variety of topics to cater for a broad range of interests. ECS7 will take place during 2022 in Lisbon, Portugal, and a successful bid to host ECS8 in Berlin, Germany, in 2023 was received. For further information on the ECS, please visit https://ecanews.org/european-crystallography-school/.

*The ECA was formally established in 1997. It succeeded the European Crystallographic Committee, which had guided the development of European Crystallographic Meetings from their inception (ECM1 in Bordeaux in 1973) through to the Prague meeting in 1998.

SPECIAL REPORT

A crystallographer's road trip "down under"



Christopher Sumby

Australian and New Zealand researchers have an enduring association with the technique of X-ray crystallography, with Adelaide in Australia being the birthplace of Sir William Lawrence Bragg and the technique being widely developed through the pioneering contributions of Arthur Lindo Patterson and Maurice Wilkins, who were both born in New Zealand [1]. Crystallography in the two countries has blossomed through the joint Society of Crystallographers in Australia and New Zealand (SCANZ) [2] and with crystallographers active in most major universities, medical research institutes and government-funded research organisations. These researchers are all supported by landmark infrastructure run by the Australian Nuclear Science and Technology Organisation (ANSTO), namely the Australian Centre for Neutron Scattering near Sydney and the Australian Synchrotron in Melbourne.



Figure 1. The Mitchell Building, the site of Sir William Henry Bragg's laboratory at the University of Adelaide, South Australia (photo credit: Chris Sumby).

With travel restrictions starting to relax worldwide, and particularly in Australia ahead of Melbourne's hosting the 26th Congress and General Assembly of the International Union of Crystallography (IUCr 2023), it seems an ideal time to think about some opportunities for travel. Australia and New Zealand, as members of the society hosting the IUCr 2023 congress, have a wealth of historical sites related to the discovery and development of X-ray diffraction, natural beauty spots displaying the fundamentals of crystallography, and visitor attractions with links to the technique. This item covers a potential "road trip," taking in some of the possible sites that crystallographers visiting the IUCr Congress in Melbourne in 2023 might want to consider. If you like the ideas here, why don't you check out the IUCr 2023's website (https://iucr2023.org/) and subscribe to their E-zine containing details of the "The Great Down Under Road Trip" for more details?

Whichever way you look at it, travel around Australia and New Zealand represents a big trip – it's around a five-hour flight from the west coast to the east coast in Australia and another three-hour flight from the eastern seaboard of Australia to New Zealand. There are lots to see, but some planning is required given the large distances involved – driving east to west or north to south in Australia is one of those "once in a lifetime" experiences given the unpopulated nature of most of the country and the distances.

As the birthplace of W. L. Bragg, Adelaide is a treasure trove of sights to interest the crystallographer. His father, W. H. Bragg, was the first Professor of Physics and Mathematics at the University of Adelaide, and his lab in the Mitchell Building of the University [3], on the main boulevard at the top of the city is still there, albeit reincarnated as the legal counsel's office (Fig. 1). The University has a vast array of documents and items from the Bragg era, and these are commonly on display. In the "new" Physics Building, busts of both Braggs are on display (Fig. 2).



Figure 2. Busts of W. L. and W. H. Bragg in the Physics Building of the University of Adelaide (photo credit: Helen Maynard-Casely).

These are copies of busts on display on North Terrance, just outside the South Australian governor general's residence. The South Australian Museum, which is also on North Terrace, has a fine collection of minerals from around Australia (Fig. 3) and a display of the Ediacaran fossils, the earliest known complex multicellular organisms [4]. Adelaide is also home to the Royal Institution of Australia (RI-Aus) [5], the sister institution to the UK's Royal Institution, and around the outskirts of the city centre, in North Adelaide and by the East Parklands, are the residences that the Bragg family called home while living in Australia.



Figure 3. Some of the mineral collection at the South Australian Museum (photo credit: Chris Sumby).

Mining the abundant natural resources of Australia is an important industry, and there are some interesting sites. About eight hours drive north of Adelaide is the town of Coober Pedy, the so-called Opal capital of Australia [6]. In this outback town, temperatures in summer can be extreme, and a number of residents live underground in caves and dugouts. Coober Pedy was once covered by an ocean that allowed silica minerals to accumulate in rock cracks and cavities and led to the formation of opals. Unlike most gemstones, though, opals are non-crystalline, but the experience of outback Australia is still an interesting one.

Heading west from Adelaide and South Australia takes one over 1500 km across the expansive Nullabor plain to Western Australia (a two to three day drive depending on where you choose to start and end) [7]. Perth is one of the most isolated cities in the world but has been a strength of Australian X-ray crystallography for many years, under the auspices of Ted Maslen, Allan White and many others [1]. A homage to quasicrystals can be found in the Bayliss Building of the University of Western Australia (UWA), where the floor is covered in a beautiful Penrose tile floor [8]. Perth was the host city when Australia first hosted the Congress and General Assembly of the International Union of Crystallography in 1987.

A trip to Australia would not be complete without a visit to the "top-end" and the spectacular national parks Kakadu [9], Litchfield [10] and Uluṟu-Kata Tjuṯa National Park [11], the last home to the sandstone monolith known as Uluru. Kakadu and Litchfield National Parks can be accessed from Darwin, while Alice Springs is the gateway to the Red Centre desert, with spectacular scenery and walks. Near Alice Springs are spectacular salt lakes, such as the 180km-long Lake Amadeus, which is twice as salty as the sea and is estimated to contain 600 million tons of salt crystals [12]. These lakes, which are typically only accessible on guided tours, glow pink in the early morning light and silver in the moonlight. Alice Springs also claims a connection to the Braggs – being named after Alice Todd, who was W. H. Bragg's mother-in-law and W. L. Bragg's grandmother.

Sticking with the theme of minerals and gemstones, the Queensland outback towns of Emerald, Sapphire and Rubyvale are found in the central highlands, inland from Rockhampton, and about 10 hours drive northwest of the state capital Brisbane [13]. There are lots of opportunities to fossick for gems and tour mine heritage sites.

Heading south from here takes you to Parkes, five hours west of Sydney, where the "The Dish" – The Parkes Radio telescope – is located. You can read all about this in the first IUCr 2023 newsletter E-Zine. Heading east to the coast again brings you to Sydney, one of the common arrival points for visitors. South of the city is Lucas Heights, home to ANSTO's OPAL reactor [14] and a suite of neutron diffraction instruments in the Australian Centre for Neutron Scattering [15]. Science Discovery Tours provide a tour of the world of nuclear science and the work ANSTO does in the areas of health, the environment and delivering solutions for industry.

There are plenty of options from here. One can push onto Victoria and the site of IUCr 2023. Alternatively, one can fly over Victoria to the southernmost state of Tasmania or head across the "ditch" to New Zealand. Tasmania, the "apple isle," is an area of significant natural beauty and home to several crystallographic sites. The tessellated pavement, just one hour's drive from the state capital, Hobart, is a picturesque natural wonder consisting of tile-like rocks along the water's edge [16]. A spectacular cubic rock, "cube rock" can be found in northeast Tasmania for those who appreciate crystals. On the slopes of South Mt Cameron, the rock is surrounded by beautiful views, including Little Blue Lake, the site of an abandoned tin mine, and views of Cameron Regional Park [17].

If you are coming "down under" for IUCr 2023, then a trip "across the ditch" before or after the conference is a must. Flights to New Zealand are available from most mainland Australian capital cities, and the South Island of New Zealand is a must-see. Down the west coast of the South Island is Punakaiki, also known as the Pancake Rocks, an area where the wild West Coast seas form blowholes amongst layers of rock [18]. These "pancakes" formed below the ocean floor as softer sandstone and harder limestone layers before the sandwiched rock was lifted out of the ocean by earthquake activity. Erosion by wind and rain led to these spectacular stacks, like the crystallographic planes of a layered crystal. Heading further south along the West Coast past, with spectacular glaciers and forest, leads one to Lake Matheson, where spectacular reflection symmetry mirrors New Zealand – Aotearoa's – tallest mountain, Aoraki (Mt Cook) in the water [19].

From Lake Matheson, near Fox Glacier, one can travel over the Haast Pass to Queenstown and then north through the Mackenzie Country or out to the east coast. If you take this route, a stop at Moeraki Boulders, a beach dotted with hundreds of nearly spherical stones half-buried in the sand is recommended [20]. The crystallographic connection is to spherically ground 2-dimethylsufuranylidene-1,3-indanedione (YLID) crystals, which are used as test crystals for diffractometer alignment and instrument testing [21].

Victoria is the final state on our crystallographer's road trip and the state capital, Melbourne, our destination. About four hours drive northwest of Melbourne is Lake Tyrrell, a 120,000-year-old shallow salt lake known for its spectacular views [22]. The drive also takes you up into the Mallee, a region named after the form of certain species of eucalyptus trees, which grow with multiple stems springing from an underground lignotuber. Alternatively, if you want something a little closer to Melbourne, then 90 minutes east of the city is Warburton and Cement Creek Redwood Forest, where 1500 Californian Redwood trees form a perfect periodic array [23]. On the way back, stop in Clayton to see the Australian Synchrotron, where "first light" was achieved in June 2006. Today, as part of the Bright project [24], seven new beamlines will be constructed to complement the existing nine. The new beamlines include MX3 for macromolecular and chemical crystallography, BioSAXS and Advanced Diffraction and Scattering Beamlines. Come 2023, several of these will be in operation.

The Australian and New Zealand crystallographic community is very excited to host IUCr 2023 and to welcome international researchers "down under" for this event. Hopefully, you can enjoy some or all of this crystallographic road trip "down under" in the lead up to or following the congress, and this article has provided some inspiration.

Thanks to Dr Helen Maynard-Casely for the inspiration for the article and to the Twitter crystallographic hive mind for their suggestions of local sights worth visiting. To get further ideas and more information, visit IUCr 2023's website (https://iucr2023.org/) and subscribe to their E-zine containing details of the "The Great Down Under Road Trip."

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OUTREACH

IYBSSD2022 given green light by United Nations



Michele Zema

International Years are proclaimed by the United Nations (UN) to mark particular events or topics in order to promote, through awareness and action, the objectives of the UN itself and, in turn, of society at large. The IUCr and the crystallographic community know this very well as they have certainly benefitted greatly from the International Year of Crystallography in 2014 (IYCr2014). Awareness about the importance of crystallography has increased enormously within the scientific community and the general public thanks to IYCr2014.

It is difficult to enumerate the many outcomes of IYCr2014:

we have seen the birth of two new regional crystallographic associations, namely the Latin American Crystallographic Association and the African Crystallographic Association, and several national crystallographic associations;

new crystallography laboratories and training centres have been inaugurated in several countries, particularly in the most disadvantaged regions of the world (see, for example, the many IUCr-UNESCO OpenLabs or the X-TechLab in Benin);

actions have been implemented for students of all ages to raise the awareness of crystallography (*e.g.* an international crystal-growing competition for schoolchildren; high-school teacher workshops; several schools and workshops for graduate, post-graduate and experienced crystallographers, which the IUCr supports through the sponsorship schemes managed by the Calendar Sub-Committee);

the IUCr is now actively involved in joint programmes with other scientific unions of the ISC network (*e.g.* the *LAAAMP* project) and in a number of initiatives in collaboration with other institutions.

It is then with great expectations that we look forward to the forthcoming International Year of Basic Sciences for Sustainable Development (IYBSSD) that will be celebrated from mid-2022 to mid-2023 – see the official announcement below. This International Year, coordinated by the International Union of Pure and Applied Physics, will focus on the links between basic sciences and the UN Sustainable Development Goals. Its main objectives are to enhance inclusive participation in science, strengthen education and scientific training, encourage increased funding of basic sciences and promote the concept of open science.

This is in fact perfectly in line with the aims of the IUCr, and the IUCr is proud to be one of the Founding Members of IYBSSD2022, as reported in an earlier issue of the *IUCr Newsletter*.

It is particularly interesting that celebrations for the Year of Mineralogy 2022, as proclaimed by the International Mineralogical Association (IMA) under the auspices of UNESCO, will be formally part of IYBSSD. The IUCr will partner with IMA in this initiative as well.

In conclusion, IYBSSD offers a new opportunity to enhance the stature of crystallography, build capacity in developing regions of the world and extend further the public understanding of science, which are the three main objectives of the “Crystallography for the Next Generation” manifesto, and to establish new collaborations within the scientific community. There are many exciting events ahead that the crystallographic community is not going to miss!

The International Year of Basic Sciences for Sustainable Development proclaimed by the United Nations General Assembly for 2022

We need more basic sciences to achieve Agenda 2030 and its 17 Sustainable Development Goals (SDGs). This is the message sent to the world by the United Nations General Assembly on 2 December 2021: Member States approved by consensus the resolution 76/A/L.12 promulgating the year 2022 as the International Year of Basic Sciences for Sustainable Development (IYBSSD2022).

With this resolution, the United Nations General Assembly ‘invites all [its] Member States, organizations of the United Nations system and other global, regional and subregional organizations, as well as other relevant stakeholders, including academia, civil society, *inter alia*, international and national non-governmental organizations, individuals and the private sector, to observe and raise awareness of the importance of basic sciences for sustainable development, in accordance with national priorities’.

The United Nations General Assembly motivated its decision with ‘the high value for humankind of basic sciences’, and with the fact that ‘enhanced global awareness of, and increased education in, the basic sciences is vital to attain sustainable development and to improve the quality of life for people all over the world’. It also stressed that ‘basic sciences and emerging technologies respond to the needs of humankind by providing access to information and increasing the health and well-being of individuals, communities, and societies’. The successes and difficulties of the global fight against the COVID-19 pandemic have been for two years a stark reminder of this importance of basic sciences, such as (but not limited to) biology, chemistry, physics, mathematics and anthropology.

The vote is the result of the mobilization of the international scientific community, led since 2017 by the International Union of Pure and Applied Physics (IUPAP), CERN (the European Laboratory for Particle Physics), and 26 other international scientific unions and research organizations from different parts of the world, under the auspices of UNESCO. Over 90 national and international science academies, learned societies, scientific networks, research and education centres are also supporting this initiative. They will organize events and activities all over the planet during this special year, to showcase and improve the links between basic sciences and the 17 SDGs.

The resolution was proposed to the United Nations General Assembly by Honduras, and co-sponsored by 36 other countries. Its vote confirms resolution 40/C 76 adopted unanimously by the UNESCO General Conference on 25 November 2019.

The International Year of Basic Sciences for Sustainable Development (IYBSSD2022) will be officially inaugurated with an opening conference 30 June–1 July 2022 at the UNESCO headquarters in Paris, France. Events and activities will be organized around the world until 30 June 2023.

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For more information, including the member organizations of the IYBSSD2022 Steering Committee and the full list of countries that co-sponsored the resolution, please visit https://www.iybssd2022.org.

MEETING REPORT (IUCR SUPPORTED)

6th European Crystallographic School



Petra Bombicz

The 6th European Crystallographic School (ECS6), the school of the European Crystallographic Association under the auspices of the IUCr, was held from 4 to 10 July 2021. ECS6 was organized as an online event by Hungarian crystallographers. The school would have taken place in Budapest in 2020 but had to be postponed for a year and then it had to be moved to the virtual space because of the COVID-19 pandemic. That is the reason we can not provide lovely photographs of the participants. Instead, a photomontage of the organizers can be seen below.



Photomontage of the ECS6 team (from left to right): first row: Petra Bombicz (Chair), Nóra V May (Secretary), Sourav De (ChemCrystLab); second row: AKCongress (PCO) and Hotel AVS (technical support) with Krisztina Tóth in the middle; third

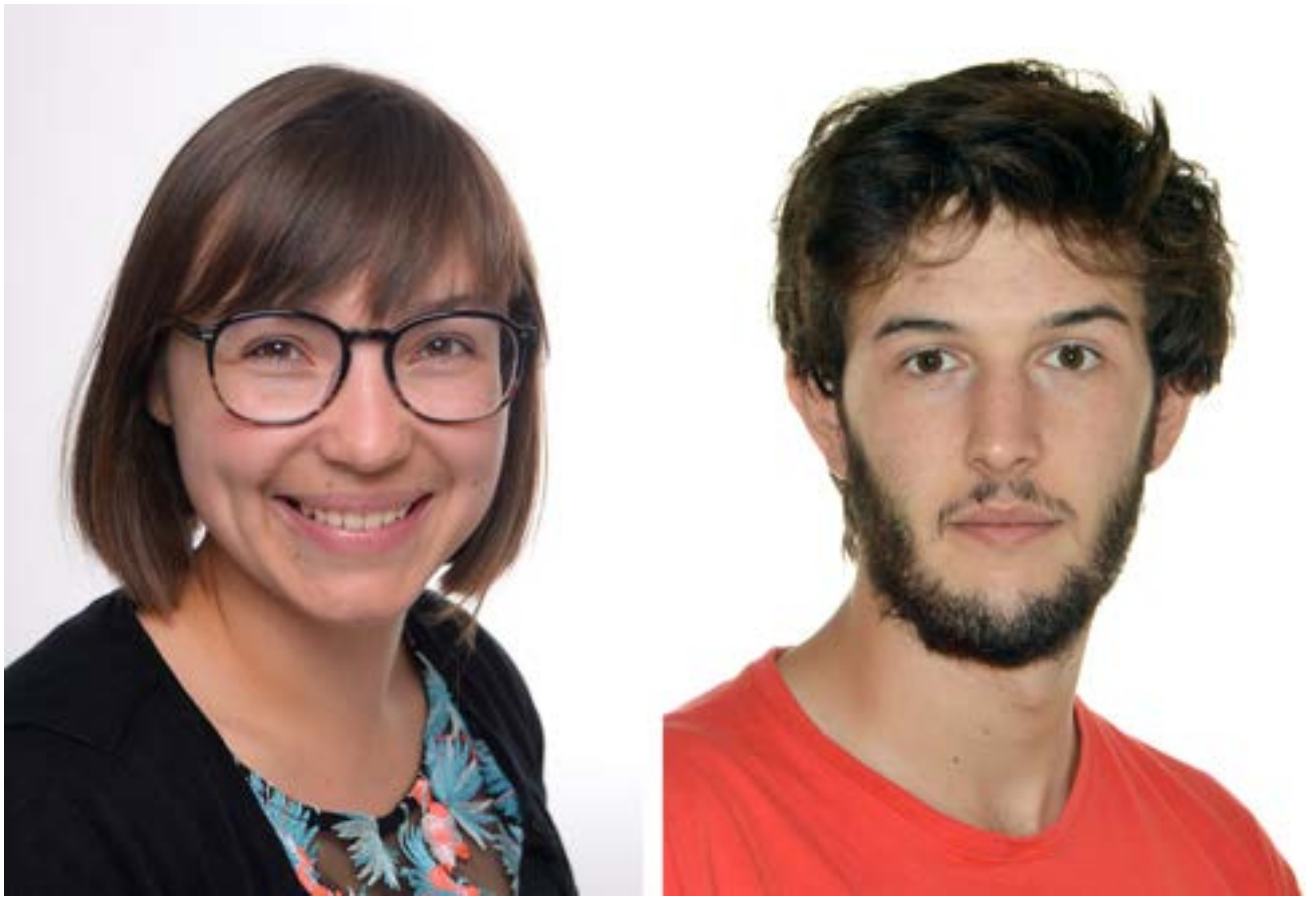
row: behind-the-scenes technical facilitator, Laura Bereczki (ChemCrystLab), Tamás Holczbauer (ChemCrystLab).

The five full busy days were extended with a preparation day before and with an excursion day after the teaching period. There were excellent lectures from eminent scientists, vivid discussions, a hands-on tutorial and four laboratory practicals. An overview of the very broad field of crystallography was provided, covering diffraction physics, symmetry, reciprocal space, instrumentation and experimental techniques, structural chemistry, non-ambient conditions, structural biology, data validation and quality, and so on. The lectures covered emerging techniques, like XFEL and electron diffraction, as well as the role of the CSD and PDB databases. Extra information on solution chemistry, on how to publish and on structural aspects of COVID were also given.

Nine scientists each from Hungary and the UK, five from Germany, three from Italy and one each from Poland, Portugal, South Africa and Switzerland accepted our invitation to teach at ECS6. The contribution of Professors Christian Lehmann, John Helliwell and Manfred Weiss, who delivered several lectures on different aspects during the week, has to be highlighted.

The 90 students arrived from four continents: Europe, North and South America, Africa and Asia: quite a number of the participants took the challenge to follow the long, busy days from different time zones. The gender distribution of the ECS6 students coincided with the natural population, half of the students were female, half of them male. In terms of proficiency, 45% of the students were beginners in crystallography, 32% had 1 to 2 years of experience and the rest had even more experience. The student survey revealed that most of the attendees were interested in molecular structure and chemical properties, powder diffraction, crystallography of functional materials and macromolecular crystallography. The topics of electron crystallography, molecular recognition and interaction, mineral and inorganic crystallography, crystallography under extreme conditions, instrumentation and experimental techniques, and crystallographic computing were also given as research interests. It means that the ECS6 school could offer something for everyone. Students might learn in their own field and could increase their knowledge in the related fields.

As ECS6 is a school, although organized online, the lectures were completed with extended Q&A sessions. The laboratory practicals were followed by 30-minute discussion sessions. All Q&A sessions were well attended. Teaching materials were provided and the ECS6 programme was made available for the registered participants to revisit for two more months. Moving to the virtual space was a special challenge for the teachers. At the end of the school all participants could vote on the lecturer who used the chance to teaching her/his subject online in the most effective way. The best online teacher of ECS6 was elected to be Christian Lehmann. The students could also take a quiz to measure the efficiency of knowledge transfer. A total of 26 students volunteered to test her/his familiarity in crystallography. The winner, who answered the highest number of questions well, was Najlaa Hamdi from Sidi Mohamed Ben Abdelah University, Morocco.



Laura Kind (left) and Marco Vandone, winners of the IUCr Journals Poster Prizes.

ECS6 students presented their own research at two poster sessions. The presenters needed to upload a poster, might also submit a flash presentation, and live chat with the authors was also made possible. All together six poster prizes were awarded by the IUCr, CCDC, PDBe and *CrystEngComm*. The IUCr Journals Poster Prize in structural biology was awarded to Laura Kind, University of Bergen, Norway, while the IUCr Journals Poster Prize in structural chemistry was awarded to Marco Vandone, University of Milan, Italy.

We missed the busy lecture halls, the crowded laboratories, the chats during the coffee breaks. Our rooms and corridors were empty, our dreams about the school were different from when we got the opportunity to organize it. Anyhow, we had to get over the difficulties caused by the pandemic. In addition to excellent scientific education, we offered different opportunities for socializing: networking in the evenings, a concert of Chemical Singers to present the extra talent of our colleagues, and two “live” virtual tours, where the guide was walking and cycling in real time instead of us, showing the beauties of Budapest and answering our questions in the daytime and at sunset.

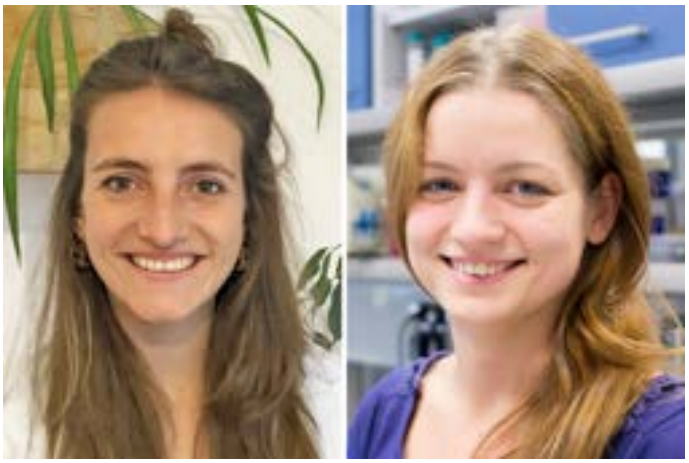
The active participation of the students was crucial to the success of the school. The school was organized for them, and they have received a huge package of new information. The most eminent scientists were working hard for months on the preparation and recording of their contributions, at the same time developing new skills in online teaching. The organizers are grateful for all the contribution and support of the ECA and the IUCr, as well as of the Italian Crystallographic Association for the bursary they offered to the student participants. The school could not have been organized without the financial support of our exhibitors: Bruker, Dectris and Rigaku (argentite sponsors), Crystal Impact and MiTeGen (molybdenite sponsors) and CCDC, PDBe, OlexSys, European XFEL, *CrystEngComm* and Molecular Dimensions (cuprite sponsors). It is a special pleasure that all members of the Hungarian crystallographic community contributed to the organization of ECS6 with their whole enthusiasm, which improved our cohesion. A special thank you has to be addressed to the members of the Chemical Crystallography Research Laboratory, Centre for Structural Science of the Research Centre for Natural Sciences.

The 6th European Crystallographic School was a magnificent event. It offered a great learning experience for the participant and valuable opportunities to interact with fellow researchers. We hope that life will soon return to its usual pre-pandemic way and that the next school, ECS7 in Lisbon, Portugal, in 2022, can be organized as an in-person event.

Petra Bombicz, Chair of ECS6, is at the Chemical Crystallography Research Laboratory, Centre for Structural Science, Research Centre for Natural Sciences, Budapest, Hungary.

MEETING REPORT

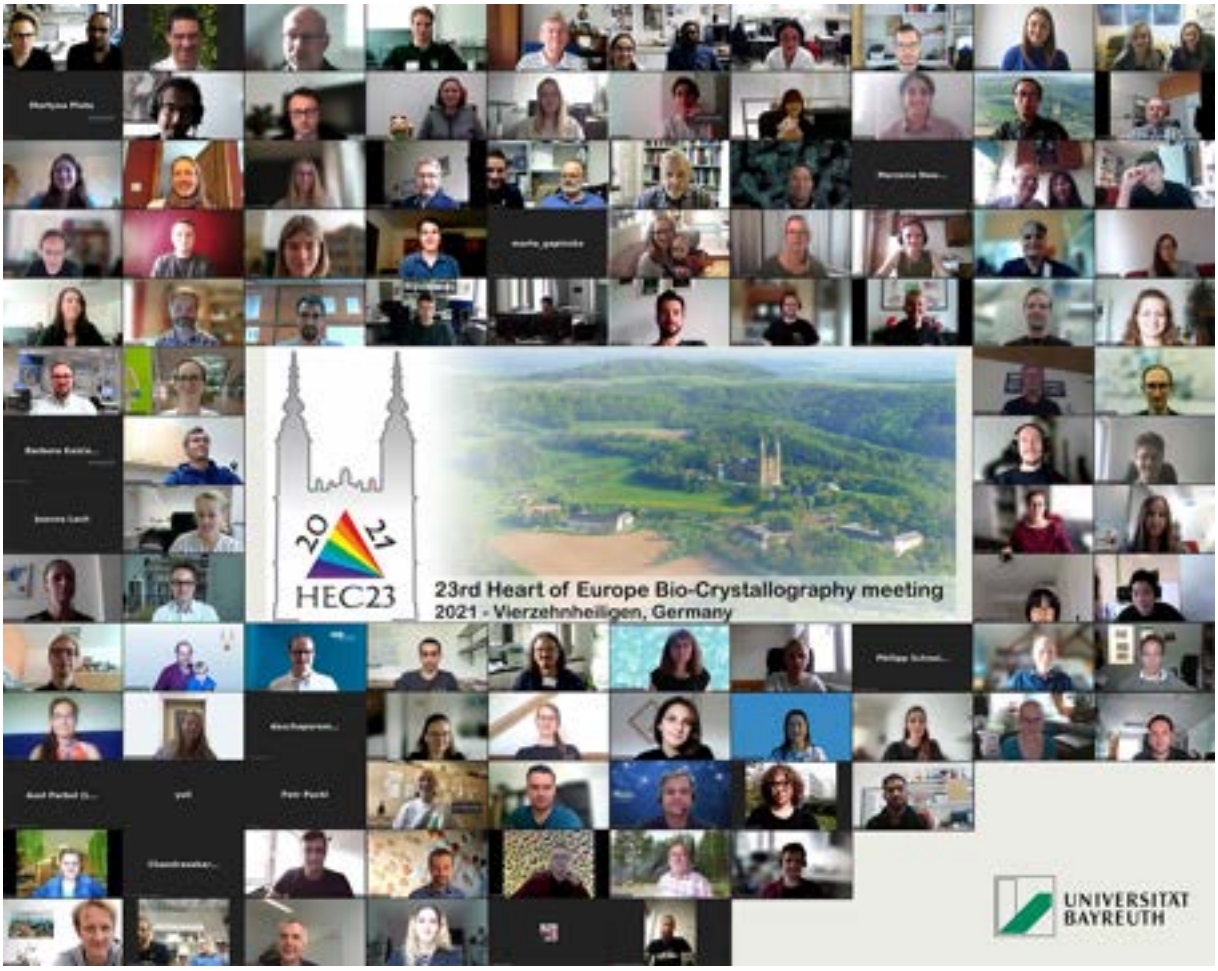
23rd Heart of Europe Bio-Crystallography Meeting



Ivana Kutá Smatanová

The 23rd Heart of Europe Bio-Crystallography Meeting (HEC23) was due to take place in Vierzehnheilingen, Germany, in September 2020. However, because of the COVID-19 pandemic, the meeting was postponed to the following year and finally took place in virtual mode (online) from 16 to 17 September 2021, organized by the group of Clemens Steegborn and his colleagues at the University of Bayreuth, Germany. Ten companies provided support for the meeting, and the European Crystallographic Association (ECA) covered registration fees for six young participants. Two student presentations were awarded IUCr Journals Prizes.

The HEC23 meeting program gathered 42 speakers from 23 research groups, in total. They delivered 21 full lectures and 12 flash talks. There was also the HEC23 Lecture and a presentation focused on the next meeting, HEC24. Company representatives gave an additional seven lectures. Professor Steegborn opened the HEC23 meeting on Thursday at 1 pm and after welcome remarks, a new HEC group of Christian Roth from MPI Potsdam and a guest group of Birte Höcker from the Bayreuth University were introduced. There followed lectures divided into six sessions aimed at bacterial enzymes and regulators, nucleic acid and interacting proteins, drug development, pathogen proteins, molecular machines and techniques, technologies and applications. Dr Herbert Nar, the Director of Structural Research at Boehringer Ingelheim, gave the HEC23 Lecture on Thursday evening. He spoke about basic concepts of structural biology applications in drug development at big pharma and illustrated these concepts with recent project examples. He finished with possible future developments in the field such as HT single-particle cryo-EM or structure prediction methods based on artificial intelligence.



Group photo of real HEC23 participants in the virtual environment.

As a tradition, there was also a place for entertainment and personal exchange. Breakout rooms gave opportunities for visiting sponsors and chatting with friends as well as for a challenging quiz and Friday night dinner entertainment.

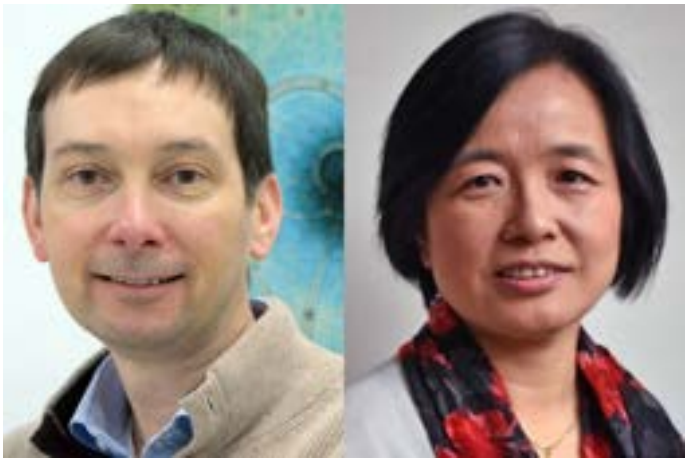
At the end of the meeting, IUCr Journals awarded prizes to two student presentations. Lena Maria Gras from the Marcus Wahl group (Germany) and Kristyna Adamkova from the Jan Dohnalek group (Czech Republic) received the IUCr Journal Prize for full and flash talks, respectively.

Finally, we would like to thank the organizers, sponsors and participants for a fascinating meeting and friendly atmosphere in the virtual environment.

The next Heart of Europe Bio-Crystallography Meeting, HEC24, will take place in South Bohemia in the Hotel Resort Relax at Dolni Vltavice on the banks of Lipno Lake and near to the Sumava mountains. The date was set as 22–24 September 2022.

IUCR JOURNALS NEWS

Introducing two new Main Editors of IUCrJ



Henry Chapman of the Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, and Xiaodong Zou of the Department of Materials and Environmental Chemistry, Stockholm University, have recently been appointed as Main Editors of **IUCrJ**. Henry Chapman, who was already a Co-editor of **IUCrJ**, will succeed the late John Spence in leading the journal section on *Physics and Free Electron Laser Science and Technology*. Xiaodong Zou will lead a new section on *Electron Crystallography*, which will act as a home within the IUCr journals for high-quality, high-impact papers in this field. We are assembling a team of Co-editors to work with Xiaodong Zou and details of this section will be provided in the next issue of **IUCrJ**.

Henry Chapman is a physicist who is a world leader in exploiting modern high-brightness X-ray sources for high-resolution structure determination and imaging of soft matter or biological systems. His work in developing experimental methods and analysis for coherent diffractive imaging of non-periodic objects includes the first experimental demonstration of X-ray ptychography, as well as his pioneering work in serial femtosecond crystallography. His international status in these FELS fields also includes his association with multiple world-class high-brightness coherent X-ray source developments around the world. Henry completed his PhD in 1992 at The University of Melbourne, Australia, for which he was awarded the Bragg Gold Medal from the Australian Institute of Physics. He explored lensless X-ray imaging at Stony Brook University (NY, USA), and first demonstrated X-ray flash imaging while at Lawrence Livermore National Laboratory in California where he also contributed to the development of extreme ultraviolet lithography. He joined DESY and the University in Hamburg in 2007 as a founding director of the Center for Free-Electron Laser Science. He was awarded the Leibniz Prize of the German Research Foundation (DFG), the Roentgen Medal, and an honorary doctorate of Uppsala University, and is a Fellow of the Royal Society (FRS).

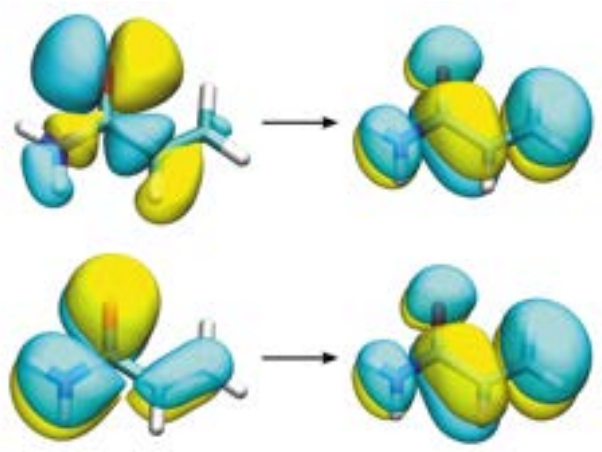
Xiaodong Zou is a leading expert in electron crystallography and porous materials. Her research interests have been developments of electron crystallographic methods and design of novel porous materials. She is one of the pioneers in establishing electron crystallography as an important technique for accurate atomic structure determination of unknown 3D crystals. Her group has demonstrated the power of electron crystallography in studying complex structures including zeolites, metal-organic frameworks, pharmaceuticals and proteins. Professor Zou has also made key contributions in design, synthesis and applications of novel zeolites and metal–organic frameworks. Xiaodong is a full professor in structural chemistry and deputy head of the Department of Materials and Environmental Chemistry, Stockholm University. She received her BSc in Physics at Peking University in 1984, and PhD in structural chemistry at Stockholm University in 1995. One of her main research interests is method development for accurate atomic structure determination of nano-sized crystals by electron crystallography. Her group has solved a number of complex structures of zeolites and mesoporous crystals by transmission electron microscopy. She is also working on synthesis, structure determination, topology analysis and applications

of inorganic open-framework materials and metal–organic frameworks. She has received several prestigious awards given by the Royal Swedish Academy of Sciences. She is an elected member of the Royal Swedish Academy of Sciences (KVA), member of the Royal Swedish Academy of Engineering Sciences (IVA), Fellow of the Royal Chemical Society (FRCS) and council member of the International Zeolite Association.

This article was originally published in *IUCrJ* (2022). **9**.

EDITORIAL

Quo vadis, quantum crystallography?



Jean Michel Gillet, Piero Macchi

In the past few issues of *Acta Crystallographica Section B*, including the current one, several articles have reported research work on quantum crystallography. Collectively they comprise a virtual special issue on the subject, the first on such an extended concept in the IUCr journals. Previously, a special issue, dedicated to Philip Coppens (1930–2017), was published in *Acta Crystallographica Section B* (August 2017). It contained many contributions in the field of charge density (as well as photo-crystallography). Originally intended to celebrate his retirement with contributions on two of the main topics developed during his career, the issue appeared just a few weeks after Professor Coppens passed away and became a kind of memorial issue.

The occasion of the present special issue is the principal authors' participation in the first online quantum crystallography meeting (QCrOM2020) held in August 2020. It was organized (and mostly improvised) to replace the sessions on this subject initially programmed for the IUCr Congress in Prague, which, as we know, was postponed to 2021. Its virtual modality (and its subsequent free of charge registration) made it possible to attract attendees from a wider range of expertise. It was the opportunity to present the latest results and reviews on the field and share opinions during fruitful discussion sessions that normally do not take place at large scale and tightly scheduled meetings like those of the IUCr Congress.

Despite all the difficulties caused by the pandemic the field is currently blooming, and the community is undergoing a generational turnover with many new young researchers involved and new groups established. The field's momentum is testified by the rather broad spectrum of studies published in this special issue, with a variety of research themes and many topics analyzed or reviewed in detail.

Quantum crystallography is a modern name for a field that started when quantum mechanics itself was put forward, coinciding with the early days of X-ray crystallography. In keeping with Peter Debye's early intuition (Debye, 1915), the discovery of X-ray diffraction offered a whole new possibility 'to establish by experiment the particular arrangement of the electrons in the atoms'. Many studies became possible thanks to the interplay between crystallographic techniques and quantum physics. For example, experimental crystallography was used to unveil the nature of electrons (waves and corpuscles; see De Broglie, 1929), to investigate the electronic structures of metals (Weiss & Demarco, 1958), to map the charge density around atoms to form bonds and molecules or solids (Coppens, 1967), and the electron polarization upon application of external stimuli (such as the electric field, see Hansen *et al.*, 2004) or upon temperature changes.

Quite remarkably, these kinds of studies are those that originally attracted the interest of quantum physicists for the emerging field of X-ray crystallography in the 1920s. At the same time, chemists also envisaged the exceptional outcome from crystallographic studies and the vast array of details useful in

developing theories of chemical bonding (Pauling, 1939).

This sentiment has always accompanied studies on accurate charge density, which has become the favourite observable for revealing the nature of chemical bonding and the supramolecular interactions, especially – but not only – within the paradigm of the quantum theory of atoms in molecules (Bader, 1990) that becomes, in the crystallographic framework, the quantum theory of atoms in molecules and crystals (Gatti, 2005).

In the past two decades, and especially in recent years, we have witnessed a renewal of the interest in a direct determination of the crystal wavefunction, which has indeed been a goal since the beginning of the X-ray diffraction era (Pauling, 1926). For example, there is growing attention being given to calculations of wavefunctions restrained to reproduce the X-ray diffracted intensities (Jayatilaka, 1998), as well as to the refinement of orbital coefficients (Tanaka *et al.*, 2008) or of reduced-density matrices (Gillet, 2007).

A search in the database of papers published in *Acta Crystallographica Section B* since 1998 (online versions), returns more than 500 papers directly or indirectly related to quantum crystallography (and overall, ~4000 in all IUCr journals). Most of them report accurate charge density studies and their applications, encompassing the technological progress which has occurred over the years, such as the availability of area detectors, the development of synchrotron sources and low-temperature devices (see for example, Iversen *et al*., 1999). Moreover, a discussion on the future of topological analysis of experimental charge density took place (Dittrich, 2017; Macchi, 2017).

The virtual special issue that we have edited seamlessly combines the recent developments and an outlook on future research in this field, highlighting fundamental questions, scientific cases and broad applications in other disciplines.

Despite the growing appeal of molecular/crystal orbital calculations, orbital-free quantum crystallography is emerging, in keeping with the emergence of orbital-free density functional theory (see Finzel, 2021; Tsirelson & Stash, 2021; Bartashevich *et al.*, 2021).

While quantum crystallography often deals with molecular aspects of electron distribution, the role of environment and of intermolecular interactions is being ever more scrutinized (see Zheng *et al.*, 2021; Macetti *et al*., 2021; Bergmann *et al.*, 2021; Forni *et al.*, 2021; Kleemiss *et al.*, 2021).

Although scientists often think of electron density as the mere distribution of charge in a molecule/crystal, one should not forget that electrons do have a spin as well and that molecular or extended systems may feature an overall spin magnetic moment. Thus spin-density models are essential (see Souhassou *et al*., 2021), especially in view of the increasing development of spintronics. The paper by Souhassou *et al.* (2021) also deals with the refinement of orbital coefficients in inorganic solids, another frontier topic. The role of ligand coordination for setting the oxidation state of a metal is also discussed by Adamko Koziskova *et al.* (2021).

Landeros-Rivera, Contreras-García & Dominiak (2021) discuss refinement strategies in electron wavefunctions obtained from X-ray diffraction data while Launay & Gillet (2021) deal with the *N*-representability of reduced density matrices reconstructed from several X-ray scattering techniques. Shteingolts *et al*. (2021) instead discuss transferable aspherical atom models for improving the quality of refinements.

One of the appeals of quantum crystallographic techniques, especially in the past few years, is the possibility of using very accurate modelling (such as atomic multipolar coefficients and molecular wavefunctions) to improve the standard (bio)chemical crystallographic studies. Such a link is fundamental because quantum crystallography should be intimately connected with the rest of crystallography and all related sciences. The quest for highly accurate observations and ever more precise calculations, inherent to the most fundamental aspects of quantum crystallography, has many implications for applied science and technology. In this respect, the present state bears little difference to quantum mechanics, originally developed as a very sophisticated theory for elite scientists, which has

proved to be vital for several technological applications, up to quantum computing.

We are confident that this special issue will contribute to attracting ever-growing interest not only in the fundamental bases of quantum crystallography, but also in its applicative aspects. We also thank all the authors of contributions to this special issue for their dedication and excellent work, and the Main Editors of *Acta Crystallographica Section B* for this opportunity.

The virtual special issue is available at https://journals.iucr.org/special_issues/2021/QCrOM2020.

Acknowledgements

We would like to acknowledge the excellent work accomplished by Sara Delahaie, Hugo Julien, Antoine Marras and Nizar Melk, who were – at the time – first year engineering students at CentraleSupelec. Their enthusiasm and hard work were decisive in the organization (in such a short timeframe) of the first online quantum crystallography meeting (QCrOM2020). We also thank CentraleSupelec for their permission to use their logo for the conference (and the cover page of this issue) as well as for their essential financial and technical support.

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EDITORIAL

Submission of structural biology data for review purposes



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

The IUCr stable of journals are proponents of the FAIR and FACT principles of publishing: data should be Findable, Accessible, Interoperable and Reusable (Wilkinson *et al.*, 2016) and Fair, Accurate, Confidential and Transparent (van der Aalst *et al.*, 2017; Helliwell, 2019). This has been manifested by a number of leading contributions to the field of structural biology including publication standards for a variety of data types (Kroon-Batenburg & Helliwell, 2014; Adams *et al.*, 2019; Guss & McMahon, 2014) as well as mandatory deposition of coordinates, and subsequently structure factors, for publication of macromolecular crystal structures. This approach has largely satisfied the FAIR and FACT principles. However, a further step is required to ensure that the data deposited in a third-party database fully support the conclusions drawn from those data. This step requires the mandatory submission of data (*e.g.* coordinates and reduced diffraction data, discussed further below) to accompany the manuscript describing the work.

This action does not imply that the various databases [PDB (Burley *et al.*, 2019), EMDB (Lawson *et al.*, 2016), SASBDB (Kachala *et al.*, 2016), BMRB (Ulrich *et al.*, 2008) *etc.*] are not doing a good job of validating data submitted to them. Indeed, the validation reports produced by databases are an important pillar in the FAIR approach to structural biology. Nevertheless, it is not the role of the databases to test the extent to which the interpretations and conclusions of a manuscript incorporating structural biology research (possibly by multiple methods) are supported by the deposited data. This role belongs in the manuscript review cycle.

Authors may ask why submission of data needs to be made mandatory. After all, the Notes for Authors for *Acta Cryst. D*, *Acta Cryst. F* and *IUCrJ* all indicate that editors may request such data from the author. However, the current system causes delays in the review system when editors have to request data. The added inconvenience increases the possibility of poorly supported interpretations avoiding scrutiny and being published. In order to clarify the situation, and maintain the IUCr's position leading the field in data quality standards in structural biology, submission of deposited data for review is best practice.

Historically there has been reticence to provide data for review as this might provide a competitor with an advantage. This concern has reduced substantially over recent years as increasing numbers of macromolecular structures are released prior to publication, and complementary methods such as accurate and precise computational predictions are more widely used. Indeed, the increasing prevalence of preprint versions of papers has further expedited the release of non-peer-reviewed data. Data submitted to IUCr Journals will be mandated for review purposes only, and thus the ethical position of a reviewer receiving them is clearly defined.

The concept of data deposition can be extremely broad, so it is important that we clarify what is mandated and what is recommended. The non-negotiable starting point is that for any manuscript containing conventional structures determined by the most common techniques (crystallography, NMR, cryoEM, SAXS) the data that are deposited with the relevant database to obtain the accession code and validation reports must be uploaded prior to editorial review. This set of standard files (which may include coordinate files, reduced diffraction data, restraint lists, electron-density maps, buffer-subtracted scattering curves, along with any validation reports) should already be immediately at hand to the submitting author. Additionally, depending on the manuscript in question there are cases where additional data should be provided. For example, many crystal structures may have indications of space-group ambiguity, twinning, anisotropy, alternate unit cells or other pathologies for which the review process would benefit from the submission of scaled but unmerged intensity data. We do not mandate submission for review of primary data as this is not practicable, however we continue to recommend that such data be made publicly available (Guss & McMahon, 2014).

To accompany the requirement for data, which will apply from the start of 2022, the journals *Acta Cryst. D*, *Acta Cryst. F* and *IUCrJ* are unifying their requirements for information to be included in the standard tables for various experiment types (colloquially Table 1 for crystal structures). These new requirements will be described in detail in the revised Notes for Authors for the journals.

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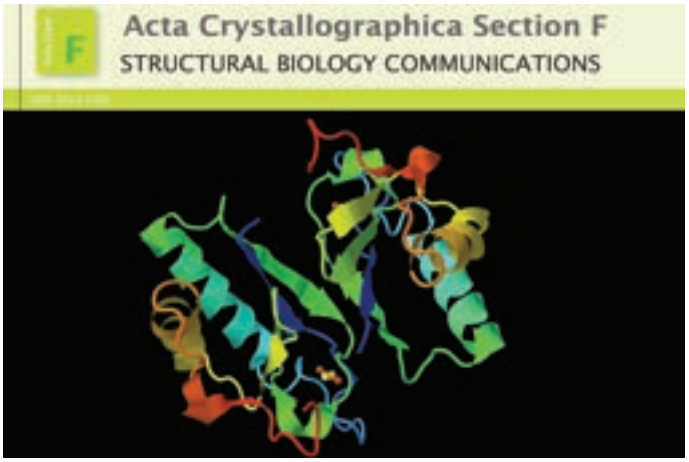
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EDITORIAL

Topical Reviews in Acta Crystallographica F Structural Biology Communications



John R. Helliwell, Janet Newman, Mark J. van Raaij

In this November 2021 issue of *Acta Crystallographica F*, we publish the first of a series of concise *Topical Reviews* on structural biology. The review in this issue discusses the crystal structures of the enzyme hydroxymethylbilane synthase (also known as porphobilinogen deaminase) and is authored by one of us (Helliwell, 2021). This article is dedicated to the 50 year anniversary of the Protein Data Bank, the macromolecular structure database to which we are proud contributors and grateful users.

Our idea, originating from John Helliwell, is to publish Topical Reviews, a category which is already described in the Notes for Authors, and to focus each review specifically on a coherent group of structures. We would expect authors to consider a typical group containing 3–20 structures (although there are no strict limits) and the resulting discussion would form a concise, up-to-date and forward-looking review of around 10 000 words. Each review would then be refereed in the usual way and, if accepted, appear prominently in the journal. The PDB holds many possibilities for the subjects of such Topical Reviews – they may be on the same enzyme, structures containing the same ligand, the same not very common co-factor or metal ion, or any kind of logical grouping of a not-too-large number of structures.

Eventually, we would like to publish at least one Topical Review per issue – and we hope that a significant number would be from this initiative (Topical Reviews on other structural biology subjects are of course also welcome!). It occurs to us that not only established scientists or group leaders would be able to write these, but also younger scientists such as postdoctoral fellows or PhD students about to submit their theses.

John Helliwell is the Guest Editor who will drive the commissioning and editing of this type of Topical Review. If you would like our feedback on the subject for a review or have a suggestion for other articles in the journal, please get in touch. Together, we look forward to receiving your ideas and your future submissions.

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COMMENTARY

Intracellular drug binding affinities by NMR

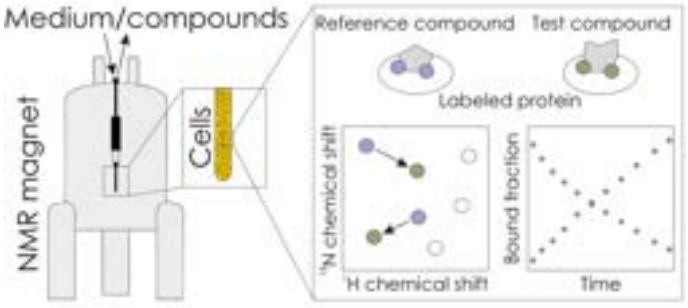


Figure 1. Scheme of in-cell determination of binding affinities using an NMR bioreactor setup.

Tobias Madl

Most small-molecule drugs fulfill their function in cells, but studying direct compound–target interactions in a cellular environment is challenging. Nevertheless, this is crucial information guiding drug development where drug engagement at the desired site of action and potential off-target binding and activity need to be assessed as early as possible. Rather than intracellular binding affinities, available approaches rely on activity-based cellular assays, and provide a downstream and indirect impact of the respective compounds on target activity. In 2006, several seminal publications proposed a first solution towards this problem by demonstrating that nuclear magnetic resonance (NMR) spectroscopy can be used to study proteins in living cells (Selenko *et al.*, 2006; Serber *et al.*, 2006). Since then, `in-cell NMR' has been successfully applied to study proteins, their (post-translational) modifications and interactions (reviewed in Luchinat & Banci, 2017; Selenko & Wagner, 2007; Pastore & Temussi, 2017; Siegal & Selenko, 2019). More recently, several groups have shown that in-cell NMR can be used to study interactions of proteins with small-molecule compounds in living cells (DeMott *et al.*, 2018; Luchinat *et al.*, 2020). However, whether intracellular compound–target interactions can be determined quantitatively in terms of binding affinities remains unknown.

In this issue of *Acta Cryst.* D, Luchinat *et al.* report that NMR spectroscopy can provide intracellular binding affinities in the nanomolar range provided that a reference compound with a known dissociation constant (K_d) is available (Luchinat *et al.*, 2021). Using the well studied human carbonic anhydrase II as a model system, Luchinat *et al.* assessed the binding and competition of a set of four small-molecule inhibitors with known binding affinities *in vitro* and in living cells. To this end, the authors expressed [^{15}N]-His-labeled carbonic anhydrase II in HEK293 T cells and followed changes in chemical shifts of ^{1}H, ^{15}N cross-peaks by NMR spectroscopy (Figure 1). This has the advantage that NMR signals specific for carbonic anhydrase II can be observed even in a complex cellular background. The authors carried out competition experiments either from a series of independent cell samples or from a single real-time NMR bioreactor run. Excitingly, Luchinat *et al.* found that the intracellular affinities were similar to those obtained *in vitro*.

Whereas it still remains to be shown whether this approach can be applied to other target proteins, these findings promise that in-cell NMR can provide a new route to the determination of intracellular ligand-binding affinities for other target proteins in the future. In principle, this approach should be applicable to all target proteins provided that (i) they can be expressed or introduced in cells isotopically

labeled at sufficient concentrations (>10 μ*M*); (ii) there is a lack of binding to other cellular components which would cause extensive broadening of NMR signals; (iii) there is sufficient protein stability; (iv) there are well separated NMR signals in the cellular background; (v) sufficient chemical shift differences are induced by ligand-binding and (iv) there is strong ligand binding. Moreover, the NMR-based approach is not limited to proteins, but could be extended to other biomolecules such as nucleotides and other isotope labeling schemes.

The real-time NMR bioreactor setup described promises to be well suited to obtain comprehensive and time-resolved datasets for cellular compound uptake and, at the same time, intracellular compound–target interactions. Remarkably, samples of HEK293 T cells could be kept viable and metabolically active for up to 60 h as shown in this study. An additional and great advantage of this setup is that concentrations of reference and test ligands can be changed easily, and the response of the intracellular compound concentrations and target binding can be followed in real-time inside the NMR spectrometer.

Identifying the intracellular details of a compound binding to a molecular target promises to become a solvable problem with the approach described by Luchinat *et al.*, provided the aforementioned requirements are met. In future studies it will be very interesting to see if in-cell NMR can be used for compound screening, for example by testing ligands or ligand mixtures with unknown cellular uptake or target affinity. Off-target compound binding is a common problem faced during drug development, and might be tractable by in-cell NMR. It remains to be investigated what the requirements for detectable off-target binding are, for example in terms of binding affinities and expression levels of off-targets. Given the flexibility of NMR spectroscopy, future studies might even go beyond compound-centered disease-related studies and enable time-resolved and quantitative binding studies with other compounds, such as metabolites, in a (patho)physiological environment.

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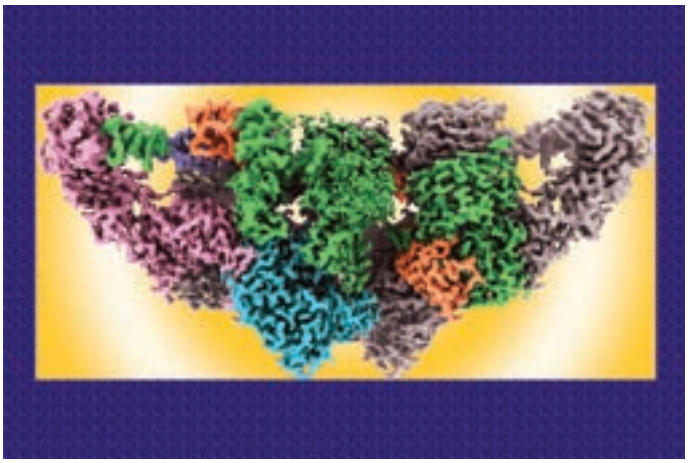
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COMMENTARY

Thyroxine hormones visualized by the cryo-EM structure of bovine thyroglobulin



Dušan Turk, Gregor Gunčar

In vertebrates, iodine has a unique role. Its circulation regulates metabolism and many other fundamental processes, including neuronal tissue growth (Caravalho & Dupuy, 2017; Di Jeso & Arvan, 2016). The cycle begins with the intake of iodine from the bloodstream into thyroid follicles by the Na^+/I^- symporter (Dai *et al.*, 1996), where tyrosine residues of thyroglobulin (TG) are iodinated for iodine storage and hormone production. The coupling of two iodinated tyrosine residues forms the thyroid hormones T4 and T3, also called thyroxines. Hence, this giant molecule, TG, is used for the synthesis of the tiny thyroid hormone molecules. TG is a dimeric molecule and is known to every biochemist as it is used as the high molecular weight standard (330 kDa) for molecular weight determination by SDS–PAGE, yet its first 3D structure was determined only recently (Coscia *et al.*, 2020). Although the human TG structures were 93% complete, the obtained density maps lacked the resolution that could enable insight into such structural details. Moreover, the material obtained either from thyroid glands of patients with goitre or recombinant TG expressed in HEK293T cells was not iodinated.

In the cryo-EM structure of bovine TG from natural sources presented in this issue of *Acta Cryst. D* (Kim *et al.*, 2021), we see for the first time the intermediate of thyroxine hormone formation, the precursor of T4, composed of two iodinated tyrosine residues, together with all iodine atoms resolved in the map (Fig. 1). The structure provides unambiguous insight into the coupling of two pairs of tyrosine residues: acceptor Tyr24 and donor Tyr149, and acceptor Tyr2575 and donor Tyr2542. Moreover, the absence of density beyond the CB atom of residues Tyr149 and Tyr2542 in well resolved parts of the density maps is strong structural evidence for their donor role in hormonogenic reaction. These findings corroborate previous results of biochemical studies such as Lamas and coworkers (Lamas *et al.*, 1989) and site-directed mutagenesis of human TG (Coscia *et al.*, 2020), which identified four rather than two hormonogenic sites, including the alternative pairing of Tyr24 with Tyr149 and Tyr234. The Tyr234 residue was not iodinated in the bovine TG structure.

These differences may arise from differences between the bovine and human thyroids and may also reflect the availability of iodine under *in vivo* conditions and those made available under the *in vitro* conditions of iodination assays (Coscia *et al.*, 2020). Kim *et al.* did not observe the presence of mono-iodinated tyrosine residues in the bovine TG structure. Similarly, biochemical assays performed by Coscia *et al.* did not reveal the presence of T3, the active form of thyroxine hormone. Hence, direct synthesis of T3 still needs to be demonstrated. The bovine TG structure exposes another interesting issue potentially related to the regulation of the redox potential of thyroid follicles. TG structures contain numerous cysteine residues, many of which are present in the cysteine-rich thyroglobulin type domains.

In the human TG structure, all cysteine residues are linked by disulfide bonds. Due to the limiting resolution of density maps, this conclusion was often only supported by their proximity. In contrast, the bovine TG structure contains cysteine residues not involved in disulfide bridges despite their proximity, as described by Kim *et al.*

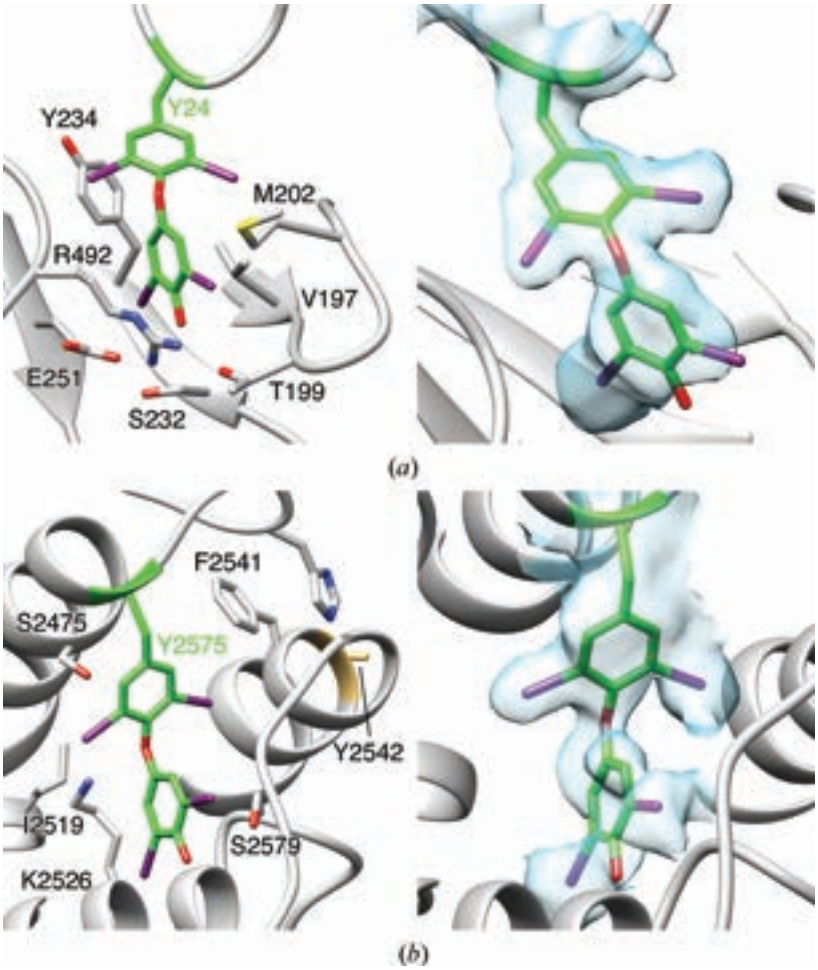


Fig. 1. Iodotyrosines in bovine TG. Side chains and cryo-EM map density fit for thyroxinated side chains at Tyr24 (*a*) and Tyr2575 (*b*). Map contour level 0.032. Reproduced from Fig. 2 of Kim *et al.* (2021).

Although TG has been extensively studied, its three-dimensional structure could not be determined for decades. Isolation of purified TG (Heidelberger & Palmer, 1933) enabled the determination of its molecular weight (Heidelberger & Svedberg, 1934). The first complete sequence of TG was deduced from cDNA of bovine TG and contained 2769 amino-acid residues (Mercken *et al.*, 1985). Yet, a successful determination of a 3D structure requires sufficient amounts of homogeneous material and technology that makes the determination possible. The material has to be stable enough to sustain treatment by crystallization conditions or during the preparation of grids. It is not customary to publish unsuccessful attempts, but we believe that determination of the bovine TG structure was at least as long-lasting as that of its human homologue. Indeed, we know from personal experience how difficult this project was to bring to fruition. The structure of human TG was the culmination of about two decades of long endeavour, the seeds of which were planted by the crystal structure of MHC class II-associated p41 invariant chain fragment bound to cathepsin L (Gunčar *et al.*, 1999). The p41 fragment revealed the fold of thyroglobulin type-1 repeats, containing six cysteine residues and the CWCV signature (Molina *et al.*, 1996).

For a long time, we struggled with attempts to crystallize TG from natural sources. Porcine material appeared to behave the best and was the easiest to isolate in large amounts. However, we were unable to obtain material that was stable over longer periods of time or reproducible crystals diffracting beyond 15 Å at a beamline such as the microfocus beamline at ESRF. During one visit (by DT) to MRC LMB, Jan Loewe suggested tackling the structure with electron cryo-microscopy, which was becoming capable of

resolving the structures of macromolecules in atomic detail. Indeed, we progressed from porcine to purchased and later recombinantly expressed human thyroglobulin (Coscia *et al.*, 2020). As Kim *et al.* stated, the bovine TG material at first also appeared unstable on the grids. They hypothesized that the instability was caused by the interactions at the solvent–air interface and that a small addition of detergent already successfully applied in other studies (Noble *et al.*, 2018; Chen *et al.*, 2019) would prevent sample denaturation. Indeed, they observed that the addition of CHAPS (CMC of ~0.49%; GoldBio) prior to vitrification of the samples on the grid significantly improved the micrographs and resulted in a data set of 2.6 Å resolution. In addition to visualizing the T4 structure on the backbone of its precursor, the structure of bovine TG by Kim *et al.* is a triumph of sample preparation and the maturation of electron cryo-microscopy. The structure demonstrates that structural details of biologically important chemical reactions can now be visualized by electron cryo-microscopy.

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COMMENTARY

Finding order in chaos – nanocrystals in amorphous protein gels

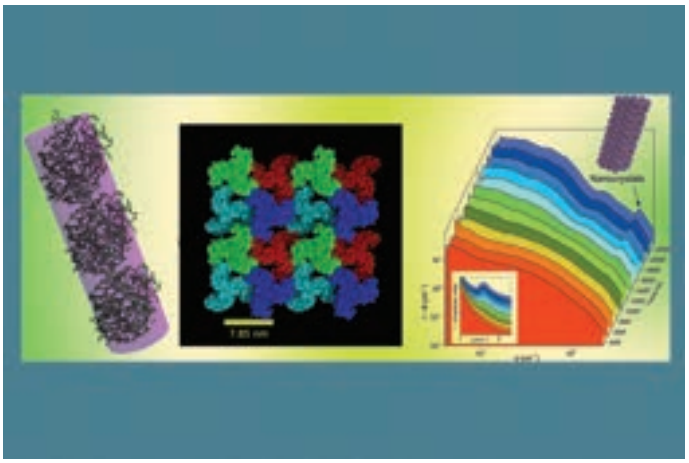


Fig. 1. Left to right: lysozyme, RNAse A and ovalbumin. Images reproduced from Greene *et al.* (2021).

Matthew W. Bowler

Methods to coax macromolecules into ordered lattices are bread and butter to the readers of *Acta Crystallographica Section F*. This is far from an easy process, and when it succeeds there is an enormous variety in the size, shape and order found within these crystals (Svensson *et al.*, 2019). Tens of thousands of trials are often needed to find the components of a supersaturated solution that will induce the formation of crystals; can anything be salvaged from all the failed crystallization experiments? Amorphous material is often found during screening, and can blaze a trail to crystallization, but is there order in the chaos? In this issue, Greene and colleagues (Greene *et al.*, 2021) add to their discovery that dense phases of ovalbumin contain highly ordered regions (Greene *et al.*, 2015), by showing the same phenomenon in a number of other proteins.

The dense phases that proteins form during the crystallization process of salting-out have been largely ignored with respect to their macrostructure. The rise of the XFELs (Chapman *et al.*, 2011; Spence, 2017), and more recently microED (Mu *et al.*, 2021; Wolff *et al.*, 2020), has made the collection of data from ordered structures on the nanometre scale a real prospect. This justifies the investigation of nanocrystals in order to gain atomic details of macromolecules that can be hard to crystallize. By detailed characterization using X-ray and neutron scattering techniques, combined with electron microscopy and modelling, the authors beautifully demonstrate a variety of microstructures that can be formed within protein gels. The researchers investigated three proteins, all adopting different microstructures: RNAse A that forms nanocrystalline sheets, immunoglobulin G that forms hexagonally packed tubes and lysozyme that forms short ordered chains. Each of these examples show similarities to the packing observed in fully fledged crystals, demonstrating that this phase is likely a step towards large crystals and, more importantly, could be common to this type of ‘amorphous’ protein gel.

While the number of examples is still perhaps limited, this study clearly shows that protein gels tend to contain microstructures. This can therefore be exploited to gain structural insights into systems that have proved difficult to crystallize and may shed light on the processes of crystallization itself. We look forward to seeing the first diffraction images from these fascinating protein phases.

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COMMENTARY

Mapping completeness

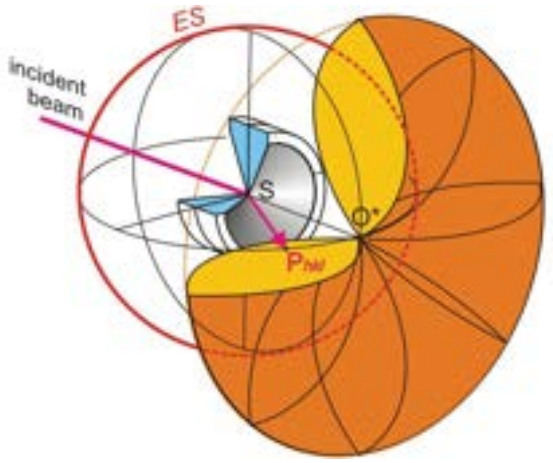


Figure 1. Illustration of accessible reciprocal space through a diamond anvil cell with a conical opening angle α. The colored toroidal volume V_{DAC} is given by $V_{DAC} = 4\pi/\lambda^3[\sin\alpha(\alpha - \sin\alpha\cos\alpha)]$ (Merrill & Bassett, 1974; Miletich *et al.*, 2000). Tchoń & Makal (2021) quantify systematically how a sample crystal of given symmetry needs to be oriented relative to the DAC in order to maximize the number of independent reflections in the toroidal volume. Figure modified after Miletich *et al.* (2000).

Martin Kunz

Diamond anvil cells (DACs) are simple devices that allow experiments involving electromagnetic radiation as a probe to be performed in the visible, IR and hard X-ray range at pressures between ~10^8 and 10^{11} Pa. Like almost anything of significance in the realm of DACs, their use for single-crystal X-ray diffraction was pioneered by Bill Bassett in Cornell in the 1970s (Merrill & Bassett, 1974). These simple devices allowed a pressure dimension to be added to crystallography for the first time, thus providing an invaluable tool in the quest to experimentally explore the nature of the chemical bond in chemistry, physics and mineralogy. Not surprisingly, DACs found immediate acceptance and countless groups all over the world adopted this simple but powerful concept for high-quality structural studies at high pressures, which led to further refinements of DAC design and use (Allan *et al.*, 1996; Finger & King, 1978; Kudoh *et al.*, 1986; Miletich *et al.*, 2000). For high-pressure single-crystal diffraction data to be of sufficient quality to enable accurate bond lengths, bond angles and displacement parameters to be extracted, a series of experimental artifacts and difficulties specific to DACs have to be overcome. These include precise crystal centering with reduced optical access (King & Finger, 1979), diamond absorption (Angel *et al.*, 2000), gasket shadowing (Katrusiak, 2004) and intensity modulation through diamond anvil diffractions (Loveday *et al.*, 1990).

An intrinsic limitation on data that comes with single-crystal diffraction in ancillary equipment is the restriction of accessible reciprocal space, thus making the collection of a complete set of unique diffraction intensities either difficult or impossible. In the case of DACs, this restriction was quantified for the first time, true to my comment above, by Bill Bassett (Merrill & Bassett, 1974) who found that the accessible reciprocal space forms a toroidal annulus (Fig. 1) whose volume is determined by the accessible *q*-range (*i.e.* wavelength and maximum diffraction angle) as well as the conical opening angle α of the DAC. Consequently, attempts to improve the completeness of high-pressure diffraction data were primarily directed towards improved DAC design (Allan *et al.*, 1996; Kantor *et al.*, 2012; Miletich *et al.*, 2000) and improved diamond design (Boehler & De Hantsetters, 2004) to maximize the effective opening angle α and thus the toroidal subspace of the reciprocal lattice (Fig. 1).

One important aspect that crucially affects data completeness and is complementary to hardware development, and which was also already mentioned in Merrill & Bassett (1974), is the orientation of the

sample crystal relative to the DAC geometry. This has never been fully quantified in a systematic way. Tchoń & Makal (2021) in this issue of **IUCrJ**, close this gap with a comprehensive and thorough study that systematically assesses the relative contributions of sample orientation, X-ray energy and DAC opening angle to the completeness of the diffraction data as a function of Laue class (symmetry). The level of completeness for a given experimental arrangement (*i.e.* combination of $2\theta_{max}$, X-ray energy/wavelength, sample Laue class, DAC opening angle α and crystal orientation relative to DAC geometry) is quantified by a 'Potency' *P* that is the ratio between the 'classical' completeness as defined in *International Tables Volume G* and an 'applicable' completeness which depends on the experimental set-up (i.e. accessible reciprocal space and sample orientation). The results are visualized for a series of important Laue classes and in-house experimental conditions in the form of heat maps projected on a unit sphere. These heat maps are of real immediate practical value for any high-pressure crystallographer in that the maps allow them to get a quick sense of the sensitivity of their experiment to crystal orientation. They furthermore allow for a rough quantitative estimate of the best crystal orientation. An obvious and important relatively low hanging next step based on this work is to create an app to assess the Potency (*i.e.* achievable completeness) of a given experimental set-up and make the app available to the crystallography community as an on-line tool. And the equally logical but harder to achieve step after that is to develop a set of micromanipulation tools in conjunction with orientation photographs of the sample to achieve the perfect sample orientation of a ~100-µm crystal on a diamond culet of slightly larger dimensions. This for the time being is still reliant on the skills and calm hands of invaluable graduate students and postdocs.

Besides these practical aspects, the results of the numerical simulations also demonstrate – somewhat surprisingly – that the energy range chosen is only of secondary importance for the completeness of the dataset. This conclusion may well be biased by the limited energy range considered (20 keV versus 22 keV), as those two energies are relevant for in-house laboratory X-ray sources, and will probably have to be revisited once synchrotron-accessible energy ranges (up to 40 keV, ~0.3 Å) are taken into consideration.

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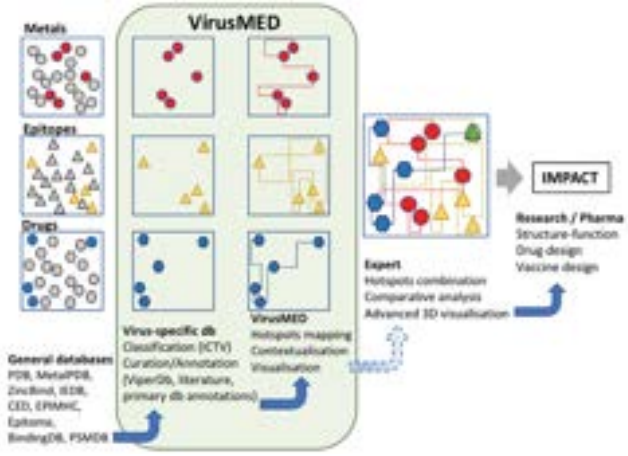
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COMMENTARY

virusMED: your travel guide to the virus world



Fasséli Coulibaly

The virus world is wide and vast. And we have just started venturing further in our explorations through metagenomics studies and the characterization of the multitude of variants in viruses relevant to human health.

Fortunately, help is coming to explore the virosphere – another term used to describe the virus world – in the form of a new server called virusMED (*M*etal binding sites, antigenic *E*pitopes and *D*rug binding sites, https://virusmed.biocloud.top) developed by Wladek Minor, Heping Zheng and their collaborators (see Zhang *et al.*, 2021, in this issue of **IUCrJ**).

To understand the scale of the task at hand, viruses infecting bacteria, called phages, alone represent the most abundant biological entity on earth, outnumbering cellular organisms by a factor of 10 (Dion *et al.*, 2020). They have been less studied than their medically relevant counterparts but a flood of data has begun, owing in part to the renewed interest in phage therapy to combat antimicrobial resistance (Gordillo Altamirano & Barr, 2019) and the proposed role of phages in regulating the population dynamics of bacteria playing an important role in carbon capture (Suttle, 2005). Sampling of our oceans, soil and even our own gut has already expanded our view of phage diversity and generated masses of viral and virus-like sequences (Paez-Espino *et al.*, 2016; Camarillo-Guerrero *et al.*, 2021; Dion *et al.*, 2020).

The search for viruses that infect eukaryotes is equally raging. For some discoveries, like mimiviruses and related giant viruses (La Scola *et al.*, 2003), the biological significance is complex but they represent a wealth of new proteins, novel biological processes and almost infinite research questions. For others, the impact is immediately evident such as the characterization of the RNA virome in animals that represent known reservoirs for zoonotic viruses such as flaviviruses, haemorrhagic fever viruses, influenza viruses and coronaviruses.

As a tool for exploration, sequencing is extremely powerful in organizing viruses into families and setting up a robust classification of these organisms in the ever-growing Taxonomy of Viruses (https://talk.ictvonline.org). A complementary approach has focused on the determination and cataloging of three-dimensional structures produced by viruses. Indeed, structure determination of intact viruses has been at the forefront of developments in structural biology since its birth (Harrison, 2015; Rossmann, 2013). These structures are made freely available to all through the Protein Data Bank (Johnson & Olson, 2021), which celebrates 50 years of existence this month, as well as the virus particle explorer database (VIPERdb; http://viperdb.scripps.edu) (Montiel-Garcia *et al.*, 2021). These invaluable resources are highly curated and constant efforts have been made to improve the quality of their content and make it more

accessible to all despite exponential growth (Smart *et al.*, 2018; Montiel-Garcia *et al.*, 2021).

While these resources are free, analysis of each viral structure is onerous and requires expertise in several inter-connected fields such as biochemistry, chemistry, molecular virology and immunology. This is where virusMED comes in to save the day. Think of it as your GPS navigation app that will guide you quickly and safely to your destination. Like a navigation app, it taps into tools that are readily available elsewhere: primary databases with sequence information, 3D structures, functional sites, metal and drug binding sites, and epitope repositories. The power of the server is to help researchers combine information from these different sources and make sense of it for the specific goal of understanding and combating viruses [Fig. 1(*a*)].

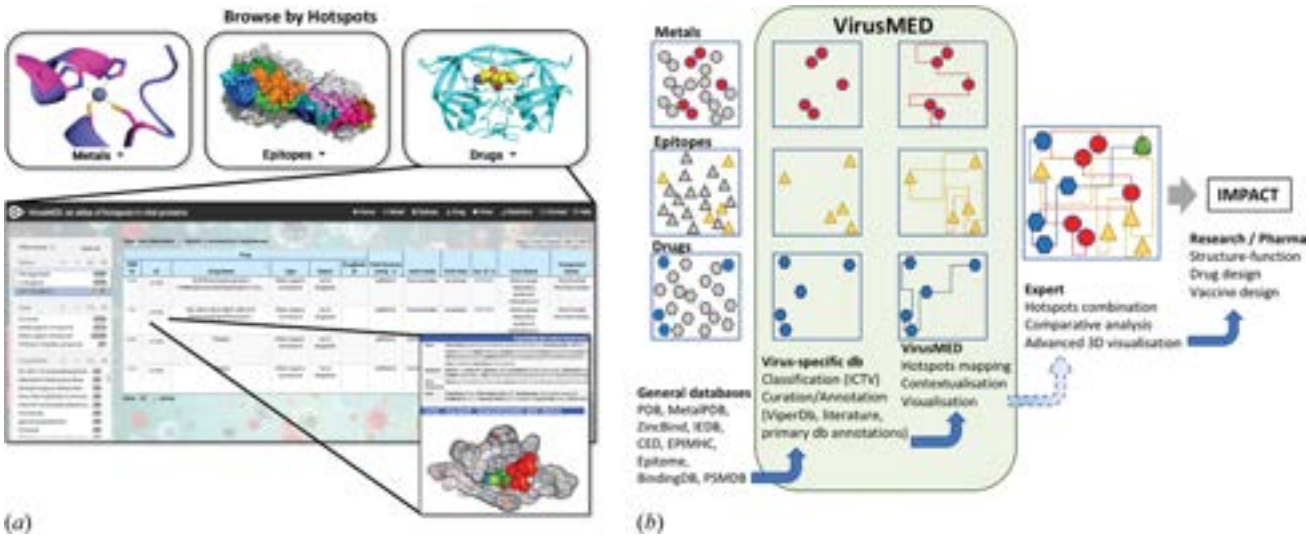


Figure 1. (*a*) virusMED is an atlas of hotspots present in viral proteins that correspond to metal binding sites, epitopes and drugs/small molecules. It is searchable by virus (not shown) and type of hotspot (top panel). Results are presented in a tabular form that can be filtered (middle panel) and mapped onto the 3D structure, providing context and a detailed view of the hotspot. (*b*) Schematic loosely based on a DIKW hierarchy. virusMED provides a navigation tool tailored to molecular virology that consolidates curated data available in various databases. This atlas is likely to facilitate research for viral families with a high volume of data, where expert analysis is time-consuming (coronaviruses, HIV, influenza viruses *etc.*). The dotted lines indicate possible future developments that will further integrate the individual atlases and facilitate comparative analysis (*e.g.* overlapping drug and epitope hotspots shown in green).

Taking SARS CoV-2 as an example, in the space of 21 months (February 2020–October 2021) over 117 000 publications were made available in PubMED and 1555 structures in the PDB. This represents an average of over 180 articles and 2 new structures every day. Organizing, curating and providing visualization tools for this large amount of data is essential to extract the most relevant information in a format that will help generate novel insights [Fig. 1(*b*)].

virusMED provides an integrated portal to navigate through 7041 structures across 75 viral families. One can browse the database using several pre-set entry points or design specific searches to rapidly gain an overview of where and how metals and small molecules bind to a specific target. Many of these ‘hotspots’ will be important functionally and may represent targets for drug development. With drug repurposing in mind, the results can be filtered to focus only on known drugs found in Drugbank or those that are already FDA approved.

The same portal allows mapping of antigenic sites in viral proteins, providing a database of more than 5000 B- and T-cell epitopes for 329 individual proteins. These can be combined to determine the antigenic landscape of viral proteins, identify variants likely to escape vaccination or reveal targets for potent and broadly neutralizing epitopes.

As the database grows, future developments can be anticipated such as more complex visualization options and an integrated search engine allowing the comparison of new structures with known hotspots. Data on binding sites for other viral proteins and cellular factors accumulate rapidly (Goodacre *et al.*, 2020; Gordon *et al.*, 2020) and, while a huge task, would deserve a similar atlas. For now, there is little

doubt that many in the structural virology community will adopt this tool to accelerate their research and facilitate the development of antiviral strategies.

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HISTORY OF CRYSTALLOGRAPHY

Celebrating the life and career of Kaarle Kurki-Suonio



Kaarle Kurki-Suonio (left) with the late Jim King (IUCr Executive Secretary 1969–1993) at the "hunting cottage" museum of Marshal Mannerheim, some 100 km north east of Helsinki, Finland, in spring 1986, prior to that summer's Executive Committee meeting in the UK. This and the other photos in this article were contributed to the IUCr gallery by S. E. Barnes.

Pilvi Sihvonen, with an IUCr perspective by Malcolm Cooper

Merkitykset ovat ensin, professori Kaarle Kurki-Suonio – didaktisen fysiikan maestro (in English, *Meanings are first, Professor Kurki-Suonio, the Maestro of Didactical Physics*) is the title of a new book that celebrates Professor Kurki-Suonio’s life and achievements. It will be published in January 2022.

In the book, the Professor’s colleagues and students sincerely express their appreciation for the assistance and encouragement they have received from Kurki-Suonio with their studies, research and work. The book also discloses the Professor's inspiring impact by playing classical music together with colleagues and students as well as his enthusiasm for wildflowers and athletics.

A central theme of the book is Professor Kurki-Suonio's unique work as a developer of physics teacher education in Finland. In addition, the book contains articles about his decades-long career, research and achievements in crystallography.

Kurki-Suonio began studying mathematics in 1950 at the University of Helsinki. The actual Eureka moment of learning took place in the first year of his studies at a physics lecture. “I was in my own thoughts, as I often was in lectures. Suddenly, I realized that I could derive formulas by using differential geometry. I understood that the formula follows an understood meaning – and not the other way around,” Kurki-Suonio relates.

This experience initiated the development of the learning philosophy of Kurki-Suonio (Kurki-Suonio, 2011), which still continues. Later, when Kurki-Suonio focused on the development of physics teacher education at the University of Helsinki, the thoughts of that moment condensed into the main motto of physics teaching, “Meanings are first”.

His dissertation on mathematical crystallography was completed in 1959 when Kurki-Suonio was 26 years old. In the 1960s, the physicists Timo Paakkari and Pekka Suortti, from the University of Helsinki, began actively seeking international contacts. Kurki-Suonio says that their work also gave wings to his international career as a crystallographer.

Finnish representation at conferences in the field of crystallography expanded in the 1970s. At the same time, Kurki-Suonio became acquainted with the French academician Erwin Bertaut, who strongly pushed Kurki-Suonio's research forward. In the 1970s and early 1980s, Kurki-Suonio was a member and then Chair of the IUCr Commission on Charge, Spin and Momentum Densities (now Quantum Crystallography), and General Secretary and Treasurer of the IUCr from 1981 to 1987.



"Old and new" members of the IUCr Executive Committee at St George's College, University of Western Australia, at the 14th IUCr Congress in Perth in 1987. From left: V. I. Simonov, Jerry Karle, Theo Hahn, Mario Nardelli, Alajos Kálmán, Kaarle Kurki-Suonio, You-qi Tang, Asbjørn Hordvik and André Authier.

It is astonishing that while Kurki-Suonio did his research in crystallography and was active in the IUCr, he was able to focus on the development of his teaching philosophy and physics teaching. It is noteworthy that already in 1973, he was nominated as a professor whose duty, among many others, included physics teacher education. Kurki-Suonio took the task seriously and dedicated himself to physics teacher education and research.

Together with his wife, Riitta Kurki-Suonio, and his colleagues, Kurki-Suonio wrote many university physics books, two series of secondary school physics books and a book of his teaching philosophy and didactical physics for teacher education. Between the years 1980 and 2013, 13 didactical physics dissertations, 16 licentiates and 223 master’s theses were completed at the University of Helsinki.

Professor Kurki-Suonio's teaching philosophy aroused interest not only in Finland but also abroad. In Germany, father-and-son researchers Karl Hayo and Hayo Siemsen studied the significance of the philosophy developed by Kurki-Suonio. According to their intensive research, interviews and discussions with many science educators from universities, schools and government bodies, Hayo Siemsen (2010) stated that a main result of the empirical success of Finnish science education was based on Machian ideas implemented in the method of Kurki-Suonio. At that time, about 600 physics teachers, around 20% of Finnish physics teachers, had studied the philosophy and didactical physics of Kurki-Suonio.

Kurki-Suonio “reached the age limit of statutory senility”, as he humorously wrote in his farewell lecture (Kurki-Suonio, 1998), in 1998. In the same year, Kurki-Suonio lost his wife, who had had a profound impact on his life. Nevertheless, he continued his work in the development of didactical physics, *e.g.* planning seminars, supervising theses and discussing innumerable issues of physics and its teaching that concerned various teachers and students, *e.g.* in the email discussion group. In 2011, the professor gave six lectures on the empirical basis of modern physics in an in-service course for physics teachers organized by the Department of Physics of the University of Helsinki and the LUMA Center (science education network of Finnish universities).

Today, visitors to Kurki-Suonio may be greeted by beautiful tunes, created when he skillfully dances his fingers over the keys of his grand piano, and become acquainted with the beautiful flowers in his garden. However, in between, there is a great opportunity to discuss, for instance, interaction, which Kurki-Suonio argues/states is a key concept in “almost everything possible” or in how our worldview is constructed.

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Kaarle Kurki-Suonio and the IUCr

Malcolm Cooper

It is a pleasure to recall the contribution that Kaarle Kurki-Suonio made in two major roles within the IUCr. First and foremost he was General Secretary and Treasurer (GS&T) of the organisation, a very senior role, for the period 1981 to 1987, and secondly he chaired its Commission on Charge, Spin and Momentum Density between 1978 and 1981 and was in fact a member of this commission for six years. The GS&T has responsibility for the finances and general governance of the IUCr, which has an important business arm publishing journals (notably the *Acta Crystallographica* series) and reference works (specifically *International Tables for Crystallography*) for the benefit of the crystallographic research community. The IUCr’s support for crystallography worldwide, specifically through financial support for young scientists travelling to international conferences, schools and workshops plus other “good works” depends utterly on the profits from its publishing business.

In his time at the helm as GS&T, together with the Executive Secretary and the triennially elected Executive Committee, he oversaw a significant journal publishing operation with an editorial staff complement of just a handful, based in Chester in the UK. When he took over as the GS&T the IUCr had assets of just around one million Swiss francs. He set up a Finance Committee with Bob Diamond as its first Convenor. The Committee’s remit was to advise him and the IUCr Executive Committee on the Union’s finances. I am delighted to say that I have now had the privilege of being Convenor for over two decades, during which time I have come to appreciate well the changes that Kaarle implemented in the Union’s financial strategy in the 1980s. He saw immediately that the journals were significantly under-priced and that the current contract with the publisher, Munksgaard, was very disadvantageous to the Union. He renegotiated the contract and raised the subscription prices significantly, with the result that in three years the IUCr’s assets had doubled. Then they approximately doubled again in the next triennium, all under his stewardship; indeed no further rises in journal subscriptions were needed until 1990, and the IUCr was able to fulfil its remit to liberally support crystallography worldwide. Staff who were employed in the Chester office when Kaarle was GS&T make the point today that he took a real interest in them personally as well as their working roles. He was instrumental in recruiting people who have remained with the IUCr to this day, and who were closely involved in the rapid development of the publishing business as it emerged into the digital era. Perhaps it is not surprising that a portrait of Kaarle, unveiled in 1998, still adorns the walls of the IUCr offices!



From left: Asbjørn Hordvik, Ted Maslen, Anne Cawley, Kaarle Kurki-Suonio and Mike Dacombe in the Vienna woods in August 1988.

The IUCr's Commission on Charge Spin and Momentum Density was the natural home for Kaarle's early research interest in the multipole analysis of electron density distribution in solids, a subject for which he had built up an international reputation and developed a research group based in the Helsinki University Physics Department. Within his department he also oversaw the novel development of complementary research work to study the momentum distribution of those electrons through the Compton effect by his colleagues (notably Osmo Inkinen, Timo Paakkari, Seppo Manninen and Pekka Suortti): it was this latter research line, which was also my speciality, that brought me into close contact with his Department at the University of Helsinki, especially with the late Seppo Manninen, and facilitated me meeting Kaarle for research discussions on many occasions in the beautiful city of Helsinki. He joined the IUCr's Commission on Charge, Spin and momentum Density in 1975 at the time of the IUCr's Amsterdam Congress.

It was largely through his efforts that the Commission's 1976 triennial conference was held at Kiljava in Finland and attended by leading researchers and young scientists from around the world. This conference was part of a triennial series called the Sagamore conferences after the location of the first two (1964 and 1967) at Sagamore in Upper New York State, USA. They were traditionally in remote countryside locations with formal sessions restricted to mornings and evenings, and afternoons reserved for informal discussions and relaxation in the fresh air, following the pattern also developed by the Gordon conference series. This formula was perfectly adhered to at Kiljava, a lakeside and forest conference venue to the delight of all participants who quickly appreciated the pleasures of the Finnish way of life, including sauna and freshwater swimming. Kaarle's Sagamore conference stays fresh in the memory of many of those who were there to enjoy it.

In conclusion, very many people outside of Finland around the world have reason to be grateful for Kaarle's scientific and educational work. Not just the scientific work he did himself, which was substantial, but also for the achievements he inspired in others. I am grateful to my colleagues in the IUCr, past and present, for their input into this brief article. Those of us who are involved with the IUCr and especially its finances, have good cause to praise Kaarle Kurki-Suonio and enjoy this opportunity to

join in celebrating his life.

Malcolm Cooper is Emeritus Professor of Physics at the University of Warwick, Coventry, UK, and Convenor of the IUCr Finance Committee.

FEATURE ARTICLE

Herbert Hauptman's stained glass models



Istvan Hargittai

The Nobel Laureate Herbert A. Hauptman (1917–2011) was a co-creator, together with Jerome Karle, of the direct methods in X-ray crystallography. In this communication, though, the focus is on his hobby of making stained glass polyhedral models and filling them with spheres. This hobby was not unrelated to crystallography either.



Herbert A. Hauptman in 1985 at the time of the Nobel Prize announcement (photo courtesy of Herbert A. Hauptman). He was a mathematician, yet a chemistry Nobel laureate for his achievements in crystallography.

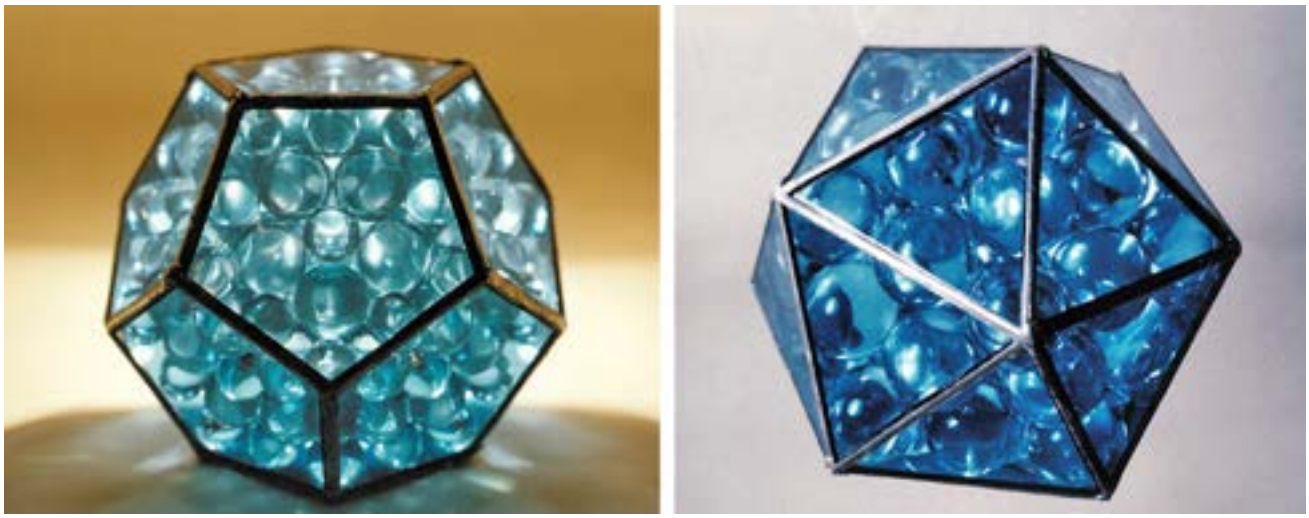
First, a brief biographical sketch. He was born in New York City into an East European immigrant family. He graduated from Townsend-Harris High School. His family was poor, and the time was the height of the Great Depression, but he could attend City College of New York because it was free, except for the 50-cent library fee. He enrolled when he was 16 years old and graduated with a BS in 1937. Afterward, he

attended Columbia University and earned a master's degree in mathematics in 1939. However, Columbia and a host of other schools turned him down when he applied for support to do his doctoral studies. There was anti-Semitism, which he later also experienced while serving in the Navy during World War II. He was settling down when he landed a job in 1947 with the Naval Research Laboratory (NRL) in Washington, DC. It was a physicist's job, but he would return to mathematics when it proved impossible for him to work for a physics PhD.

At the NRL, he worked together with Jerome Karle, and they jointly developed the so-called direct methods for solving the phase problem in X-ray crystallography. This happened in the early 1950s, and it has a vast literature. Suffice it to say that, before, it was considered impossible, but when they solved it, for many years, it did not break through in the crystallography community. Some of those who used to ridicule them eventually became the most important supporters of the technique. It made it possible to solve increasingly complex structures and, among them, those of biological importance.

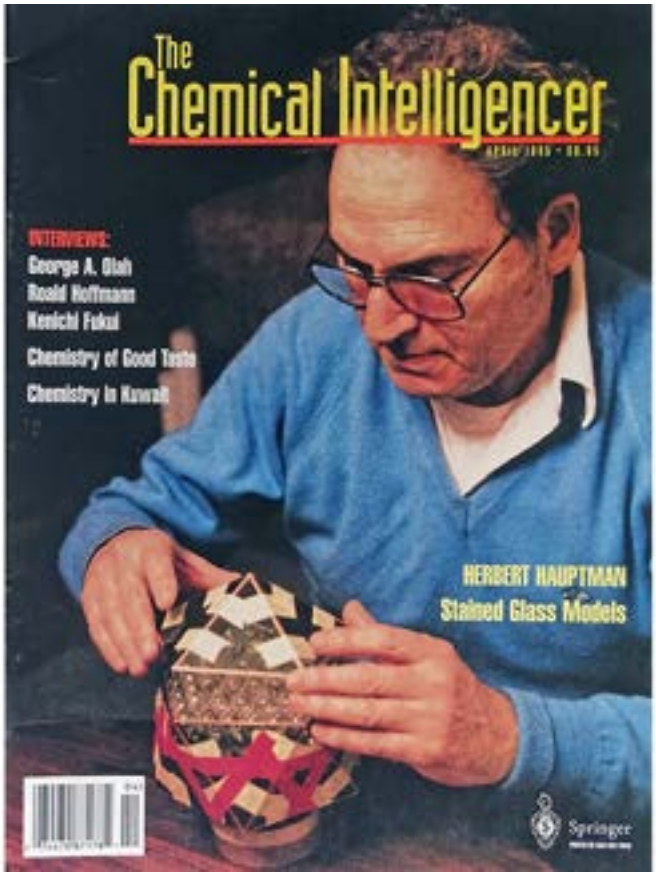
Hauptman never left the work on dealing with the improvement of the direct methods. Still, when it was no longer a burning issue, he returned to acquiring a PhD, which he finally succeeded in mathematics from the University of Maryland in 1955. His dissertation was an *n*-dimensional Euclidean algorithm. He introduced some geometrical approaches to the understanding and application of the Euclidean algorithm.

About 30 years after first introducing the direct methods, Hauptman and Karle were awarded the Nobel Prize in Chemistry in 1985 "for their outstanding achievements in the development of direct methods for the determination of crystal structures." By then, Hauptman was at the Medical Foundation of Buffalo, where he moved from NRL in 1968. This institute is now called the Hauptman-Woodward Medical Research Institute in Buffalo.



Two of Hauptman's stained glass models with spheres packed inside them. Left: a pentagonal dodecahedron; right: an icosahedron (both courtesy of Herbert A. Hauptman).

In the early 1980s, Hauptman took a class working with stained glass, and when he mastered it, he started making stained glass polyhedra. When he was 8 or 9, one of his favorite books taught him how to make the Platonic solids, and this interest never left him. He prepared about 40 regular and semi-regular polyhedra. Soon he became interested in packing spheres inside them. He put equal-size spheres into a regular tetrahedron, and these packed in the hexagonal close-packing arrangement. The cube and the octahedron could be filled up too with equal-size spheres. However, the icosahedron and the dodecahedron could not.



Herbert A. Hauptman preparing an icosahedral model with sphere packing as displayed on the cover of the April 1995 issue of *The Chemical Intelligencer* (the photograph was courtesy of Herbert A. Hauptman).

As a result of many experiments, he determined that spheres of two sizes would suffice in filling the icosahedron, and the ratio of their diameters would always be the same. Roughly, the small sphere has 9/10 of the radius of the large sphere. For the dodecahedron, two or even three different sizes did not suffice, and so he had to employ spheres of four different sizes, which did work. The Nobel Prize put an end to these studies and to the Hauptmans' quiet life. Ten years later, I persuaded him to write up his experience with packing the spheres in a regular icosahedron (Hauptman, 1995). The interest in learning how to make stained glass polyhedral models and then in playing with them may have been an indication of his gradually preparing for retirement in the early 1980s. This was then. When I asked him in 2001 about retirement, he told me about a new 9-year project of a significant grant from the NIH providing about a million dollars annually. So, obviously, at the age of 84, he did not think much about retirement.



The Hauptmans (on the left) and the Hargittais (on the right) in Buffalo in 1995 (by an unknown photographer).

Over the years, I had some good interactions with Hauptman, and our wives took well to one another. We visited each other in Buffalo and in Budapest, and I recorded two long conversations with him, one in Buffalo in 1995 and another in Erice, Sicily, in 2001. We blended the two conversations *via* correspondence, and the result appeared in 2003 (Hargittai, 2003). Perhaps the two most interesting segments in these conversations were about the painful gradual acceptance of the direct methods by the crystallographic community and about the painful, complicated relationship between Herbert Hauptman and Jerome Karle. I am happy to say that we had the most pleasant, friendly interactions with Isabella and Jerry Karle as well. Our interactions reached back to the mid-1970s. Perhaps, another vignette could be devoted to them.

Literature

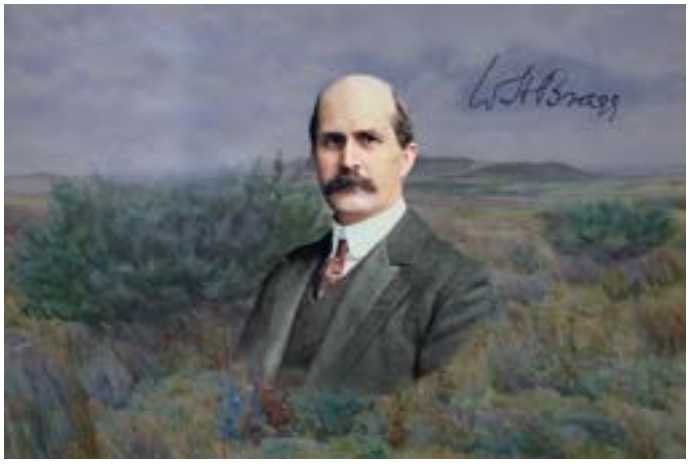
Herbert A. Hauptman (1995). “On the Packing of Spheres in the Regular Icosahedron.” *Chemical Intelligencer*, April 1995, pp. 26–30. *The Chemical Intelligencer* was a Springer magazine about the culture of chemistry, which I initiated and edited during its six-year existence (1995–2000). A collection of its best papers has appeared: Balazs Hargittai and Istvan Hargittai (2015). Editors. *Culture of Chemistry.* New York: Springer.

Istvan Hargittai (2003). *Candid Science III: More Conversations with Famous Chemists*, edited by Magdolna Hargittai, ch. 21, “Herbert A. Hauptman”, pp. 292–317. London: Imperial College Press.

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

FEATURE ARTICLE

New exhibition explores the legacy of Sir William Henry Bragg at the University of Leeds



Rebecca Higgins

Sir William Henry Bragg, and his son William Lawrence, changed how we understand the world around us, all from a laboratory at the University of Leeds. A new exhibition, ‘Shaping the course of modern science: William Henry Bragg and his legacy at the University of Leeds’, uses material from the University’s Special Collections and key loans from the Bragg family and the Royal Institution to reveal the story of Bragg’s Nobel Prize-winning work, and his continued legacy. The exhibition opened on 26 October 2021 and will run until 5 March 2022, coinciding with the opening of the new Sir William Henry Bragg building and as part of the Bragg Cultural Programme.



Sir William Henry Bragg joined the University of Leeds in 1909 as Cavendish Professor of Physics. In Leeds, he undertook pioneering research on X-rays and crystals with his son Lawrence. They became the first, and so far only, father and son duo to be awarded the joint Nobel Prize for Physics in 1915. The prize was awarded for their work at Leeds, developing the techniques of X-ray crystallography which allowed scientists to deduce the position of atoms within crystals using Bragg's equation, $n\lambda=2d\sin\theta$, first found by Lawrence Bragg.

Some of the items displayed as part of the exhibition include the original notebooks used by William Henry and Lawrence Bragg to record the results of their 1913 experiments, containing the handwritten discoveries which led to the Bragg equation. Bragg's original spectrometer, on loan from the Royal Institution, is also on display. This special piece of equipment was built in a University of Leeds workshop by C. H. Jenkinson, and helped the father and son team to work out the structure of many crystals, including sodium chloride and diamond. These items are displayed for the first time alongside William Henry's Nobel Prize medal, kindly loaned by the Bragg family.

The guest curator, Dr Stella Butler, comments that "William Henry Bragg and his son Lawrence formed a fantastic scientific partnership. The father brought amazing experimental skill, the son theoretical genius. Together they provided the springboard for scientific discoveries that would eventually reveal the secrets of nature."

Alongside highlighting William Bragg's work at Leeds, the exhibition also delves into his legacy that still lives on today. William Astbury, Bragg's student and protégé, joined the University of Leeds in 1929, pioneering the investigation of large biological molecules. His laboratory became one of the UK's most important centres for crystallography and his camera, used to produce the first X-ray diffraction studies of wool, is displayed in the exhibition. It was at this centre in Leeds where Astbury's research student Florence Bell wrote the thesis which contained one of the first X-ray photographs of DNA, the carrier of genetic information. Bell's original thesis is also on display.

The exhibition highlights another of William Bragg's protégés, Dame Kathleen Lonsdale. Her crystallographic work at the University of Leeds between 1927 and 1930 established that the benzene ring of six carbon atoms was a flat structure, with the six atoms sharing their outermost electrons as a 'cloud'. A model of benzene is on display alongside a copy of Lonsdale's *Structure Factor Tables,* both loaned from the Royal Institution, the latter being important in simplifying the complex and lengthy calculations involved in the determination of crystal structures. Lonsdale was awarded an honorary degree by the University of Leeds in 1967, and the exhibition also includes letters and photographs relating to this happy occasion. Crystallography also caught the *zeitgeist* of post-war Britain, with crystal structures inspiring designs at the Festival of Britain in 1951. Helen Megaw, a student of J. D. Bernal, himself a student of William Bragg, was responsible for suggesting crystallographic designs for the Festival. An example of one of the fabrics is shown alongside Lonsdale's work in the exhibition, loaned by Mike Glazer, Emeritus Professor of Physics at the University of Oxford.



In the 1950s, Gordon Cox and Durward Cruickshank introduced new computational methods to the University's crystallographic research, prompting the purchase of Leeds' first computer, a Ferranti Pegasus. It was now possible to work on much larger molecules, and in the 1980s, Simon Phillips, working at Leeds, was part of the international team which produced the first computer-generated 3D images of an antigen–antibody complex. The methods pioneered by the Braggs remained central even as computers 'took over' the calculations. Images in the exhibition have been provided by Professor Simon Phillips, the first Director of the Leeds-based Astbury Centre for Structural Molecular Biology established in 1999.

Finally, whilst X-ray crystallography is William Henry's most famous achievement, he is also remembered as a strong believer in the power of science and scientific education to do good in society and continued to champion this vigorously throughout his life. He was particularly known for his ability to explain complex scientific ideas to lay audiences, notably in his Royal Institution Lectures, and was seen as one of the main scientific voices in the interwar era. To his family, he was unassuming and modest, a much-loved father and grandfather who loved to paint and play sports, particularly lacrosse, golf and tennis. The Bragg family have kindly loaned rare family photographs, a selection of William's pencil sketches and one of his watercolour paintings in order to illustrate the man behind the science.



The crystallographic methods pioneered by William Henry Bragg and his son Lawrence have formed an important platform for research for over a century, ultimately contributing to uncovering the secrets of life itself. The molecular structures that have been determined using X-ray crystallography have led to life-changing treatments and vaccines, such as the COVID-19 vaccine, impacting the lives of everyone across the world. This new exhibition honours all of the different facets of William Bragg’s life and legacy.

AWARDS AND PRIZES

Call for nominations for the thirteenth Ewald Prize



The IUCr invites your nominations for the Ewald Prize for outstanding contributions to the science of crystallography. The Prize is named after Paul P. Ewald, in recognition of his significant contributions to the foundations of crystallography and to the founding of the IUCr. Professor Ewald was the President of the Provisional International Crystallographic Committee from 1946 to 1948, the first editor of the IUCr journal *Acta Crystallographica* from 1948 to 1959 and the President of the IUCr from 1960 to 1963.

The Prize is presented once every three years during the triennial International Congresses of Crystallography and consists of a medal, a certificate and a financial award. The recipients to date are as follows:

Year

Place

Recipient(s)

1987

Perth, Australia

Professor J. M. Cowley and Dr A. F. Moodie

1990

Bordeaux, France

Professor B. K. Vainshtein

1993

Beijing, China

Professor N. Kato

1996

Seattle, WA, USA

Professor M. G. Rossmann

1999

Glasgow, UK

Professor G. N. Ramachandran

2002

Geneva, Switzerland

Professor M. M. Woolfson

2005

Florence, Italy

Professor P. Coppens

2008

Osaka, Japan

Dr D. Sayre

2011

Madrid, Spain

Professor E. Dodson, Professor C. Giacovazzo and Professor G. M. Sheldrick

2014

Montreal, Canada

Professor A. Janner and Professor T. W. J. M. Janssen

2017

Hyderabad, India

Professor T. L. Blundell

2020

Prague, Czech Republic

Dr Olga Kennard, OBE FRS

The thirteenth Prize, for which nominations are now being invited, will be presented at the Melbourne Congress in August 2023.

Scientists who have made contributions of exceptional distinction to the science of crystallography are eligible for the Prize, irrespective of gender, nationality, age or experience. The Selection Committee will give careful attention to the nominations of outstanding scientists who have not yet won a Nobel Prize. Either an exceptionally distinguished scientific career or a major scientific accomplishment may be recognised. Current members of the Selection Committee and the President of the IUCr are not eligible. No restrictions are placed on the time or the means of publication of the nominee's contributions. The prize may be shared by more than one contributor, but no more than three, to the same scientific achievement.

Nominations for the Ewald Prize should be submitted electronically using the Ewald Prize Nomination Form to the IUCr Executive Secretary at execsec@iucr.org. The closing date for nominations is **31 August 2022.**

OBITUARY

Zofia Kosturkiewicz (1928–2021)



Mariusz Jaskólski

On 1 October 2021, the day of the Inauguration of the New Academic Year, Professor Zofia Kosturkiewicz suffered a massive cerebral stroke and four weeks later, on 29 October, without regaining consciousness, died peacefully in a hospice. Her death is a painful loss to her numerous friends and former students, many of whom owe her the formation of their personalities and scientific career. Especially those to whom she has always been, and will remain to be, The Boss (Szefowa).

Professor Zofia Kosturkiewicz was a woman of stature. As a young girl, she served as a liaison courier in the underground resistance (Armia Krajowa = The Home Army) during WWII. After the war, her family moved to Poznań, where she completed high school (begun in wartime underground education) and in 1947 entered Poznań University as a chemistry student. She started brilliantly as an organic chemist working on the stereochemistry of cinchona alkaloids (MSc in 1951, PhD in 1960).

However, in 1953, formally as an organic chemistry assistant, she was asked by the University to create, from scratch, a teaching curriculum in crystallography for chemistry students. She accomplished this daunting task with spectacular success. Her teaching programs became the standard for crystallography teaching curricula in practically all academic institutions in Poland and abroad. She was an accomplished enthusiastic lecturer. Her lectures attracted many students despite the difficulty of the subject. She also became an expert on chemistry curricula of the Ministry of Higher Education.

Along with teaching, Dr Kosturkiewicz also developed a research program in the structural crystallography of organic compounds. Poznań was the first place in Poland where the X-ray structure of organic and bioorganic compounds was established. In 1963 she spent a sabbatical in the laboratory of the famous scholar, one of the pioneers of structural organic crystallography, Professor Aleksandr Kitaigorodskii, in Moscow. With the acquisition of one of the first single-crystal X-ray diffractometers (Syntex $P2_1$) in Poland, the research program in Poznań really took off, leading to the creation of a powerful school of organic structural chemistry, later extended to protein crystallography as well. Professor Kosturkiewicz was instrumental in creating and organizing the famous Polish Schools of Crystallography, attracting the elite of the crystallographic world and of the popular Symposia on Organic Crystal Chemistry.



Zofia Kosturkiewicz (right) with Dorota Adamiak (left) and Dorothy Hodgkin at the Third Polish Summer School on X-ray Crystallography in Jabłonna in 1972. Photo contributed to the IUCr gallery by W. L. Duax.

Professor Kosturkiewicz supervised over 150 MSc theses and 11 PhD theses. Her laboratory was a popular place for internship and instruction for numerous students and collaborators from within and outside Poland. During 1970–1974 Dr Kosturkiewicz also taught crystallography to a small group of three PhD students at the Technical University of Gdańsk, 350 km away from Poznań. She used to travel to Gdańsk, sometimes several times a month, with models, teaching aids and other accessories, to give lectures, classes and guide the research projects (and brilliant students) there.

Professor Kosturkiewicz published 110 research papers, two books and countless popular articles. She guest-edited the issue of the *IUCr Newsletter* dedicated to Crystallography in Poland (2007). For a number of years, she represented Poland in IUPAC.



Mike Glazer (Editor of the *IUCr Newsletter*) walking with Zofia Kosturkiewicz in Poland in 1983.

In her younger years, Professor Zofia Kosturkiewicz was a sworn excellent rock climber. On a par with all-male teams, she climbed the most difficult routes of the Tatra Mountains. She cherished a passion for mountains until her last day.

Till time heals the sore, her empty desk will remind all of us who were close to her of the loss. But perhaps more important than personal grieving is the lasting legacy left by Professor Kosturkiewicz: very strong organic and biological crystallography in Poznań, and a network of her students and collaborators scattered all over the world.



For a list of papers by Professor Kosturkiewicz appearing in IUCr journals click here.

OBITUARY

John D. Westbrook Jr (1957–2021)



Christine Zardecki, Stephen K. Burley

John D. Westbrook Jr (1957–2021), Research Professor at Rutgers University and Data & Software Architect Lead for the RCSB PDB, passed away on 18 October 2021.

He was incredibly beloved and respected by his colleagues at Rutgers and worldwide, known for his dry wit and endless enthusiasm for thinking about all aspects of data and data management.

John had a long and highly successful career developing ontologies, tools, and infrastructure in data acquisition, validation, standardization, and mining in the structural biology and life science domains. His work established the PDBx/mmCIF data dictionary and format as the foundation of the modern Protein Data Bank (PDB) archive (wwPDB.org).

More than twenty-five years ago, while still a graduate student, John recognized the importance of a well defined data model to ensure high-quality and reliable structural information to data users. He was the principal architect of the mmCIF data representation for biological macromolecular data. Data are presented in either key-value or tabular form based on a simple, context-free grammar (without column width constraints). All relationships between common data items (*e.g.* atom and residue identifiers) are explicitly documented within the PDBx Exchange Dictionary (https://mmcif.wwpdb.org). The use of the PDBx/mmCIF format enables software applications to evaluate and validate referential integrity within any PDB entry. A key strength of the mmCIF technology is the extensibility afforded by its rich collection of software-accessible metadata.

The current PDBx/mmCIF dictionary contains more than 6200 definitions relating to experiments involved in macromolecular structure determination and descriptions of the structures themselves. The first implementation of this schema was used for the Nucleic Acid Database, a data resource of nucleic acid-containing X-ray crystallographic structures. Today, this dictionary underpins all data management of the PDB. Since 2014, it has served as the Master Format for the PDB archive. It also forms the basis of the Chemical Component Dictionary (https://wwpdb.org/data/ccd), which maintains and distributes small molecule chemical reference data in the PDB.

In 2011, the Worldwide Protein Data Bank (wwPDB) PDBx/mmCIF Working Group was established to enable the direct use of PDBx/mmCIF format files within major macromolecular crystallography software tools to provide recommendations on format extensions required for deposition of larger macromolecule structures to the PDB. This was a key step in the evolution of the PDB archive, which enabled studies of macromolecular machines, such as the ribosome, as single PDB structures (instead of split entries with atomic coordinates distributed among different entry files). In 2019, mandatory submission of PDBx/mmCIF format files for deposition was announced (Adams *et al.*, 2019).

To ensure the success of the PDBx/mmCIF dictionary and format, John worked with a wide range of community experts to extend the framework to encompass descriptions of macromolecular X-ray crystallographic experiments, 3D cryoelectron microscopy experiments, NMR spectroscopy experiments, protein and nucleic acid structural features, diffraction image data, and protein production and crystallization protocols. These efforts have recently focused on developing compatible data representations for X-ray free electron (XFEL) methods and integrative or hybrid methods (I/HM). I/HM structures, currently stored in the prototype PDB-Dev archive (https://pdb-dev.wwpdb.org), presented new challenges for data exchange among rapidly evolving and heterogeneous experimental repositories. Proper management of I/HM structures in PDB-Dev also required extension of the PDBx/mmCIF data dictionary to include coarse-grained or multiscale models, which will be essential for studying macromolecular structures *in situ* using cryo-electron tomography and other bioimaging methods.

John contributed broadly to community data standards enabling interoperation and data integration within the biology and structural biology domains. His efforts have included (i) describing the increasing molecular complexity of macromolecular structure data, (ii) representing new experimental methodologies, including I/HM techniques, and (iii) expanding the biological context required to facilitate broader integration with a spectrum of biomedical resources. John’s work has been central to connecting crystallographic and related structural data for biological macromolecules to key resources across scientific disciplines. His efforts have been described in more than 120 peer-reviewed publications, one of which has been cited more than 21 000 times according to the Web of Science (Berman *et al*., 2000). Eight of his most influential published papers have appeared in the *International Tables for Crystallography*.

John has also done yeoman service to the crystallographic community over many years and was recognized with the inaugural Biocuration Career Award from the International Society for Biocuration in 2016.

For the International Union of Crystallography, John served on the Commission for Maintenance of CIF Standard (COMCIFS), the Working Group on Data Diffraction Deposition (DDDWG), and the Committee on Data (CommDat). He also served as a Co-editor for *Acta Crystallographica Section F*.



John Westbrook (second from left) at the COMCIFS Dictionary Management Workshop at Warwick University, UK, in August 2013. Other participants: far left: Peter Murray-Rust. Front row: Brian Toby, James Hester, Frances Bernstein,

Saulius Gražulis. Behind: John Bollinger (in green shirt), David Brown, Herbert Bernstein, Mark Könnecke, Ian Bruno. At rear: Doug Du Boulay (in black shirt), Mike Hoyland, Nick Spadaccini, Simon Coles, Brian McMahon.

John was a long-standing member of the American Crystallographic Association and served on the Data, Standards & Computing Committee. He also served on the Metadata Interest Group for the Research Data Alliance.

John is survived by his wife, Bonnie J. Wagner-Westbrook, Ed.D. and his devoted Mother-in-Law, Joan N. Wagner of Clinton Twp., NJ; many cousins including Chandler Turner (of Portsmouth, VA), Ann (Turner) Heyes (of Tasmania, Australia), and Louise (Turner) Brown (of Oakland, CA).

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This article was originally published in *Acta Cryst.* (2021). D**77**, 1475–1476.

A tribute to John has been written by Jill Trewhella for the IUCr Commission on Small-Angle Scattering: https://www.iucr.org/resources/commissions/small-angle-scattering.

OBITUARY

Uwe Grimm (1963–2021)



Uwe Grimm, in his capacity as retiring Chair of the IUCr Commission on Aperiodic Crystals, meeting with the IUCr Executive Committee during the 24th IUCr Congress in Hyderabad, India, in 2017. Photo contributed to the IUCr gallery by R. Kužel.

Michael Baake, Ronan McGrath, Rudolf A. Römer

Uwe Grimm, Professor of Mathematics at the Open University, Milton Keynes, died suddenly and unexpectedly on 28 October 2021. Uwe was a leading mathematical physicist, well known for his work on quasicrystals. These non-periodic solids (discovered in 1982 by Dan Shechtman and earning him the 2011 Nobel Prize in Chemistry) share many properties with better understood periodic crystals but also exhibit properties more often associated with non-periodic and randomly structured materials. Uwe's 2013 book *Aperiodic Order*, written and edited with his friend and long-time collaborator Michael Baake of Bielefeld University, is one of the most up-to-date and authoritative guides to this still relatively young research field. The book contains a preface by Roger Penrose, whose famous tiling continues to play a big role in the field. Uwe authored around 150 scientific articles, starting originally with studying the solutions and (conformal) symmetries of one-dimensional integrable systems while a PhD student in Bonn, Germany, under the supervision of Vladimir Rittenberg. He then spent eight years as a postdoctoral researcher in Melbourne, Amsterdam and Chemnitz before coming to Milton Keynes in late 2000.

Uwe's interest in quasi-periodic systems emerged around 1990, when he realized how interesting conformal symmetries in integrable systems with quasi-periodic couplings can be, and how non-trivial concepts from algebra and geometry show up in the spectral theory of aperiodic Schrödinger operators. He quickly became fascinated with emerging aperiodic structures not only in one-dimensional systems, but also with the beauty that is inherent in two- and three-dimensional aperiodic tilings. Visualizing the intriguing patterns that seemingly extend indefinitely without ever truly repeating was one of his 'professional hobbies' and many of his publications are a treasure trove of visual as well as mathematical beauty.

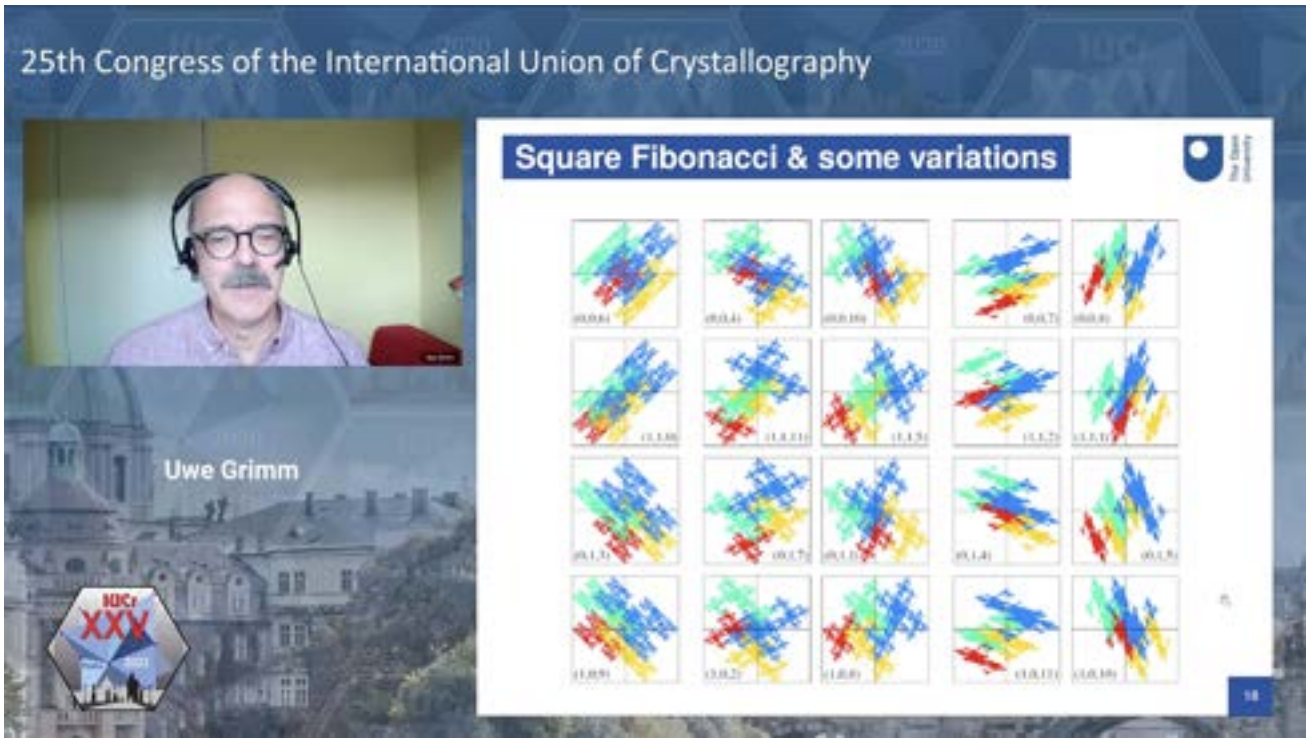
Early on in his career, Uwe became interested in communicating this beauty to a wider audience. Among other activities, he co-organized and participated in Royal Society Summer Exhibitions, in 2004 with his friend and colleague Ronan McGrath from the University of Liverpool, and in 2009 with colleagues from the Open University and others. He wrote general overview articles for the wider science community and even 'Beat the Brain' as a member of the Weapons of Math Instruction Open University Maths team in a 2015 BBC show. He used his Twitter account @RealLateStarter as a further and quite successful means of engaging as a scientist with the wider public.

At the Open University, Uwe was a valued member of staff, leading the formation of the aperiodic order research group. He successfully funded his research by obtaining several major grants as Principal Investigator from UK funding agencies. He served as Head of the School of Mathematics and Statistics, and as Associate Dean (Research) he helped the university shape its wider profile. He discharged these duties with a light touch, supreme modesty and a great sense of respect for colleagues and students.

Uwe was also a much-valued Co-editor for *Acta Crystallographica Section A* and a Consultant for and Chair (2014–2017) of the International Union of Crystallography's Commission on Aperiodic Crystals. He was elected Fellow of the Institute of Physics (IOP), was a former Honorary Secretary and Chair of the IOP's Mathematical and Theoretical Physics Group Committee, and a member of the London Mathematical Society. He also organized many influential meetings and conferences, including APERIODIC'09 in Liverpool, again jointly with McGrath. Recently he had instigated and organized regular online meetings of the UK aperiodic academic community to help maintain research connections during the COVID-19 pandemic. Uwe loved Australia since having been a postdoc there in the mid-1990s. He was an Honorary Associate of the University of Tasmania, Hobart, and he and his family spent a fondly remembered sabbatical on the island.

Uwe was trained as a physicist and mathematician. He developed our knowledge of aperiodic order but also worked on problems including the mathematical structure of groups and point sets, the theory of long-range order, the physics of electronic transport and evolution in parasites. He was also a talented pianist, juggler, and a jovial board-game enthusiast. He is survived by his wife Kathrin and two sons, Jasper and Moritz.

We, his friends, co-authors and colleagues, will miss him greatly. Our thoughts and condolences go to his family.

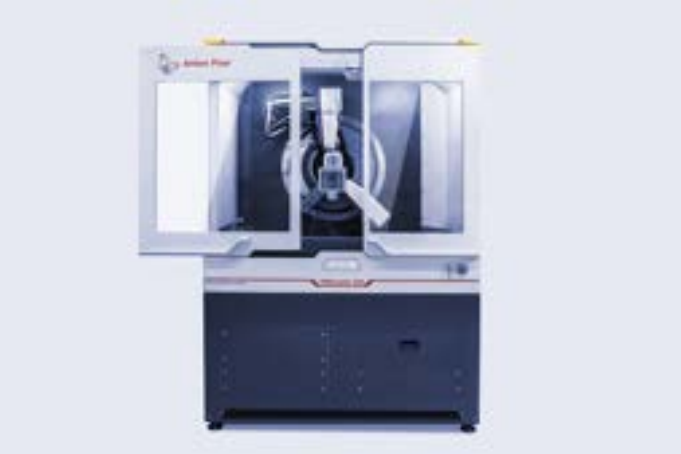


Uwe Grimm delivering his Keynote Lecture "Diffraction from aperiodic crystals: the state of the art" at the 25th IUCr Congress in August 2021.

This obituary was originally published in *Acta Cryst*. (2022). A**78**.

NEW PRODUCTS

Driving XRD: Anton Paar launches powder diffractometer XRDynamic 500



Anton Paar introduces its own powder diffractometer after supplying non-ambient XRD attachments and pioneering the SAXS sector for many years. XRDynamic 500 is a fully automated multipurpose X-ray powder diffractometer for the laboratory combining unbeatable data quality with up to a 50% increase in measurement efficiency.

The core of XRDynamic 500 is the unique TruBeam™ concept, which includes a large goniometer radius offering best-in-class measurement resolution for high-quality XRD data. Also, the beam path is evacuated – a first amongst laboratory powder diffractometers – to minimize air scattering and maximize signal-to-noise ratio. Together, these two features eliminate compromise between measurement speed and data quality. Excellent data can now be collected under standard conditions.

TruBeam™ delivers flexibility and convenience for the user *via* fully automated X-ray optics together with automated instrument and sample alignment routines. Automatic switching between up to three different beam geometries at the click of a button allows measurement of different samples with different instrument configurations without any user input.

The high degree of automation along with component recognition and simplified workflows in the XRDdrive control software make XRDynamic 500 both easy to use for beginners and flexible for advanced users, reducing the risk of potential errors. Even novices can collect high-quality XRD data without the need for extensive training.

XRDynamic 500 is a true multipurpose diffraction platform enabling collection of data on many different sample types for various analytical tasks. Whether the sample is a powder, a solid or a nanomaterial, a prime measurement solution is always possible *via* an extensive range of components and sample stages. This includes the latest pixel detector technology from CERN and Anton Paar's world-leading non-ambient XRD attachments, which function with a built-in control unit and optimal non-ambient infrastructure in the radiation-safe instrument enclosure. A dedicated SAXS configuration with fully evacuated beam path from source to detector delivers data with the quality of a stand-alone line-focus SAXS instrument with a q_{min} of 0.05 nm^{-1} for advanced nanostructure analysis.

For more information and technical specifications, see www.anton-paar.com

For further information, please contact gerhard.ehmann@anton-paar.com, tel.: +43-316-257-1350

About Anton Paar

Founded in 1922 in Graz (Austria) by Anton Paar, the company has combined precise mechanical production with the latest achievements in the fields of research and development for many decades. In recent years, Anton Paar GmbH has invested up to 20% of its annual turnover in research and development. The company offers analytical solutions that are produced within the nine producing sites (in Europe and USA).

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