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LETTER FROM THE PRESIDENT

Proud of our past, focusing on the future



Hanna (in red jumper) with Main Editors at the 2023 IUCr Journals Management Board meeting in Chester in March. Left to right, back: Sean Parkin (*Acta Cryst. E*), Kristina Kvashnina (*Journal of Synchrotron Radiation*), Mark van Raaij (*Acta Cryst. F*); middle: Sandy Blake (*Acta Cryst. B*), Randy Read (*Acta Cryst. D*), Bill Harrison (*IUCrData*), Thomas Proffen (Commissioning Editor), Loes Kroon-Batenburg (*IUCrData*); front: Janos Hajdu (*Journal of Applied Crystallography*), Elspeth Garman (*Acta Cryst. D*), Andrew Allen (IUCr Editor-in-chief), Simon Billinge (*Acta Cryst. A*). Paul Raithby (*Acta Cryst. C*) was not present for the photo. Photo by Ed Morgan, IUCr.

Hanna Dąbkowska

The 26th IUCr Congress is approaching fast. We are proud of the abstracts submitted already and I encourage you to take advantage of adding poster abstracts before the 31 May deadline. Posters are an amazing way of connecting with peers and colleagues; please make an effort during the meeting to talk to poster presenters about their work. Many of us have already booked our flights and accommodation in Melbourne. There are already about 1450 Early Bird registrants to the Congress. Please check the program at the Congress website, there are some groundbreaking presentations and very interesting workshops. The deadline for standard registration is 23 June but if you submit a poster and register by 31 May, you will receive the early bird rate!

I am looking forward to meeting Commission Chairs, this time in person, to discuss the many changes and updates that have happened since the Prague Congress. I am also looking forward to chatting with many of you as this is what I missed most in the last six years (since the Hyderabad Congress). I hope to hear your plans for this Union and for your own careers. I hope they are going in the same direction.

Once a triennium a great honor is bestowed on the IUCr President to inform the winners of IUCr Prizes about their achievement. I am very grateful to the many colleagues who took the time and effort to nominate the candidates. The competition was fierce and all four formidable Prize Committees had a challenging job in picking the final winners.

The **13th Ewald Prize** was awarded to Professor Wayne Hendrickson from Columbia University (USA), who transformed and moved forward structural biology as he discovered and perfected resonant diffraction methods for determining the atomic-level structures of biological molecules, MAD (multiwavelength anomalous diffraction) and its single-wavelength variation SAD, critical for developing the field of structural genomics. Professor Hendrickson will present his award talk in person at the Opening Ceremony of the 26th IUCr Congress in Melbourne on Tuesday 22 August.

The **2nd W. H. & W. L. Bragg Prize** was awarded to Professor Arkadiy Simonov from ETH Zürich (Switzerland) for developing the three-dimensional difference pair distribution function (3D-ΔPDF) and

applying it to solving important problems in materials science. This is the first general approach for refinement of the diffuse scattering contribution to single-crystal diffraction patterns. Professor Simonov will present his talk at the Congress on Monday 28 August.

The **Struchkov Prize** was awarded by the IUCr for the first time but it is a continuation of that established in 1997. It was granted to Dr Robert R. Fayzullin, from Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center (Russia) for his work on real-space interpretation of chemical bonding by combining one-electron potentials and associated force fields derived from high-resolution X-ray diffraction data.

Jian-Min Zuo from University of Illinois at Urbana-Champaign (USA) wins the 2023 Gjønnes Medal, awarded by the IUCr Commission on Electron Crystallography, for his outstanding contributions to the development and application of quantitative electron diffraction. His talk will be also presented at the Congress on Monday 28 August.

The **Memorandum of Understanding** (MoU) **signed in January 2023 between the IUCr, UNESCO and CNRS** is the result of hard work by many respected colleagues [Claude Lecomte, Africa Initiative; Michele Zema, IUCr Executive Outreach Officer, *LAAAMP*; Andreas Roodt (SA); Patrice Kenfack (Cameroon) (see AFRAMED article in this issue); to name just a few]. This MoU will formalize the interactions of this document's signatories to determine the terms and modalities according to which they will cooperate for implementation of the project on “Providing Remote Access to Laboratory Equipment and Infrastructures for Africa.”

Please note that the next edition of the IUCr Crystal growing competition for schoolchildren has already been announced, with a deadline of 19 November 2023. Now is a good time to encourage children to get involved in science!

In mid-March, some of us met in Chester for a Journals Management Board meeting. The Editors and Managing Editors discussed how to make our 10 journals more attractive not only to this community but also beyond. As usual I encourage you all to publish at least once a year in IUCr Journals. All the activities developed by this not-for-profit Union, all the schools, meetings, outreach activities and the awards are financed by the income from the Journals and – on a much smaller scale – by personal donations. If you have any ideas of what new subjects should be introduced into the Journals please contact the Editor-in-chief, Dr Andrew Allen; the Executive Managing Editor, Peter Strickland; or the specific Journal.



The IUCr Finance Committee and Chester staff met in March 2023 in Aarhus, Denmark. Left to right: Bo Brummerstedt Iversen, Luc Van Meervelt, Santiago García-Granda, Joseph Ferrara, Hanna Dabkowska, Peter Strickland, Malcolm Cooper, Alex Stanley and Andrew Allen.

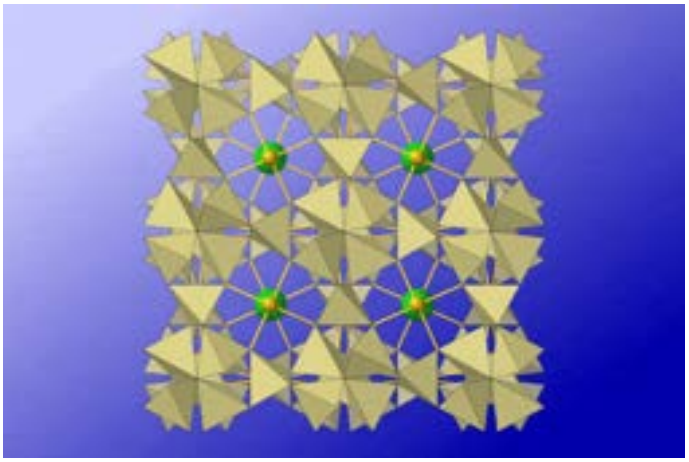
The IUCr Finance Committee met last week, discussing plans for the future in these challenging times. A slow post-COVID recovery and a recession looming in many countries call for limiting spending in different areas of our activities, which is never an easy decision.

Last but not least I would like to acknowledge the hard work our CEO is putting into this organization. Dr Alex Stanley joined the Chester staff in 2022, a pre-Congress year, which is always the most challenging time not to mention the added pressures imposed by the worldwide recession. Alex is doing an excellent job, she is full of enthusiasm and goodwill. I hope with your help she will be able to implement all her interesting ideas to modernize and push this organization into the fourth quarter of its centennial existence.

I wish you all the best this spring. Many challenges face each of us and the IUCr but together we will continue to achieve all our goals.

EDITORIAL

Editorial



Mike Glazer

Here we are, one year on from the invasion of Ukraine, and it remains to be seen what the outcome will be. For sure, whatever it is, the international situation will be changed. However, it is my hope that as far as our science of crystallography is concerned, we shall be able to return to some sort of normality. The IUCr exists to further cooperation between all countries in our science, treating all members equally and with respect, no matter our private feelings. I look forward to the time when I can again greet my colleagues and many friends in Russia. I hope it will not be too long.

This summer, our triennial IUCr Congress will take place in Melbourne. The organisers have been extremely busy and have put together an exciting programme. The IUCr Congresses usually have attendances of about 2000 or more, so organising such an event is challenging. However, I am sure that it will be a great success. If you can make it to Melbourne, please do so.

I recall my first Congress. This was in 1966 in Moscow. Yet, despite it being at the height of the cold war, I was able to befriend several Soviet colleagues, and that visit has always stuck in my memory. I recall traveling with fellow PhD student, Howard Flack, and our PhD supervisor, Kathleen Lonsdale. We were due to arrive at Moscow Sheremetyevo Airport, but for some reason, we landed at Moscow's other airport, Vnukovo. Professor G.S. Zhdanov was supposed to meet us at the airport, so we had to wait a long time to allow him to travel across Moscow to get to Vnukovo. On the car ride into the city, our interpreter taught us a lot of awful Russian swear words (Howard and I often used them in signing off messages to each other!). My impressions of the country then were mainly one of chaos: arrangements failed to be made, and hotels declared that they had never heard of us. Frustrating, I know, but we relied on the generous help of our crystallographic friends. One of them, Sergei Soloviev, spoke excellent English and translated several Russian talks at the Congress, and we struck up a good friendship, meeting up often at conferences in the years that followed. We disagreed on our politics, but nonetheless, armed with the occasional bottle of vodka, we enjoyed each other's company. I last saw him during a European meeting in Moscow many years later. At the time, he was working at the Chornobyl reactor as part of the team trying to deal with the problems that had been caused there. He had heard, somehow, that I was in Moscow, and so he made a special trip to come and see me. Unfortunately, he died not long after. Since the Moscow Congress, I have been able to attend every IUCr Congress, apart from the one in Prague. I hope to make it to Melbourne, but I must confess that age makes the idea of 23 hours in an aircraft a bit more challenging than in the past.

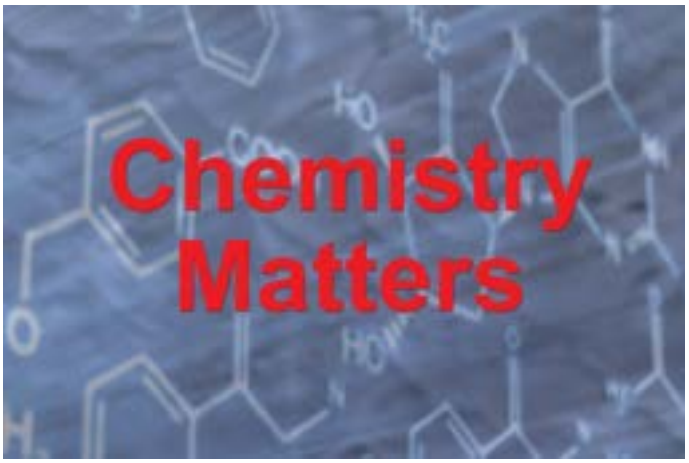
In this issue of the *Newsletter*, the Hargittais once again have sent us a fascinating account, this time on the structural helix and its role in the now famous (or is it infamous?) story of the solution of the DNA structure. Istvan and Magdolna seem to have an infinite number of great stories to tell us, and they are always worth reading.

We also have several meeting reports from several countries: France, Korea, Argentina, Japan, Costa Rica, and two from Africa. At the SCANZ meeting in Australia, I should mention that Richard Welberry, famous for his work on diffuse scattering, received the Bragg medal. This shows nicely how vibrant the science of crystallography is and how international we are.

I am sorry to say that news has arrived in the last couple of weeks of the deaths of three great members of our crystallographic community: Olga Kennard (UK), Uri Shmueli (Israel) and André Authier (France). One of the problems with getting older is the frequency with which one starts to lose friends. We have an obituary for Olga in this issue, and I hope that we shall have obituaries for Uri and André in the summer issue of the *IUCr Newsletter*.

EDITORIAL

Acta Crystallographica Section C: Chemistry Matters



Paul R. Raithby

As I come towards the end of my term as one of the Main Editors of *Acta Crystallographica Section C*, it is appropriate to take this opportunity at the beginning of a new calendar year to provide readers with a short update on the progress that the journal has been making. I would also like to thank everyone who has contributed to the journal, including all the authors, referees, the Managing Editor and the team in the Chester Editorial Office, the Co-editors and my fellow Main Editors. It also provides me with the opportunity to welcome our two new Main Editors, Amy Sarjeant from Bristol-Myers Squibb Company in the USA and Alan Kennedy from the University of Strathclyde in the UK. They have been in post since October and are already bringing new ideas for the future development of *Acta Crystallographica Section C*.

Over the last decade *Acta Crystallographica Section C* has been continuing to transition to a journal that publishes exciting new structural science with an emphasis on molecular chemistry. Authors are encouraged to present new chemistry where there is a clear chemical story based around molecular structure. In this context, 'structure' is used loosely and is not in any way restricted to structures determined by single-crystal X-ray crystallography, but includes those determined from powder X-ray or neutron data and NMR spectroscopy, and through theoretical calculations. Structures determined using Hirshfeld atom refinement and related methods are also encouraged.

The journal continues to highlight exciting aspects of structural chemistry through feature articles and special issues. The next special issue is on *noncovalent interactions based on the sigma-hole*, that my co-Main Editor, Jonathan White, is organising with Professor Lee Brammer and two members of his group, from the University of Sheffield, as guest editors. This is a highly topical area of structural research with the importance of these noncovalent interactions in a broad range of chemistry only now being fully appreciated. The publication date will be early in 2023. Further special issues will follow later in 2023 and 2024.

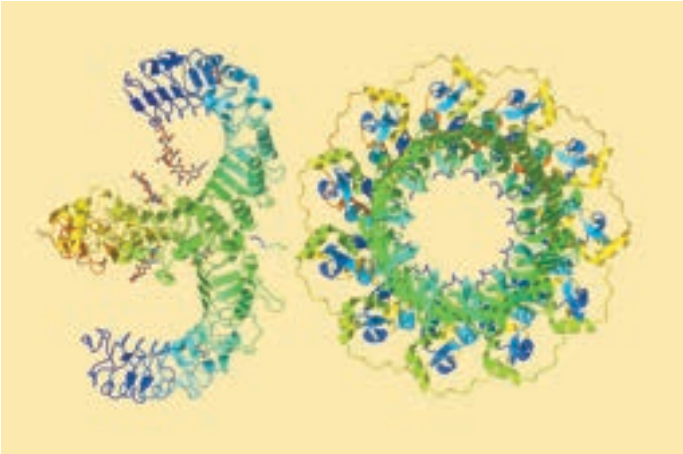
I would like to thank the contribution made by the retiring Co-editors Yoshiki Ohgo, Tong-Bu Lu, Chris Frampton and Eugene Cheung, and my particular thanks go to my co-Main Editor, Larry Falvello, who will be retiring in 2023. His contribution to the journal over many years has been enormous, and I am most grateful to him for the scientific rigour and good common sense that he applies to all matters relating to *Acta Crystallographica Section C*, and for the patience and kindness that he has always shown to me and the other editors and contributors to the journal. Finally, I would like to acknowledge all the hard work, support and friendship of the Chester Editorial Office staff during my time as a Main Editor. It is ultimately they who get the accepted manuscripts through production into the final product that we can all read and

enjoy.

This article was originally published in *Acta Cryst*. (2023). C**79**, 25.

EDITORIAL

30 years of Acta D



Elspeth F. Garman, Randy J. Read, Charles S. Bond

This year we celebrate 30 years of *Acta Crystallographica Section D*, and so have a milestone at which to reflect on its history and future trajectory. A comprehensive and detailed account of the development of the IUCr Journals can be found in the 2005 article by André Authier (Authier, 2009). Since *Acta D* was launched in 1993 (when there were fewer than 1000 entries in the PDB), approximately 16,600 different authors have submitted over 8100 articles, approximately 6650 articles have been published and the PDB has passed 200,000 entries. In the last year alone, authors from 33 different countries published in the journal, the top five being the USA, the UK, Germany, France and China.

Over 40 *Acta D* special issues have been published, most notably those arising from all the CCP4 January Study Weekends since 1998. To speed up the production of special issues we now publish the articles as they are ready and collect them together as a virtual online issue. Since 2017 *Acta D* has also published the proceedings of the CCP-EM Spring Symposium, reflecting its expanding remit in structural biology. Other special issues have included the proceedings of a number of International Conferences on the Crystallization of Biological Macromolecules, and on subjects ranging from structural proteomics to neutrons in biology to diffraction data deposition. We continue to publish special issues on all areas of structural biology. In addition, *Acta D* publishes guidelines for experimental data reporting which ensure that structural biologists continue to produce high quality, reproducible scientific results for the wider benefit of the community.

The impact factor of *Acta D* has fluctuated over the years (Fig. 1), reaching the heady heights of 14.1 in 2012, and is currently 7.65 (2022 value). The top 10 most cited papers are listed in Table 1, highlighting the importance of communicating new methods in structural biology.

Table 1. The top 10 most cited papers in *Acta D* from 1993 to present.

1

Emsley, P. & Cowtan, K. (2004). *Coot*: model-building tools for molecular graphics. *Acta Cryst.* D**60**, 2126–2132.

2

Collaborative Computational Project, Number 4, (1994). The *CCP*4 suite: programs for protein crystallography. *Acta Cryst.* D**50**, 760–763.

3

Emsley, P., Lohkamp, B., Scott, W. G. & Cowtan, K. (2010). Features and development of *Coot*. *Acta Cryst.* D**66**, 486–501.

4

Brünger, A. T., Adams, P. D., Clore, G. M., DeLano, W. L., Gros, P., Grosse-Kunstleve, R. W., Jiang, J.-S., Kuszewski, J., Nilges, M., Pannu, N. S., Read, R. J., Rice, L. M., Simonson, T. & Warren, G. L. (1998). *Crystallography & NMR System*: A New Software Suite for Macromolecular Structure Determination. *Acta Cryst.* D**54**, 905–921.

5

Adams, P. D., Afonine, P. V., Bunkóczi, G., Chen, V. B., Davis, I. W., Echols, N., Headd, J. J., Hung, L.-W., Kapral, G. J., Grosse-Kunstleve, R. W., McCoy, A. J., Moriarty, N. W., Oeffner, R., Read, R. J., Richardson, D. C., Richardson, J. S., Terwilliger, T. C. & Zwart, P. H. (2010). *PHENIX*: a comprehensive Python-based system for macromolecular structure solution. *Acta Cryst.* D**66**, 213–221.

6

Spek, A. L. (2009). Structure validation in chemical crystallography. *Acta Cryst.* D**65**, 148–155.

7

Murshudov, G. N., Vagin, A. A. & Dodson, E. J. (1997). Refinement of Macromolecular Structures by the Maximum-Likelihood Method. *Acta Cryst.* D**53**, 240–255.

8

Kabsch, W. (2010). *XDS*. *Acta Cryst.* D**66**, 125–132.

9

Chen, V. B., Arendall, W. B., Headd, J. J., Keedy, D. A., Immormino, R. M., Kapral, G. J., Murray, L. W., Richardson, J. S. & Richardson, D. C. (2010). MolProbity: all-atom structure validation for macromolecular crystallography. *Acta Cryst.* D**66**, 12–21.

10

Winn, M. D., Ballard, C. C., Cowtan, K. D., Dodson, E. J., Emsley, P., Evans, P. R., Keegan, R. M., Krissinel, E. B., Leslie, A. G. W., McCoy, A., McNicholas, S. J., Murshudov, G. N., Pannu, N. S., Potterton, E. A., Powell, H. R., Read, R. J., Vagin, A. & Wilson, K. S. (2011). Overview of the *CCP*4 suite and current developments. *Acta Cryst.* D**67**, 235–242.

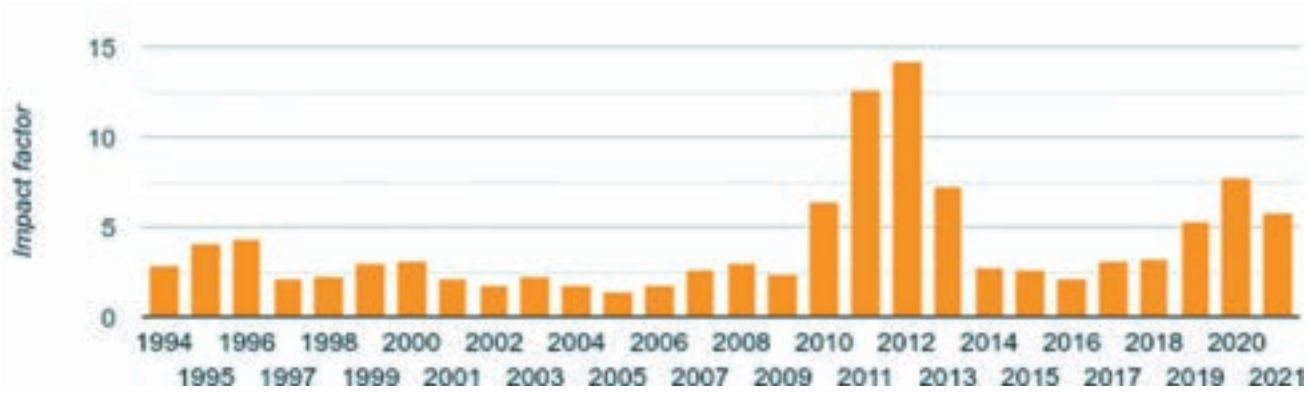


Figure 1. The impact factor history of *Acta D*.

We asked all the previous Section Editors of *Acta D* if they would like to comment on the 30th Anniversary, and were delighted to hear back from them all.

The first was Jenny Glusker, who steered the journal for ten years from 1993 to 2002 and who has kindly sent us this comment:

"It was a great honour for me to be the Editor of the new section of *Acta Crystallographica*. The number of articles of large crystal structures had been increasing and *Acta D* helped the crystallographic

community to present beautiful diagrams of macromolecules and, most important of all, three-dimensional descriptions of active sites and possibly the actual mode of action of many macromolecules. Also newly crystallized macromolecules were described. Authors were most helpful and it was generally a pleasure to interact with them. I thank them for submitting their articles and listening to my comments. We are moving forward in our understanding of the many biochemical processes in our living bodies and articles in *Acta D* will surely benefit us all."

In 2003 Ted Baker and Zbyszek Dauter took over as Section Editors, and served until 2014 and 2015, respectively. Ted remarks:

"Having no previous experience of editorship, I was delighted to take on this task, and share it with my very good friend Zbyszek Dauter. It was an exciting time, sometimes quite challenging. The number of protein structures solved began to accelerate rapidly, as did the use of automated aids for structure solution. Papers became more varied, both in terms of novel structures and in new methods; exciting for us and (I hope) of great value to the community. We also had to place quality and increasingly rigorous validation at the forefront, as less experienced structural biologists began to enter the field. Close links with the Worldwide Protein Data Bank (wwPDB) were mutually beneficial in this regard, and as was the great support and encouragement we received from Peter Strickland and Louise Jones in the Chester office. And the new looks they gave to the journal made it a special pleasure to open each new issue."

Zbyszek notes:

"Already the first issue of *Acta D* in January 1993 contained the article about direct methods phasing applied to proteins by George Sheldrick *et al.* with me as a co-author. Since then, this journal became my favourite publication venue, and now I count about 90 structural and methodological articles in *Acta D* co-authored by me. I was highly honoured and happy when I shared for 12 years the section editorship with Ted Baker, which gave me the excellent opportunity to know the newest progress in macromolecular crystallography. It has been also a pleasure to collaborate closely with such helpful and skilled professionals as Louise Jones and Peter Strickland."

Ted and Zbyszek were joined in 2013 by Soichi Wakatsuki and he served for the next four years. Soichi comments:

"During the period that I served as a Section Editor, *Acta D* expanded the scope of the journal from 'crystallography' to 'structural biology' in 2016, which I think was very forward looking and timely. I am very glad to see the evolution of *Acta D* since then, and wish it continues to be the golden standard of publishing reliable and exciting science and methodologies to serve the wider communities!"

The next new recruit was Jenny Martin, who was a Section Editor from 2014 to 2017 and who says:

"I loved my time with *Acta D*. I learned so much from my fellow editors and editorial staff, and from the authors and reviewers of the papers I was handling. I can highly recommend being an editor of *Acta D* as a way of growing networks, developing new skills and improving one's own academic writing. My time at *Acta D* was a time of change, with the journal expanding from biological crystallography to cover structural biology more broadly as outlined in our editorial on 'Expanding beyond biological crystallography' in the January 2016 issue (Martin *et al.*, 2016). Times are still a-changing with the twin revolutions of high resolution cryo-EM and high throughput AI protein structure prediction having an enormous impact on the field recently. I can't wait to read about the newest technological advance or important biological structure in *Acta D*. Here's to the next 30 years!"

Of the current Section Editors, Randy Read has served since 2014, and was joined by Elspeth Garman in 2018 and Charlie Bond in 2020.

As mentioned by Jenny Martin and Soichi above, in 2016 the remit of the journal was widened to include papers describing insights provided not only by biological crystallography but also other structural biological methods when combined with functional data. The new subtitle of *Acta Crystallographica Section D, Structural Biology* was chosen to reflect this change in scope. To quote that Editorial: "Our

over-arching aim is to ensure *Acta D* continues to be the preeminent biological crystallography journal of the IUCr. We aspire to be the journal where all structural biologists, not just biological crystallographers, send their best papers." This remains our mission today.

The future of structural biology

At the launch of *Acta D*, there were fewer than 1000 structures deposited in the PDB. Many folds were unknown and protein structure prediction was primitive, so experimental phasing methods were essential. Since that date, 99.5% of currently known macromolecular structures have been determined (thanks to structural genomics, improved methods and an expanding structural biology community) and protein structure prediction is now uncannily accurate. Many of the proteins that crystallographers would have struggled to crystallize, especially large complexes, can now be studied by cryo-EM. It is fair to say, then, that structural biology is now a relatively mature field, and that the new challenges are to be found in using it to gain an ever more sophisticated understanding of chemistry and biological processes. There are challenges in studying smaller samples, which can be achieved using more powerful synchrotron and XFEL sources. Different challenges are brought by larger samples, which can be addressed for instance using electron cryo-tomography to visualize cell sections. Dramatically improved time resolution can come from a combination of powerful sources and ultrafast detectors. At the same time, we are certain to see many advances coming from the birth of powerful machine-learning methods, such as those underpinning structure prediction algorithms such as *AlphaFold*.

It continues to be an exciting time to be a structural biologist.

References

Authier, A. (2009). *Acta Cryst.* A**65**, 167–182.

Martin, J. L., Read, R. J. & Wakatsuki, S. (2016). *Acta Cryst.* D**72**, 1–1.

This article was originally published in *Acta Cryst.* (2023). D**79**, 95–97.

EDITORIAL

Introduction to the special issue on Magnetic small-angle neutron scattering – from nanoscale magnetism to long-range magnetic structures



Electron backscatter diffraction inverse pole figure map of Eurofer97 from Ulbricht *et al.* (2022).

Sabrina Disch, Sebastian Mühlbauer, Andreas Michels, Elliot Paul Gilbert

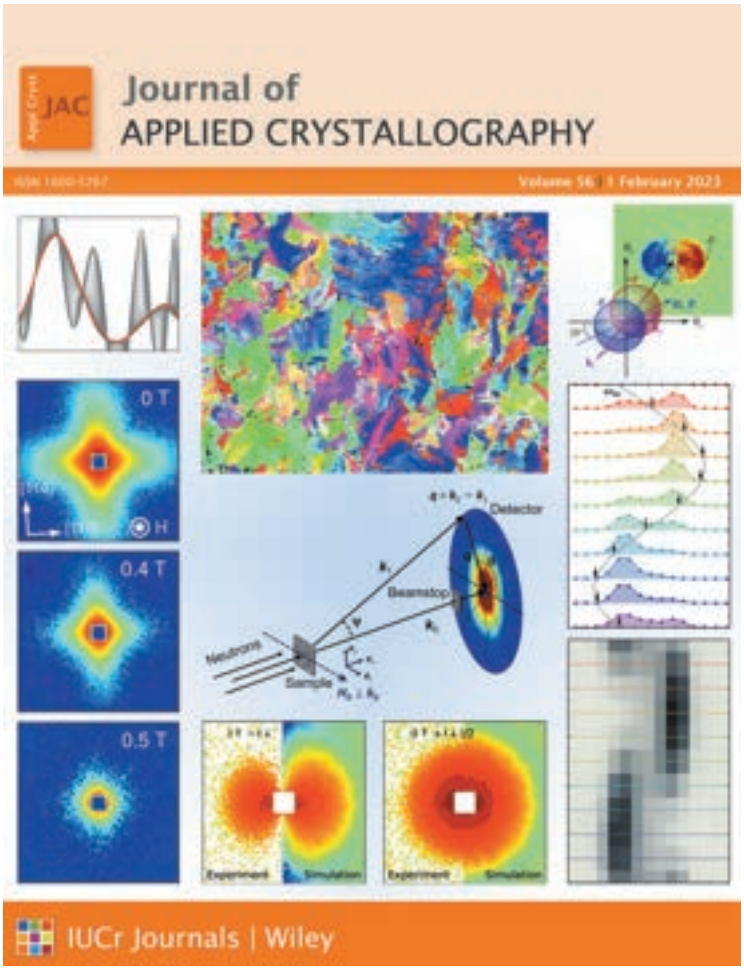
Nanoscale magnetism comprises a rich variety of physics spanning from fundamental to direct industrial application; it encompasses diverse phenomena including novel emergent magnetic structures such as skyrmion crystals, superconducting vortex lattices, exotic quantum textures in spin-ice and frustrated spin systems, and the magnetic properties of a multitude of nanotextured materials such as nanoparticles and ferrofluids, nanocomposites, permanent magnets, and magnetic steels. A common theme unifying these scientific fields is the potential for the application of small-angle neutron scattering (SANS) which, due the intrinsic magnetic moment of the neutron and its deep penetration, allows simultaneous access to the structural and magnetic bulk properties at the nanoscale.

Motivated by the success of a recent workshop (Disch *et al.*, 2021) and significant community interest in a recent review article (Mühlbauer *et al.*, 2019) and book (Michels, 2021) on magnetic SANS, the idea on this special issue was conceived, with three specific aims:

(i) To raise awareness of the range of science cases which can be addressed with the magnetic SANS technique, including for those researchers that are experienced in SANS but not currently working in magnetism.

(ii) To strengthen collaborations and create synergies between two rather disconnected research communities, namely those focused on complex long-range-ordered magnetic textures that emerge as the result of strong electronic correlations or superconductivity, and those employing the magnetic SANS method in the more classical sense to study the nonperiodic magnetization distribution caused by nanoscale structural inhomogeneity.

(iii) To address future challenges related to magnetic SANS theory, neutron instrumentation, specialized sample environment and neutron data analysis.



The 16 selected research articles in this special issue of *Journal of Applied Crystallography* represent the cutting-edge work of around 80 individual co-authors; it showcases the breadth of magnetic SANS across the full gamut of magnetic nanostructures and identifies recent and future trends, as well as instrumentation capabilities and novel simulation tools.

SANS studies of skyrmionic spin textures and skyrmion host materials are addressed by Karube *et al.* (2022), White *et al.* (2022), Causer *et al*. (2023) and Mettus *et al.* (2022). Karube *et al.* (2022) investigate the fractal magnetic domain structure in bulk crystals of the antisykrmion host $(Fe,Ni,Pd)_3P$ with a combination of SANS and magnetic force microscopy. A similar combination of scattering techniques and real-space measurements is used by White *et al*. (2022) in a study where SANS is complemented by magnetometry, magnetic diffuse neutron scattering and Lorentz transmission electron microscopy. They examine the mesoscale magnetic ordering and skyrmion phase suppression caused by compositional disorder and magnetic frustration in the chiral magnet $Co_{6.75}Zn_{6.75}Mn_{6.5}$. The consequences of reduced sample dimensions on long-wavelength magnetic modulations such as helicoids, solitons, merons and skyrmions are addressed by SANS near-surface scattering just above the critical angle of reflection by Causer *et al.* (2023) using the paradigm helimagnet MnSi. Finally, using the time-resolved stroboscopic SANS variant TISANE, Mettus *et al.* (2022) study the opportunities and the limitations of this technique to investigate the driven dynamics of skyrmion lattices on the millisecond time scale.

Two contributions are devoted to the study of superconducting vortex lattices using SANS. Louden *et al.* (2022) investigate the ordering of the vortex lattice in MgB_2 single crystals subjected to doping with Mn and C; while the vortex lattice remains qualitatively unchanged for Mn doping, C doping suppresses an otherwise field- and temperature-driven vortex lattice reordering transition, probably associated with a change of the electronic structure. Campillo *et al.* (2022) deal with the challenges of analyzing the diffraction data from mesoscopic crystals, such as the data from superconducting vortex lattices acquired in time-of-flight SANS; such studies will be highly relevant for anticipated SANS studies at the European Spallation Source.

The use of a SANS instrument for measurements of inelastic properties is the subject of the contribution by Azarova *et al.* (2023). SANS with polarized neutrons is capable of determining the spin-wave stiffness and energy gap of low-energy magnons, even for amorphous ferromagnetic samples. The role of SANS in the investigation of reentrant spin glasses close to a canonical spin glass is discussed and revisited by Mirebeau & Martin (2022), focusing on the prototypical materials $Au_{1-x}Fe_x$ and amorphous a-$Fe_{1-x}Mn_x$.

SANS studies of materials where the nanomagnetic variation is induced by nanoscale structural inhomogeneities of bulk samples are addressed in four contributions. Ulbricht *et al.* (2022) use magnetic SANS to examine the properties of low-dose irradiated Fe–Cr model alloys and the ferritic martensitic steel Eurofer97. Uniaxial polarization analysis on soft magnetic nanocrystalline alloys is used in combination with micromagnetic computations to establish the route to a general framework for polarized real-space neutron methods for magnetic microstructures by Malyeyev *et al.* (2022). Zaporozhets *et al.* (2022) follow a similar approach, extending micromagnetic SANS theory to investigate spatially inhomogeneous ferromagnets with a nonzero average uniaxial anisotropy, and apply these results to magnetic-field-annealed Vitroperm and plastically deformed nickel. Finally, magnetic nanoprecipitates and interfacial spin disorder in zero-field-annealed $Ni_{50}Mn_{45}In_5$ studied by SANS is the topic of the contribution by Bersweiler *et al.* (2022).

To complete the SANS studies on magnetic materials with structural inhomogeneities, four papers of this special issue deal with magnetic nanoparticles and ferrofluids. Zákutná *et al.* (2022) use magnetic SANS to investigate the multiscale magnetization of cobalt-doped ferrite nanocubes of similar size but varying Co/Fe ratio with a combination of polarized SANS, X-ray diffraction, Mössbauer spectroscopy and magnetization measurements. The effect of faceted nanoparticle shape on the superstructure formation in concentrated ferrofluids under applied magnetic field is studied using magnetic SANS by Bender *et al.* (2022*a*) with analysis of the two-dimensional pair distance distribution function.

Finally, two contributions showcase the impact of state-of-the-art data analysis and simulations of SANS data of magnetic nanoparticles. Bender *et al*. (2022*b*) compare the indirect Fourier transform method with a singular-value decomposition technique and an iterative algorithm to achieve model-free analysis of small-angle scattering data. The contribution by Barnsley *et al.* (2022) features a numerical algorithm based on reverse Monte Carlo simulations to model two-dimensional scattering intensities of SANS measurements, accounting for magnetic scattering, instrument resolution and particle polydispersity, making no assumptions about the underlying particle interactions.

It is hoped that this special issue of *Journal of Applied Crystallography* dedicated to magnetic SANS will serve as an enduring resource and valuable reference for the community, as well as stimulating the greater utilization of the technique in the important realm of magnetic nanostructures.

The virtual special issue is available at https://journals.iucr.org/special_issues/2023/msans.

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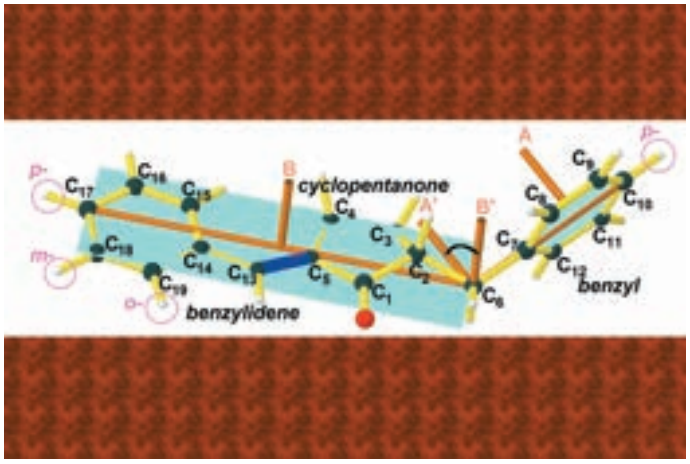
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COMMENTARY

Elucidation of molecular crystals with one-, two- or three-dimensional geometrical models



Vladislav A. Blatov

The spatial structure of molecular crystals is a real challenge for explanation and prediction. Although the general model in which such crystals are considered as a packing of molecules seems clear and unambiguous, the devil is in the details. Since organic molecules possess an unlimited diversity of sizes, shapes and active centers of specific intermolecular interactions (hydrogen bonds, halogen–halogen interactions, *etc*.), the arrangement of a particular molecule depends on many parameters. The crucial point in the rationalization of a molecular crystal structure consists in revealing these parameters and establishing their importance for the structure formation. Thus, the invention of new structural descriptors, *i.e.* concepts or magnitudes that characterize molecular crystals, is always valuable. Among them, geometrical descriptors are the simplest and most obvious and retain their importance despite the evident progress of the high-throughput computer modeling (Oganov *et al.*, 2019).

The oldest but still relevant geometrical approach to the understanding of the architecture of molecular crystals was proposed by Kitaigorodsky (1961). This approach is based on a three-dimensional model of close packing of rigid molecules, similar to the model of the closest packing of rigid atoms in inorganic crystal chemistry. Despite differences in the shape of atoms, which are considered balls, and organic molecules, Kitaigorodsky's approach exhibited its viability and revealed similarities in the structure of atomic and molecular packings. In particular, both packings prefer to have coordination number 12 and are assembled from close-packed layers with a hexagonal structure. However, this model does not account for the details of the molecular shape and specific interactions between molecules that result in a number of deviations from the general trends in the crystal organization. In particular, Kitaigorodsky (1973) mentioned that molecular coordination numbers often differ from 12 and values 10 or 14 are also widespread. To formalize Kitaigorodsky's approach, Fischer & Koch (1979) proposed representing molecules by their Voronoi polyhedra, *i.e.* the unions of the Voronoi polyhedra of atoms, which compose the molecule. Peresypkina & Blatov (2000) implemented Fischer & Koch's model into software, analyzed molecular packings in all available organic crystals and showed that coordination number 14 is the most abundant. This conclusion does not contradict the close-packing approximation if one considers the molecules as deformable and flexible objects. Thus the three-dimensional model has exhibited its efficiency in the analysis of the molecular packing as a whole; however, to reveal the details of the crystal architecture one could need other approaches.

The paper by Thomas & Hughes (2023) proposes such approaches and provides an essential contribution to the problem under discussion. The authors supplement the three-dimensional model with two other

geometrical models that treat the molecular packing at lower dimensions. The first model can be called one-dimensional since it represents a molecule as a chain of rods; each rod is directed along the longest principal axis of inertia of a selected section of the molecule. The molecules considered in the paper are represented as chains of two hinged rods, but it seems this approach can be extended to more complicated cases of chain-like molecules with many sections. Such a model is simpler than the Voronoi polyhedron representation but preserves the general shape of the molecule and enables one to clearly visualize a molecular packing. It seems however that this approach is inapplicable to discotic or polyhedral molecules, where two or even three principal axes of inertia are of equal length. The second model perceives a molecular packing as a series of two-dimensional slices. The molecules in the slices can be represented as unions of atomic van der Waals spheres, polygons built for the centers of intermolecular voids or Dirichlet domains, *i.e.* two-dimensional analogs of Voronoi polyhedra, which are constructed for the systems of molecular centroids. Such an approach enabled the authors to explore the molecular packings in more detail than the three-dimensional model permitted and to find similarities and differences in two series of organic crystals: five sulfathiazole polymorphs and 16 substituted 2-benzyl-5-benzylidene cyclopentanones. An important advantage of the two-dimensional model is that it provides a diagram showing both the densest and the rarest places of the molecular packing as well as the low-density space where the molecular ends come together ('junction zones' in the authors' terminology). In addition to the geometrical consideration, the authors estimated the intermolecular interactions using the semi-empirical potentials given by Gavezzotti & Filippini (1994).

As a result, a number of new geometrical descriptors have been proposed that provide a detailed description of molecular packings and essentially supplement the three-dimensional model. This approach seems very efficient in the analysis of series of chemically similar molecular crystals as was demonstrated by the authors. However, it is hardly applicable for an automated analysis of big crystallographic data, where the Voronoi polyhedron model is preferable (Peresypkina & Blatov, 2000).

The paper by Thomas & Hughes (2023) is quite heavy for an initial reading due to many details that the proposed approach provides for each molecular structure. I would recommend the reader to start from the paper by Thomas (2015) where some basic concepts of the approach were introduced. Then if the reader wants to have just a general idea of the approach the parts 'Method and Discussion' should be enough, while parts 3 and 4 are good for a deeper insight. On the other hand, I would encourage the authors to adjust this promising approach for a wide application by making their software *PROCUSTES* (Thomas, 2022, unpublished) available for downloading and usage. This is the spirit of the time: new theoretical approaches should be implemented into user-friendly software as soon as possible. Since the authors intend to develop this topic it would be interesting to read in their next paper(s) about the limitations and possible improvements of the approach. For this purpose, the variety of the analyzed molecular crystals should be essentially extended. That is what the authors actually promise at the end of the paper, so let us wait for their new contributions.

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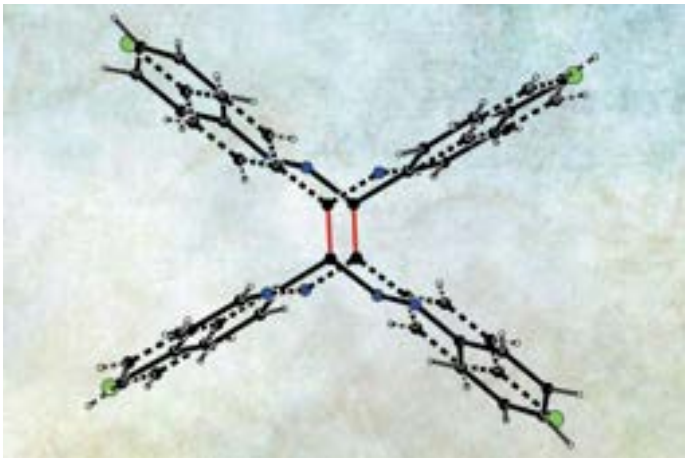
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COMMENTARY

Optimizing disordered crystal structures



Anthony Linden

Disordered crystal structures constitute about 28% of the entries in the Cambridge Structural Database (Groom *et al*., 2016). It is always exciting when a new data set comes off the diffractometer and one hopes for a rapid refinement of what is expected to be a routine structure determination, but then the discovery of disorder ruins one's day when one realises that considerable time and effort will be needed to arrive at an optimal structure model. Sometimes the disorder is only present in a solvent molecule or counterion, *e.g.* a tumbling PF_6^- anion, where it is not so critical to develop a 'perfect' model, but nonetheless, every improvement in the disorder model for such species usually improves the agreement factors and the precision of the atomic coordinates for all components in the structure, thereby leading to more precise geometric parameters, even in the non-disordered main component. For many analyses, the geometric parameters are the most tangible results of interest, so obtaining their best precision is important.

In crystal structures where the molecule or fragment of interest is disordered, the disorder might have no consequences for the understanding of the chemical species present, such as conformational variations in the puckering of a five-membered ring or in the orientation of a terminal $–CF_3$ group. In such cases, modelling the disorder is often, but not always, relatively straightforward.

At the other extreme, the challenge of dealing with extensive, subtle or even full-molecule disorder often requires much effort, because the positions of many atoms from the various disorder components are almost overlapping and it can be tricky to set up the best combination of restraints and/or constraints to allow the refinement to work smoothly while maintaining the correct chemical and geometrical logic of the species present. Full-molecule disorder can occur when the topology and polarity of the compound is such that the molecule can slot into its space in the crystal structure without caring about which way around it sits. A similar scenario can occur when more than one chemical species with similar topology is present in the crystal and they occupy the same crystallographic site; a mixture of diastereoisomers is one such example. Of course, these topological considerations are not necessarily limited to (entire) molecular species. Whether it is a molecular or an extended structure, a part of the asymmetric unit, such as a single ligand, might also fit into its cavity in more than one orientation or conformation.

A mixed-crystal full-molecule disorder situation is described in this issue of *Acta Crystallographica Section C* by Parkin *et al.* (2023). The authors revisit the product of an organic reaction published by some of the same authors (Mohamed *et al.*, 2016), which at the time was described as the *meso* isomer of (*E*,*E*)-1,10-[1,2-bis(4-chlorophenyl)ethane1,2-diyl]bis(phenyldiazene) disordered across a crystallographic centre of inversion. Some unusual geometry subsequently noticed in the original model prompted the reevaluation. The new interpretation of the data leads to the conclusion that the crystal structure is more likely to be a three-component superposition of the *meso* form with, additionally, the

S,*S* and *R*,*R* enantiomers. Such a superposition is feasible given the spatial similarities of the isomers. The matter is made more complicated by the question of whether or not the true space group is *Cc* or the centrosymmetric *C*2/*c*.

While the motivation of Parkin *et al.* (2023) is to improve on the original interpretation of the structure, the means of getting there is presented in a clear and instructive way. The article is thus a good learning example for dealing with a highly disordered structure and for what some people call 'forensic crystallography'. Not only do the authors contend with modelling the disorder, but also deduce which chemical compounds are most likely to be present and address the space-group ambiguities. Usually, this sort of problem requires many trial refinements and, in general, practitioners should not feel reluctant to try out various ideas before settling on their final model. The problem is approached from both crystallographic and chemistry points of view. That is, the models for each of the disordered components have to be geometrically logical, as it is unlikely that such organic molecules would be geometrically distorted. The models should also account for the observed electron-density distribution; the presence of Cl atoms in these molecules makes their disordered positions stand out more clearly, thereby giving a starting point for developing the models, which understandably require a significant array of restraints and constraints. As with many complex disorder problems, there is probably not a unique way to select restraints and constraints to arrive at an acceptable model. The authors themselves state: '*it is unlikely that any two crystallographers would settle on the same combination of constraints/restraints*'. Finally, the chemical origin of the enantiomers and *meso* isomer has to be understood – originally only the presence of the *meso* compound had been assumed. This highlights the importance of critical and logical thinking and a good dialogue between the crystallographer and the scientist(s) producing the substances and interpreting the other spectroscopic data, if they are not the same person. These comments are not intended as a criticism of the original work – sometimes another pair of eyes and a different viewpoint reveal things that the others have not noticed.

Coincidentally, this issue of the journal reports another disordered mixed-crystal structure where the disorder is a consequence of the superposition of two diastereoisomers, one of which is additionally conformationally disordered, at the same crystallographic site in the crystal, treatment of which requires a three-component disorder model, although full-molecule disorder is probably not present (Linden *et al.*, 2023).

Anecdotally, I was recently contacted by a young crystallographer who was struggling with the interpretation of a disordered structure that looked somewhat like the expected synthesis product, but was strange in other respects, especially some excessively long bonds. After discussing the synthesis of the material, we concluded that the crystal was a mixed-crystal composed of unreacted starting material and product, and the two species had crystallized randomly at the same crystallographic site. It was then possible to develop an appropriate disorder model for the structure, albeit still with some non-ideal geometry. I suggested that if it was at all possible still, some additional attempts at carefully optimizing the reaction and/or work-up and separation procedures might allow one to obtain the product in a more pure form. Indeed, the desired pure product was obtained subsequently and a clean crystal structure ensued, thus obviating the need to continue with or attempt to publish the mixed-crystal structure. Of course, the separation or purification of mixtures can sometimes be extremely difficult, but if tweaks to the procedures have not yet been tested, further attempts might be more fruitful than trying to continue with a messy, inferior quality, or even ambiguous, mixed-crystal structure determination.

Small-molecule crystallographers are fortunate today to have some excellent tools available to assist with the modelling of disorder. While the program *SHELXL* (Sheldrick, 2015) has long had an extensive array of restraint and constraint instructions (SADI, SAME, DFIX, DANG, SIMU, DELU and RIGU, to name just a few), manually developing the initial disorder model was sometimes cumbersome. Nowadays, the *Olex*^{2} software (Dolomanov *et al.*, 2009), as one example, has excellent and clever tools in the Graphical User Interface (GUI), which allow one, after a little practice, to split, drag and rotate fragments conveniently in order to obtain a good starting approximation to the disorder and then apply the appropriate restraints and/or constraints. The GUI of *ShelXle* (Hübschle *et al.*, 2011) can be used in a

similar way. *Olex*^{2} also has a fragment database, which can be used to help model common fragments or solvent molecules. Excellent YouTube tutorials demonstrating many of the features of both of these programs, not just disorder handling, are available online.

Further discourses on many aspects of obtaining the best results from a crystal structure determination, including the handling disordered structures, can be found in Vinaya *et al.* (2023), Clegg (2019) and Linden (2020).

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COMMENTARY

Towards the standardized presentation and publication of small-angle scattering data from biomolecules in solution

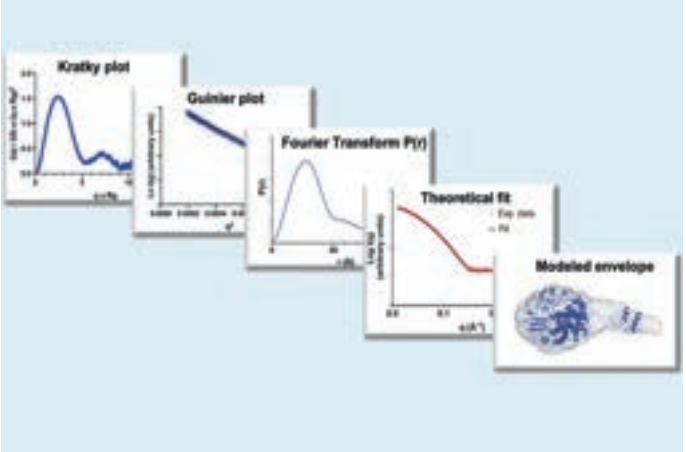


Figure 1. Schematic flow of data representations for SAXS experiments.

Mirjam Czjzek

Today Findable Accessible Interoperable Reusable, or FAIR, data principles are on everyone's lips (Wilkinson *et al.*, 2016). But how do you ensure that these principles are easy to fulfil, widespread and adapted to *your* data? It is all about standardizing experiments, data treatment, data reporting and deposition. In this context, the macromolecular crystallography community, through engagement via the International Union of Crystallography (IUCr), has been exemplary and an early pioneer, as shown by the recent celebration of the 50th anniversary of the wwPDB (Worldwide Protein Data Bank) (Burley *et al.*, 2022). Through the decades, and in correlation with the technical and methodological advances in structural methods dedicated to macromolecules such as NMR or cryo-EM, the PDB coordinate repertoire has expanded to include as many as possible experimentally determined three-dimensional (3D) structural data from biological macromolecules (https://www.rcsb.org/pages/about-us/history).

In contrast to the above-mentioned structural methods that (potentially) give access to close-to-atomic resolution, small-angle scattering (SAS) profiles, whether obtained by neutron (SANS) or X-ray (SAXS) scattering of macromolecules in solution, only give access to low resolution, and do not allow the determination of atomic coordinates that could be compatible with data deposition at the PDB. Albeit with this limitation, small-angle scattering is complementary to other methods, and is particularly powerful in combination with these other methods, leading to the emerging field of integrative/hybrid structure determination (Sali, 2021). Thanks to considerable advances in instrumentation and computational methods, the amount of SAS data has also increased dramatically over the past two decades (Fig. 1), and the need for standardized data treatment and deposition has become equally urgent and important for SAXS and SANS data. Since the wwPDB initiative that created the SAS validation task force, publication guidelines have been extended to those of SAS data (Trewhella *et al.*, 2013; Jacques *et al.*, 2012*a*,*b*), finally resulting in the Small Angle Scattering Biological Data Bank, SASBDB, (Valentini *et al.*, 2015) that today is connected to the wwPDB through PDB-dev (Vallat *et al.*, 2021).

The article by Trewhella *et al.* (2023) in this issue depicts the history of the actions commissioned by the IUCr and the SAS community, leading to best practice and publication guidelines, including template tables being published by Trewhella *et al.* in 2017. With the aim of providing an updated template, following the IUCr announcement of requirement of data deposition (including SAXS and SANS data) prior

to editorial review (Baker *et al.,* 2022), and of keeping pace with the recent methodological and technological advances, Trewhella *et al.* (2023) now provide a 2023 update of template tables for reporting biomolecular structural modelling of small-angle scattering data.

Integrating the experience gained by five years of using the template tables developed in 2017, combined with practical experience, the updated tables improve the presentation, while trying not to impose unnecessary work on researchers. While the original templates were mainly based on data from four SAXS examples, the new template tables also better integrate data coming from more complex samples (*i.e.* glycosylated proteins, DNA and RNA) and experiments, such as those from SAS contrast variation experiments (SAS-cv).

The article transparently describes the process by which the new consensus template tables were elaborated, highlighting the major changes and proposing the standardization of nomenclature to describe the components. The article then describes the reasons for reorganization of some of the sample details, or changes in reporting specific data-collection parameters, such as wavelength or beam geometry.

Finally, the newly developed table is tested for its utility using a published complex DNA–protein SAXS study (Pozner *et al.*, 2018), for which all reported items populate the template and are subsequently commented on in the context of how to analyse and interpret the given values.

A second objective of Trewhella and coworkers was the creation of a SAS-cv template table, to include the required additional parameters for this type of experiment. Again, Trewhella *et al.* (2023) describe which items have been added and why, with the aim of allowing a broadened applicability, without increasing the workload. To test the relative ease of use and utility of the template, it was populated with data and modelling from a combined SAXS/SANS-cv experiment, deposited in the SASBDB, of a protein complex consisting of a histidine kinase with bound protein inhibitors that were partially deuterated (Whitten *et al.*, 2007). The reader is then guided through the resulting table on how to read and interpret the given data, how the figures can complete the information obtained, and what assessments can be made by a reader/reviewer given the quality of the data presentation. The examples discussed nicely demonstrate the utility of such a standardized presentation, and the template tables will not only facilitate a critical assessment to readers and reviewers, but also largely support the experimenter to prepare, perform and present their SAS data in a concise but complete manner.

As a conclusion, the authors point out that it is evident a single template table cannot account for all the different kinds of SAS experiments involving biomolecules that can be set up or thought of. However, discussions are already ongoing in the SAS community to follow the examples presented here and develop templates for SAS experiments involving nanoparticle/micelle/bicelle-type structures (Trewhella *et al.*, 2023).

Taken together, these efforts are of great importance to enhance the confidence with which the scientific community can rely on biomolecular SAS data and build upon them for further investigations. And I sincerely believe that the structural biology community will strongly welcome the template tables and use them extensively for future publications.

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COMMENTARY

Towards automating single-particle cryo-EM data acquisition

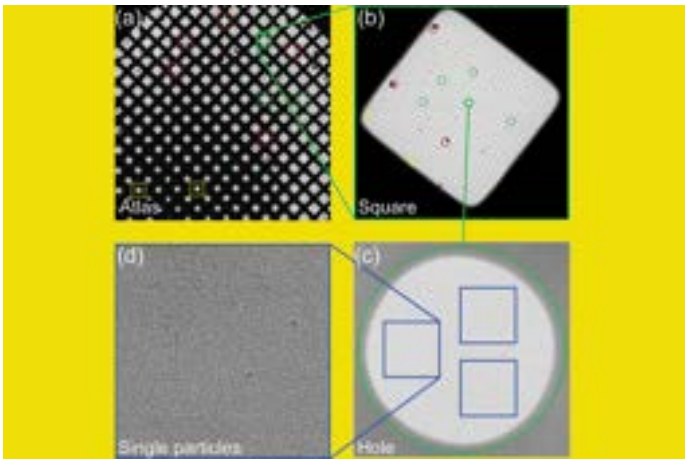


Figure 1. Required target selection steps during single-particle cryo-EM data acquisition. (*a*) Low magnification overview (Atlas) of a cryo-EM grid. Human operator choices for squares that are suitable for imaging are marked with green boxes. Yellow and red boxes represent operator choices of squares with thick ice layers or broken support film, respectively. (*b*) Square with examples of operator choices of holes that are suitable for cryo-EM imaging marked with green circles. Yellow and red circles mark operator choices of holes that have suboptimal ice thickness or are covered by ice contamination, respectively. (*c*) High-magnification image of a hole with a thin ice layer. Areas for cryo-EM data acquisition are marked with blue boxes. (*d*) Cryo-EM image acquired under optimal conditions and in thin ice showing single particles of good density.

Christian Dienemann

Cryogenic electron microscopy (cryo-EM) of single particles is a powerful technique for the structural determination of biological macromolecules and significant advances in the field have been made over the last two decades (Kühlbrandt, 2014; Nogales, 2016). Improved electron detector technology (McMullan *et al*., 2016) and data analysis algorithms (Scheres, 2012; Punjani *et al.*, 2017; Grant *et al*., 2018; Tegunov & Cramer, 2019), as well as specialized microscope software that streamlines data acquisition (Carragher *et al*., 2000; Mastronarde, 2005) have increased the accessibility of cryo-EM as a method for structure determination. Therefore, the number of protein and protein complex structures determined by single-particle cryo-EM is constantly increasing (see https://www.rcsb.org/stats/growth/growth-em).

For cryo-EM, a protein solution is frozen as a thin layer of vitrified ice that is embedded within a holey support film on an EM grid (Weissenberger *et al.*, 2021). Freezing of cryo-EM grids usually needs to be extensively optimized for ice layer thickness, as well as protein particle concentration and integrity, by repeating cycles of cryo-EM screening and altering sample preparation (Passmore & Russo, 2016; Noble *et al.*, 2018). Once the sample is optimized, a large number of randomly oriented particle images are acquired, classified, aligned and eventually reconstructed to a volume representing the coulomb potential density of the protein particle (Sigworth, 2016).

During cryo-EM grid screening and data acquisition, the microscope operator needs to manually pick suitable regions (squares) based on a grid overview (atlas) and select target holes with suitable ice thickness based on their appearance (Fig. 1). In many cases, ice thickness has to be chosen carefully to avoid broken or preferentially oriented particles (Noble *et al.*, 2018; D'Imprima *et al.*, 2019). Especially for the acquisition of large datasets, manual square and hole selection can be very time-consuming and

less experienced operators may have difficulty targeting grid regions that yield high-quality data (Li *et al.*, 2022). Nowadays, data analysis is done 'on-the-fly' during acquisition (Thompson *et al.*, 2019), which gives valuable real-time information about data quality, and the microscope operator can adjust target selection based on the outcome. However, such trial-and-error strategies lead to the inefficient use of instruments that are in high demand and are expensive to maintain. Automation of the targeting of squares and holes during cryo-EM screening and data acquisition, therefore, has great potential to increase the throughput as well as the success rate of cryo-EM experiments for researchers of all experience levels.

In this issue of **IUCrJ**, Kim *et al.* (2023) present the software toolbox *Ptolemy*, which uses machine learning to automate the task of selecting target regions in single-particle cryo-EM screening and data collection. The algorithms within *Ptolemy* were pre-trained using metadata from annotated human operator microscope sessions. *Ptolemy* first addresses the automatic selection and ranking of suitable squares for data acquisition. To do so, *Ptolemy* uses a convolutional neural network [CNN, reviewed in Dhillon & Verma (2020)] classifier to predict the 'collectability' of squares on an atlas and can reproduce human expert operator selections on samples unknown to the neural network. *Ptolemy* then automatically finds holes on these squares using a neural network with U-Net (Ronneberger *et al.*, 2015) architecture and 2D lattice restraints for the hole positions. The U-Net not only reproduces human operator selections with high precision, but the probabilities the U-Net assigns for a hole also appear to be suitable measures for the collectability of a hole. Altogether, *Ptolemy* provides an all-in-one solution for reliable and accurate automatic targeting of squares and holes on single-particle cryo-EM grids. This is a big step towards the full automation of cryo-EM screening and data collection and is readily implemented in the microscope operation software *Leginon* [for details of the implementation, see Cheng *et al.* (2023), also published in this issue of **IUCrJ**].

While *Ptolemy* uses specifically tailored and tuned CNN and U-Net machine-learning approaches to achieve high accuracy for recognizing and ranking squares and holes, other software have approached the problem of automatic data acquisition in slightly different ways. A conceptually similar approach was taken by *SmartScope* (Bouvette *et al.*, 2022), which utilized dedicated square and hole finders to select targets for the operator. In comparison to *Ptolemy*, the *SmartScope* square and hole recognition procedures are based on an R-CNN with ResNet50 architecture and a YOLOv5 model with CSPNet backbone for square and hole recognition, respectively. It remains to be seen which deep-learning implementation yields better performance in real-life cryoEM imaging sessions. Notably, *SmartScope* implemented *Ptolemy* as an alternative to their own square and hole recognition algorithms (Bouvette & Viverette, 2022), so direct comparison will be possible.

A conceptually different approach is taken by *cryoRL* (Li *et al.*, 2022). Instead of attempting to generate a complete selection of suitable squares and holes prior to cryo-EM imaging, *cryoRL* treats the selection of imaging targets as a path-planning problem where the algorithm is rewarded when imaging good targets. Currently, a target is considered good when it yields a cryo-EM image with high information content, which inversely correlates with ice layer thickness. However, the thinnest ice layer possible might not be a suitable target for acquiring data of sensitive or very large protein complexes (D'Imprima *et al.*, 2019; Noble *et al.*, 2018). Instead, other results from 'on-the-fly' data analysis, like complex integrity, particle number per image or the orientation distribution of particle views in the 3D reconstructions, could represent suitable quality targets.

It seems likely that combining the approaches taken by *Ptolemy*, *SmartScope* and *cryoRL* will lead to very powerful automatic cryo-EM data acquisition tools. Such tools would first generate highly accurate initial collectability rankings of squares and holes, whereas the process of data collection would be guided by sample-specific 'on-the-fly' decision-making that is based on data analysis results.

Acknowledgements

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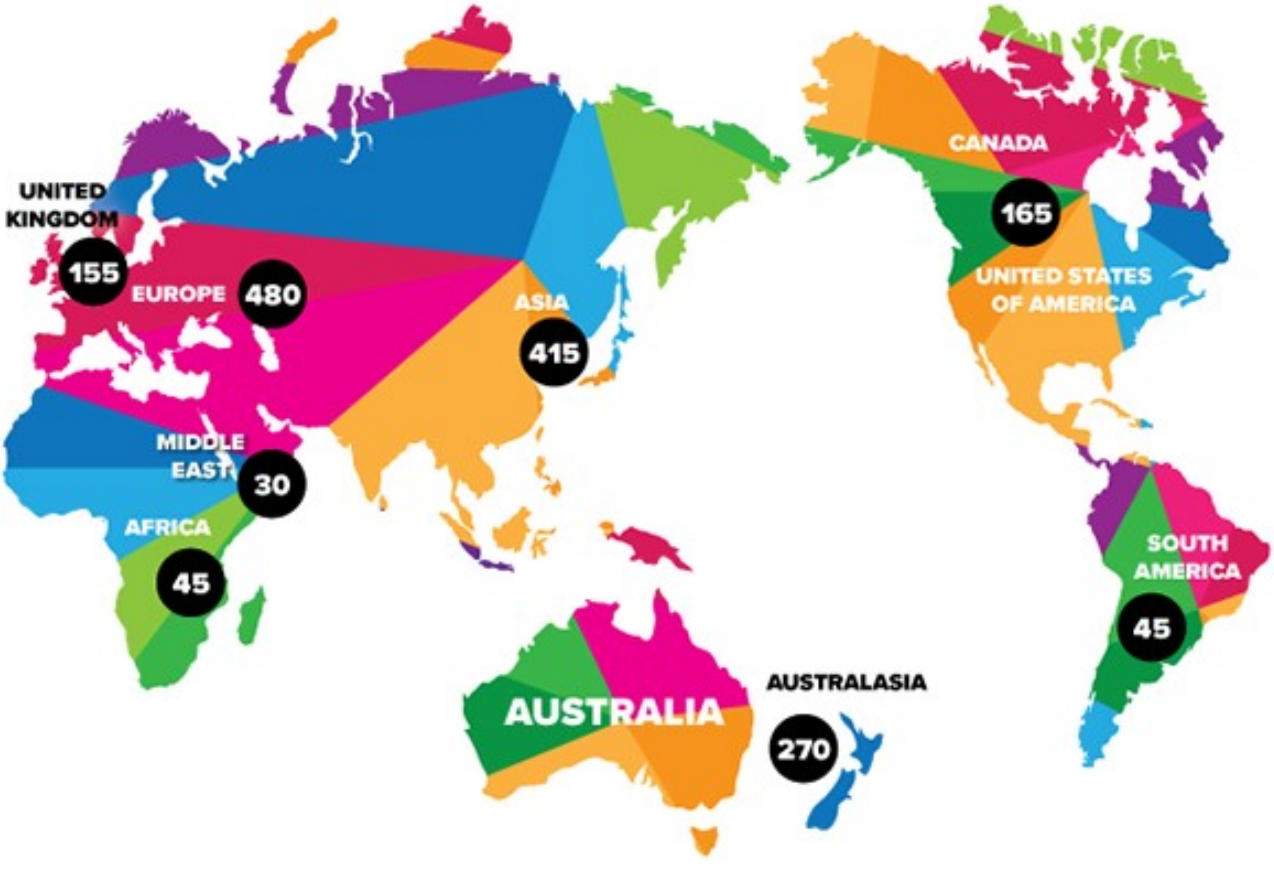
This article was originally published in *IUCrJ* (2023). **10**, 4-5.

IUCR CONGRESS

IUCr 2023: latest news



The IUCr 2023 organisers would like to acknowledge and thank the more than 1600 authors who responded to the Call for Abstracts (see the geographical distribution below), and all those who have taken advantage of early-bird registration.



Due to the size and capacity of the venue, we are happy to report that we have extended the space and are now in a position to accept additional submissions for Poster presentations. Therefore, the Organising Committee now invites prospective authors to submit poster abstracts for the Congress by 31 May.

We are also excited to release some details regarding the IUCr 2023 Social program. For the duration of the Conference, daily morning, lunch and afternoon tea breaks are included in your registration fee. The traditional Welcome Function on Tuesday 22 August will be hosted at the Melbourne Convention and Exhibition Centre amongst our valued sponsors and exhibitors. We plan to provide some Australian treats

and fine beverages on this occasion.

Rounding off the social program and celebrating the near end of the Conference on Monday 28 August, we will host the Gala dinner event “A Night at the Museum” at the famous Melbourne Museum. This is an event not to be missed. We promise this will be something special and includes access to the Dynamic Earth Exhibit, which is befitting for a dynamic crystallography group. All social functions, plus catering and transfers, are included in your registration. Please note that standard registration ends on 23 June but if you submit a poster and register by 31 May, you will receive the early bird rate!

For a chance to win a complimentary full registration, why not enter the Photo 51 - IUCr 2023 Photographic Competition? For the Coffee Category, we invite you to take a picture of *yourself* that best represents coffee OR art & culture in your hometown. We encourage you to think a little differently, have fun and be creative. Entries, which will be judged by the Melbourne Convention Bureau, will close on 15 June. Good luck!

Key dates

Call to action

Date

Poster abstracts close

31 May 2023

Standard registration deadline

23 June 2023

Accommodation booking deadline

22 July 2023

IUCr 2023 pre-Congress workshops

21 & 22 August 2023

IUCr 2023 Congress

23–29 August 2023

OUTREACH

IUCr crystal growing competition for schoolchildren



After an enforced break of three years, we are delighted to announce that the IUCr Crystal growing competition for schoolchildren is back!

The competition is open to all schoolchildren (maximum age 18) and aims to introduce students to the exciting, challenging and sometimes frustrating world of growing crystals. This initiative was originally launched in 2014 as part of the celebrations for the International Year of Crystallography.

The winners of the **2023 edition of the IUCr Crystal growing competition** will be those who most successfully convey their experiences to the panel of judges in a video report. Each contribution should clearly show or mention the experimental work carried out by the participants during the growing of their single crystals (compounds and methods used are free of choice). Furthermore the contribution should reflect in a *creative* way on the experimental work and theoretical background and/or applications.

Videos submitted to local competitions during 2022 may be also submitted to the IUCr competition.

The winning contributions in each category will receive 'Young crystal growers' certificates and medals.

Important dates

Closing date for submissions: **19 November 2023**

Notification of winners and launch of 2024 edition: **29 January 2024**

For more information, please visit the competition web page.

MEETING REPORT (IUCR SUPPORTED)

Robert Stewart School 2: Spin and charge densities modelling



Nicolas Claiser, Mohamed Souhassou

The second Robert F. Stewart Electron Density School, named in honour of one of the fathers of high-resolution crystallography, took place from 20 to 22 August 2022 at the Faculty of Science and Technology of Vandoeuvre-les-Nancy, France. The school was organized by the CRM2 laboratory, with whom Robert Stewart had collaborated.

The school's aim was to enable doctoral students from Europe and abroad to acquire new skills in the field of experimental modelling of electron and spin densities. Thus, a series of practical courses were devoted to current software, including that developed at CRM2 (*MoPro*, *MOLLYNX*).

The 30 participants comprised 15 supervisors, teachers and researchers and 15 young scientists from all over Europe but also from Africa, who were able to take advantage of this event for scientific exchange with each other and with recognized scientists.

IUCr funds supported the attendance of five young scientists from Egypt, Germany and Poland.

MEETING REPORT (IUCR SUPPORTED)

17th Conference of the Asian Crystallographic Association



Rachel M. Williamson

The 17th Conference of the Asian Crystallographic Association (AsCA2022) was held between 30 October and 2 November 2022 on the island of Jeju, South Korea, and was followed by satellite meetings on 3 and 4 November. The conference venue, the Ramada Plaza, proved to be an excellent choice by the organisers, with outstanding oral and poster presentation facilities, and an exhibition space with a wonderful sea view proving to be a very popular networking space at coffee breaks.

During the Opening Ceremony on Sunday 30 October, delegates were promised an exciting program, with three plenaries, nine keynotes and 18 microsymposium talks distributed between the three general streams of Structural Biology, Chemical Crystallography and Materials Science, and Specialized Techniques. It was clear that the organising committees had worked extremely hard during challenging times to bring together a strong lineup of 107 speakers, with an emphasis on great diversity and gender equity. The scientific program included plenary lectures by Hanna Yuan (Taiwan), Hiroshi Kitagawa (Japan) and Hyotcherl Ihee (Korea), as well as keynote lectures by Michael J. Eck (USA), Hoi Ri Moon (Korea), Pimchai Chaiyen (Thailand), Feng Shao (China), Partha S. Mukherjee (India), Makina Yabashi (Japan), Begoña Heras (Australia), Hyunjung Kim (Korea) and Yanming Ma (China).

The conference launched with a plenary by Professor Hanna Yuan (Academia Sinica, Taiwan) on “Structural Insights into the Decay of Mitochondrial RNA and DNA in Health and Disease”. Professor Yuan detailed the role of mitochondrial enzymes in removing damaged or degraded mtRNA and mtDNA, in particular the role of endonuclease G in maintaining mitochondrial genome integrity. Endonuclease G activity is associated with various diseases, including neurodegeneration and cancer. Unpublished results were shared, showing several crystal structures of human endonuclease G in complex with small polyphenol compounds. As an aside, Professor Yuan described some crystals as taking half a year to grow. This is an effort well worth the wait, as these enzyme–polyphenol complexes provide a molecular basis for targeting a key mitochondrial enzyme and treating diseases that arise from its diminished or increased activity.

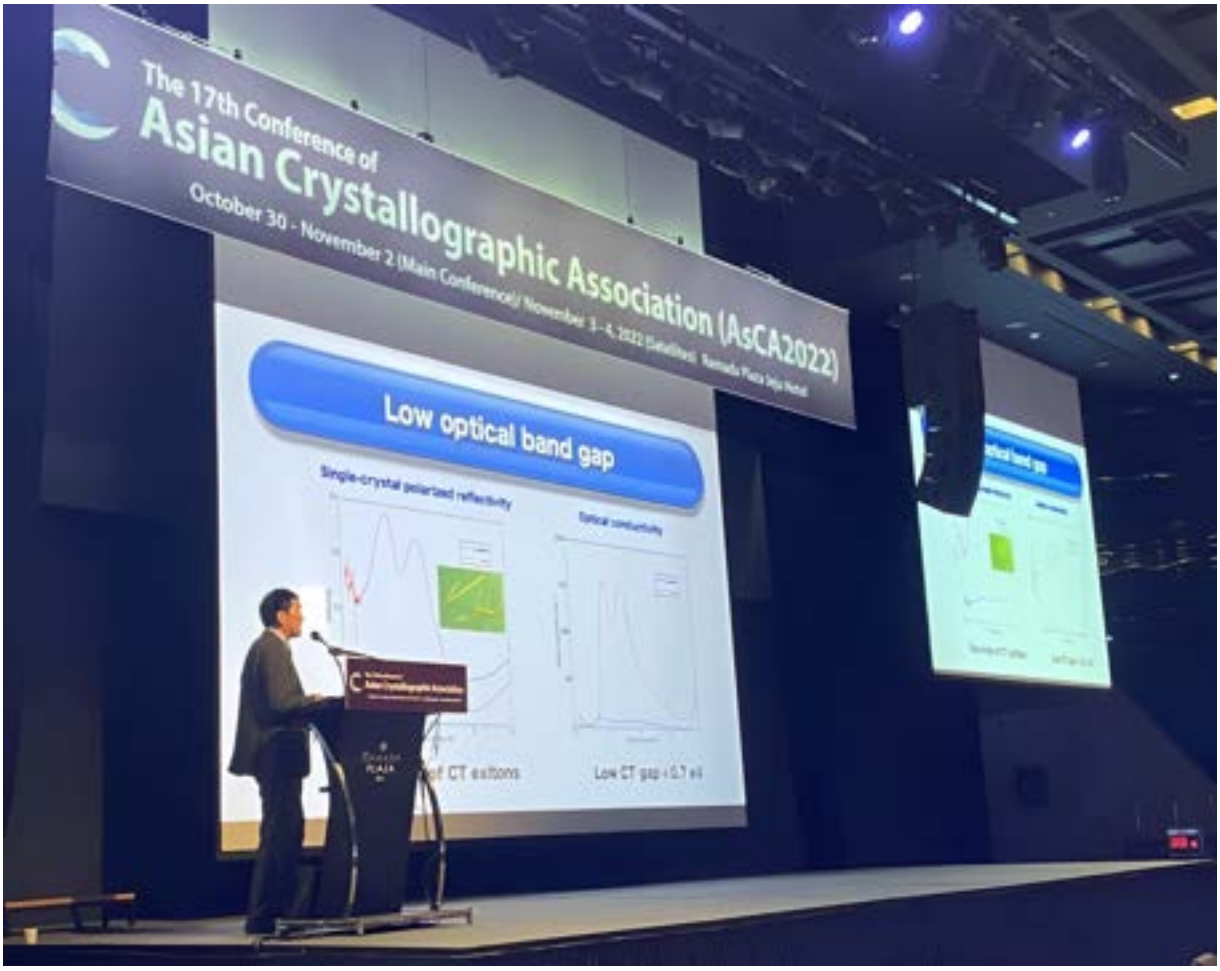
Another highlight in the Structural Biology stream was Professor Begoña Heras’s (La Trobe University, Australia) keynote lecture on “Structural Insights into the Function and Inhibition of Bacterial Virulence Proteins”, in which she detailed her group’s work in studying autotransporters, the largest group of surface adhesins in Gram-negative bacteria and drivers for biofilm formation. Professor Heras presented recent results and structural work that has led to a recently patented biofilm inhibitor.



Some of the Australian contingent at AsCA 2022, including the author. Left to right: Janesha Maddumage (PhD student, La Trobe University), Dr Rachel WILLIAMSON (Australian Synchrotron), Professor Begoña Heras (La Trobe University), Dr Mihwa Lee (La Trobe University) and Dr Chathura Suraweera (Monash University). Photo supplied by Professor Heras.

The Chemical Crystallography and Materials Science stream had a plethora of interesting talks. Emily Meekal, a doctoral candidate working in the Goodwin Group at the University of Oxford, UK, gave a fascinating talk on her work on TRUMOF-1, an example of a crystalline metal–organic framework (MOF) in which there is scope for chemical control of the occupational and orientation disorder present as a way of tuning physical and chemical properties. Ms Meekal showed that the disordered network of TRUMOF-1 could be elegantly mapped using the concept of Truchet tiles. TRUMOF-1 is the first example of a functional material exhibiting this topology, although others will surely follow.

Professor Hoi Ri Moon's (UNIST, Korea) keynote address on "Rational design of MOF@MOF" showed the power of using a joint computational/experimental workflow to screen thousands of MOFs and identify optimal MOF pairs capable of seamlessly connecting *via* the co-ordination of the metal nodes of one MOF with the linkers of the second MOF. The successful synthesis of cubic/cubic and cubic/hexagonal MOF@MOFs was described, as well as composites of dimensionally (2D and 3D) and functionally (conductive and porous) different MOFs in the form of well-integrated core–shell structures. Professor Moon's lecture concluded with a special treat for attendees: a musical MOF mash-up, *i.e.* a movie of a multitude of hetero-interpenetrated MOF@MOFs with musical accompaniment.



Professor Hiroshi Kitagawa from Kyoto University delivering one of the plenary lectures. Photo supplied by Professor Hoi Ri Moon.

The care and thought that the organisers of AsCA2022 put into the program could be seen in details such as arranging a free afternoon on Tuesday 1 November to allow conference delegates an opportunity to network and explore their surroundings, before returning refreshed to attend the evening's Plenary by Professor Hiroshi Kitagawa (Kyoto University, Japan) on "Low-Dimensional Electrons Systems in Coordination Networks". This was followed by a superb conference dinner, notable for delicious food and extremely prompt service.



AsCA 2022 conference dinner. Photo supplied by Professor Hoi Ri Moon.

The strong level of support given to young scientists at AsCA2022 was obvious at the Closing Ceremony when eight Rising Star and seven Travel awards were presented to very well-deserving recipients. Prizes for the various Exhibitor competitions were then awarded to much excitement in what proved to be an extremely lively way to close out AsCA2022 in Jeju.

Feedback from attendees emphasised that AsCA2022 was a highly successful meeting and a welcome return for many to in-person conferences.



AsCA2022 Council meeting.

Dr Rachel Williamson is Principal Scientist MX at the Australian Synchrotron, ANSTO-Melbourne, Australia.

CRYSTALLOGRAPHY IN AFRICA

Appui à la formation et la recherche à travers les mesures à distance (AFRAMED): a recent and ambitious project for the development of crystallography in Africa



Seham K. Abdel-Aal, Patrice Kenfack Tsobnang, Adam Bouraima, Ayi Djifa Hounsi, Emmanuel Wenger, El-Eulmi Bendeif, Claude Lecomte

Motivation for the AFRAMED project

Crystallography is a powerful science in helping to understand the world around us. It can determine the atomic-level structure of materials, and researchers use this knowledge to explain why things behave the way they do. This can be used to improve the properties of materials and contribute to developing new ones and drugs with improved properties. On the African continent, this science is in the early stages of development thanks to the IUCr Africa Initiative, the African Crystallographic Association (AfCA), UNESCO, ISC, CNRS and the national crystallography associations in South Africa, Algeria, Morocco, Tunisia, Cameroon, Congo Brazzaville and Senegal. One of the tools used to tackle the lack of equipment, which is the main factor responsible for the delay in the development of crystallography in particular and science in general on the continent, was the existence of OpenLabs. Different types of OpenLabs exist: OpenLab type I, OpenLab type II, the Travelling Lab and the OpenFactory.

The OpenFactory took place in Grenoble (France) and Darmstadt (Germany); type I and II OpenLabs were held in Senegal, Cameroon, Tunisia, Algeria, Morocco, Benin, Ghana, Côte d'Ivoire, Gabon, Congo Brazzaville, Mauritania and Kenya. The details of these four types of OpenLabs are given on the IUCr website.

With the COVID-19 pandemic, it was no longer possible to organize these OpenLabs and continue to train our African colleagues on the African continent. The idea to use diffractometers remotely was proposed, and the CNRS IRN (International Research Network) "AFRAMED" project was launched by the chair of the IUCr Africa Initiative, Professor Claude Lecomte, and his team in Nancy (France).

The launch ceremony of AFRAMED



Inauguration of AFRAMED at the Faculté des Sciences et Technologie, Université de Lorraine (Nancy, France).

AFRAMED (**A**ppui à la **F**ormation et la **R**echerche en **A**frique par des **Me**sures à **D**istance) is a project financed for five years (2022–2026) by the Centre National de la Recherche Scientifique (CNRS). It aims to help African researchers and university teachers whose field of research depends on crystallography – chemists, physicists, geologists and biologists – to carry out diffraction experiments from their home laboratories using a French diffractometer remotely for research or teaching activities. During the five years of the project, at least three representatives from different African countries, who hold permanent positions in their universities, will be trained in the laboratories of the French partners of the project for at least one month. Then these representatives will connect to the diffractometer remotely for about 100 hours per year from their respective countries. This time is used for X-ray diffraction measurements of new crystals and for the training of students and other interested permanent lecturers. At the end of the project, at least 15 national representatives in Africa will be trained and at least 15 African countries will be involved in the project. The project was launched on 31 August 2022 in the Conference room of the Faculté des sciences of Université de Lorraine with three CNRS French laboratories (CRM2 Nancy, LCC Toulouse and Institut Européen de Chimie et Biologie Bordeaux) and six African countries (Cameroon, Gabon, Egypt, Togo, Cote d'Ivoire and Senegal) in the presence of many personalities: Professor Alain Schuhl, CNRS science director (Directeur general délégué à la science); Professor Christelle Roy, CNRS Director of Europe and international affairs; Dr Edwige Elmer-Laurent, Regional CNRS delegate; Dr Helene Boulanger, President of the University de Lorraine; Professor Karl Tombre, Vice President in charge of international cooperation; Professor Amal Kasry, head of Capacity Building at UNESCO; and Professor Delia Haynes, President of AfCA.



Professor Claude Lecomte officially launching the AFRAMED project.

The AFRAMED project objectives are that, after training in the French laboratories, all 15 applicants can independently perform X-ray diffraction measurements. For this purpose, African national representatives are trained in the host laboratory in selecting crystals, mounting and centering them, collecting and reducing data, and then solving the crystal structures. After the training, the applicants are able to perform their own diffraction experiments in the French laboratory remotely; the crystalline samples studied (sent previously to the French laboratory partner of AFRAMED) are centered on the goniometer by a researcher in the French laboratory who allows the applicants to remotely operate the diffractometer. Cameras installed around the diffractometer provide visual feedback of the experiment to the distant operator; such remote experiments allow applicants to perform their experiment in precisely the same way as if they had a diffractometer in their own laboratory. It also offers a new way to teach experimental sciences as the students are able to manipulate a large instrument (in this case a diffractometer) for the first time in their university study course, under the supervision of their professor. For the first year of the project, four representatives from Cameroon, Egypt, Gabon and Togo attended the training session on the PMD2X Bruker D8 Venture diffractometer at the CRM2 laboratory in Nancy (UMR CNRS 7036/Université de Lorraine).

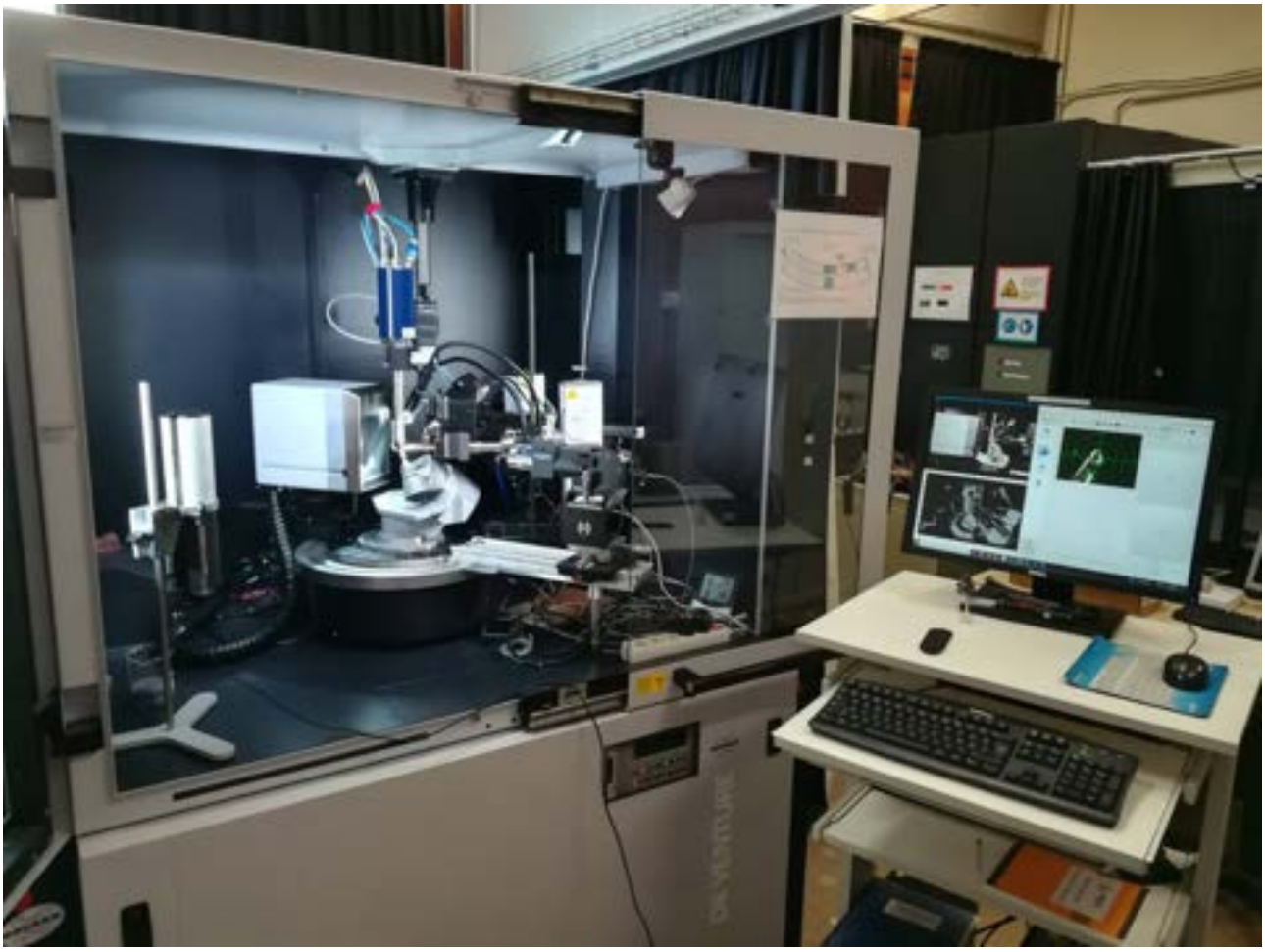


Photo of the Bruker D8 Venture diffractometer (equipped with two cameras) used at PMD2X-CRM2 for the remote measurements in the framework of the AFRAMED project.

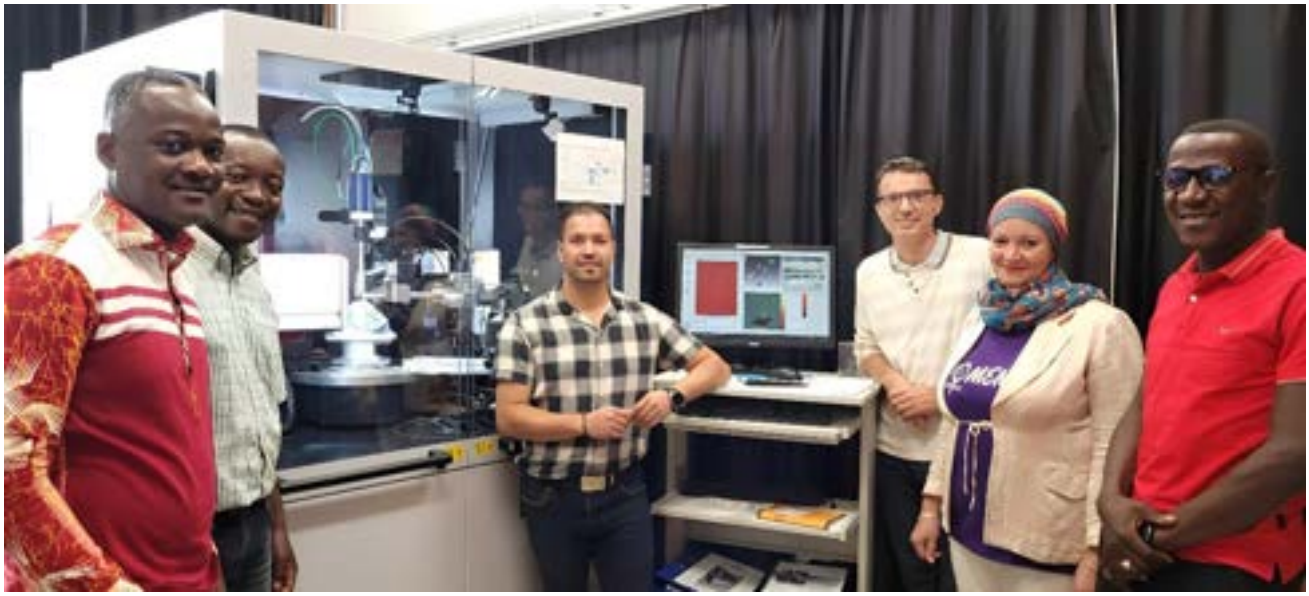
The 2022 AFRAMED training

The 2022 training session of AFRAMED took place on 1–30 September 2022, and started with the welcome inauguration presentations of the applicants (Dr Seham K. Abdel-Aal, Egypt; Dr Patrice Kenfack Tsobnang, Cameroon; Dr Adam Bouraima, Gabon; and Dr Ayi Djifa Hounsi, Togo). The African researchers' scientific backgrounds were crystallography, inorganic and coordination chemistry, and materials sciences for various applications (energy storage, conversion of solar energy to electricity, gas sorption, removal of pollutants with clay material *etc.*).



Photos taken during the 2022 training session at CRM2.

First, applicants were trained to select suitable single crystals (size, shape, quality) and to mount them on the sample holder (a loop). They then learned to center the crystal and to use the Bruker *APEX4* program. Data reduction was also taught by Dr Emmanuel Wenger and Dr El-Eulmi Bendeif (who are in charge of the CRM2 diffractometers).



Left to right: Ayi Djifa Hounsi (Togo), Patrice Kenfack Tsobnang (Cameroon), El-Eulmi Bendeif (France), Emmanuel Wenger (France), Seham K. Abdel-Aal (Egypt) and Adam Bouraima (Gabon) at the 2022 AFRAMED training session.

Single crystals of sucrose, paracetamol, sodium chloride and sodium nitroprussate were measured during the session, starting from selecting suitable single crystals; mounting them on the loop; centering; then

screening, collecting and reducing the data; and finally solving and refining the crystal structure using the *Olex2* program. During the training, the African researchers also attended lectures on the basics of crystallography. The principles behind structure resolution and refinement, electron-density modeling, analysis of intermolecular contacts using Hirshfeld surface analysis, and contact enrichment ratio descriptors were covered. Lectures on software used for structure interpretation at the atomic and subatomic levels, with emphasis on *Olex2* and *MoPro etc.*, were given by Professor Claude Lecomte, Professor Christian Jelsch, Dr Emmanuel Wenger and Dr El-Eulmi Bendeif.

In the last stage of the training, the software for remote measurements was installed on the computers of the four African participants, which they successfully used to measure diffraction data remotely from the African crystals.



The first remote experiment in the CRM2 laboratory located above the diffractometer room.

During the closing ceremony, certificates were given to the four African researchers who attended this 2022 session, and an evaluation meeting was organized between the four applicants and the teaching staff of the AFRAMED project.



Photo of the trainees showing their certificates during the 2022 training session of AFRAMED, with Emmanuel Wenger and Claude Lecomte in the fourth and fifth position from left to right.

Some points were raised during this discussion to facilitate and improve the 2023 training sessions. These points were related to the period of the year in which to run the training, the involvement of UNESCO in the project and the increase in the time allocated to each country involved in AFRAMED. Requests have also been made to consider other instruments in the project.

MEETING REPORT (IUCR SUPPORTED)

50th Annual Meeting of the Argentinean Biophysical Society



María Natalia Lisa, Rodolfo Rasia

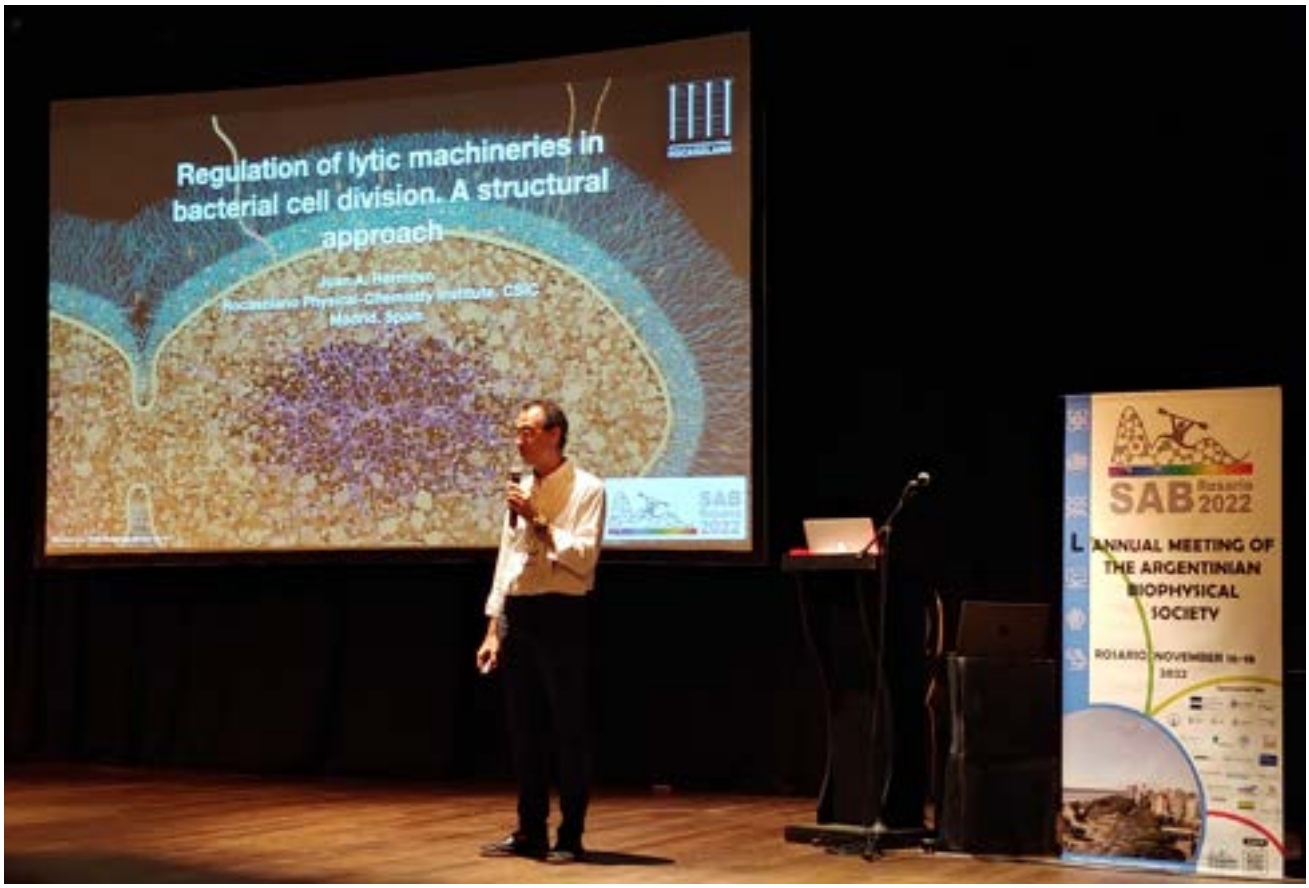
The 50th Annual Meeting of the Argentine Society of Biophysics (SAB for short in Spanish) was held on 16–18 November 2022 at Rosario, with a record 242 participants, 10 plenary lectures, 5 symposia (with 5 international speakers) and 161 poster presentations (including the oral communications that were presented in both formats). A grant received from the IUCr allowed a high participation of Latin American PhD students.



IUCr grantees.

During SAB2022 the biophysical community of Argentina and members of the Latin American scientific community got involved in very fruitful discussions on recent advances in all fields of biophysics and structural biology, with the participation of international experts. We had the privilege of listening to the latest work of Dr Emanuele Buratti (ICGEB, Trieste, Italy), Dr Eva Nogales (University of California, Berkeley; Howard Hughes Medical Institute; and Lawrence Berkeley National Laboratory, USA), Dr Juan Hermoso (Institute of Physical Chemistry "Rocasolano", CSIC, Madrid, Spain; **IUCr sponsored**), Dr

Shahriar Mobashery (University of Notre Dame, IN, USA), Dr Ariel Kaplan (Faculty of Biology, Technion, Israel Institute of Technology, Israel), Dr Valeria Levi (Departamento de Química Biológica- FCEN - UBA/ IQUIBICEN-CONICET), Dr Natalia Wilke [Centro de Investigaciones en Química Biológica de Córdoba (CIQUIBIC), CONICET; Universidad Nacional de Córdoba], Dr Gonzalo Prat Gay (Fundación Instituto Leloir and IIBBA-CONICET) and Dr Luciano Abriata (École Polytechnique Fédérale de Lausanne EPFL, and Swiss Institute of Bioinformatics, Lausanne, Switzerland). Five symposia were organized by the SAB Organizing Committee to feature the state-of-the-art research of renowned Argentinean and international investigators, and oral presentations delivered by young researchers, postdocs and PhD students that were selected from the presented poster abstracts by the Scientific Committee. The result was an exciting series of symposia that prompted ample debates with participation of both senior and young researchers and of PhD students. Some participants highlighted that some talks in the symposia could have been plenary lectures, some examples being those of international participants Dr Chris Bahl, Dr Carlos Bustamante, Dr Cesar Ramirez Sarmiento and Dr Alexis Aspee, among many other excellent researchers from Argentina, including Dr Stefani [Centro de investigaciones en Bionanociencia (CIBION), CONICET].



IUCr Plenary Lecture – Dr Juan Hermoso.

Scientific discussions were also extremely plentiful during the poster sessions: it was extremely pleasing to see young Argentinean and Latin American researchers showing their research to senior scientists (Argentinean and international researchers), who dedicated ample time to analyse posters and suggest new experiments to tackle obstacles or address unanswered hypotheses. Dr Nogales participated in an extremely successful CEBEM (Mercosur Centre of Structural Biology) Speaker Corner with students and young researchers. Scientific and friendly discussions extended to the welcome cocktail and the coffee breaks. On the evening of Thursday 17 November, we had a hospitality dinner for SAB lecturers at Holiday Inn.

SAB2022 concluded on Friday 18 November with an extremely interesting and enlightening presentation by Dr Capitolina Diaz Martinez (Universidad de Valencia, Spain), in which she addressed two dimensions of equality in research and innovation: a) analysis of sex/gender in research and b) gender equality in the

research team and management personnel. She also presented several successful practices on how to make scientific activity, its management, and decision-making in this regard more egalitarian. She also covered the position taken by some scientific publishers and their requirements regarding the inclusion of the gender dimension for the originals they receive. Her presentation was the preamble to the Women in Science roundtable, which was moderated by Dr Erica Hynes (Member of the Chamber of Deputies of the Province of Santa Fe, Argentina, and former Minister of Science, Technology and Productive Innovation of Santa Fe and the first woman in Argentina in charge of a Science portfolio). The roundtable involved Dr Soledad Celej (President of SAB), Dr Maria Eugenia Francia (PI at Institut Pasteur, Montevideo, Uruguay), Dr Valeria Levi [Vice-Dean of the School of Exact and Natural Sciences (FCEN) - University of Buenos Aires], Dr Eva Nogales and Dr Capitolina Diaz Martinez.

In all, we think we have amply achieved our goals and were able to provide all members and non-members of our society with an excellent environment in which to show their research, learn about state-of-the-art research in biophysics and related areas, and even establish some new collaborations. For the first time in SAB, we awarded a special grant to support the participation of women with children from 0 to 2 years.



SAB2022 participants.

Last but not least, SAB encourages initiatives from students and young researchers, and sponsors the Young Initiative on Biophysics (YIB), which is a group formed by students and young researchers in 2015 with the spirit of building a network of undergraduate students, PhD candidates and postdoctoral researchers working on the diverse and rich fields of biophysics to share ideas, inspiration and practical advice. SAB2022 provided the venue and covered all costs of the VI YIB Meeting, which was held on 15 November, with a record attendance of 90 participants. The activities fostered collaborations and networking among young researchers, and strengthened bonds of camaraderie and friendship. In addition, YIB organized the YIB Symposium, which took place during the SAB meeting, with three oral communications from PhD students and young researchers.

MEETING REPORT (IUCR SUPPORTED)

The Third Pan-African Conference on Crystallography



The Third Pan-African Conference on Crystallography, PCCr3, was held in Nairobi, Kenya, from 15 to 21 January 2023, under the auspices of the African Crystallographic Association (AfCA). The conference, which took place at Bomas of Kenya, was organised under the theme *Harnessing Crystallography for Africa's Research and Technology Transformation*. A total of 70 delegates from four continents (Africa, Europe, South America and North America) participated in this year's PCCr. The conference was made possible with sponsorship from the IUCr, NRF Kenya, Cambridge Crystallographic Data Centre (CCDC), ICDD, Bruker, Rigaku, Oxford Cryosystems, Dectris, *Crystal Growth & Design*, *CrystEngComm*, the RSC Pan Africa Chemistry Network, NACOSTI, ESTEC, Kenya Nuclear Regulation Authority, Mandini Kenya, ESTEC, MRS Kenya and Multimedia University.

The purpose of the conference was to stimulate economic growth in Africa by building synergy between funding agencies, industry and academia through the exploitation of crystallography to enhance research and innovation. The conference provided a platform for African crystallographers to exchange ideas and collaborate around the use of crystallography in advancing science on the African continent.



Participants in the Third Pan-African Conference on Crystallography (photo credit: Conrad Wafulah).

Scientific sessions

The conference included the following sub-themes:

Inorganic and Industrial Materials

Crystal Engineering and Structural Chemistry

Crystallography and Life Sciences

Diffraction Physics and Phase Transformations

Crystallographic Databases

Application of Crystallography in Materials Science, Agricultural Science and Geological Science.

There were several excellent plenary lectures covering a wide range of topics. These were delivered by Emmanuel Nji, Len Barbour, Michele Zema, Sylvain Ravy and Elspeth Garman. A variety of invited lectures were also presented, by a truly global group of speakers: Eunice Nyawade, Kenya; Seham Kamal, Egypt; Patrice Kenfack Tsobnang, Cameroon; Gift Mehlana, Zimbabwe; Beatriz Guimaraes, Brazil; Prisca Kouakou, Côte d'Ivoire; Andy Maloney, UK; El-Eulmi Bendeif, France; Abou Akoun, Côte d'Ivoire; and Dietmar Stalke, Germany.

The conference kicked off with an opening ceremony that was addressed by the Vice Chancellor of Multimedia University, Professor Festus Kaberia, who hosted the meeting. The Vice Chancellor stressed the importance of promoting crystallography in Africa through the provision of basic and research equipment for both industry and academia. Also in attendance were the secretary of the European Crystallographic Association, Andy Maloney, and the CEO of the IUCr, Alex Stanley, who also gave unwavering assurance towards supporting AfCA to achieve its mandate on the African continent and beyond. The president of AfCA, Delia Haynes, presented a brief history of AfCA and its roles in promoting the advancement of crystallography in Africa.



The president of AfCA, Delia Haynes, addressing delegates at the opening ceremony of PCCr3 (photo credit: Conrad Wafulah).

The first plenary lecture was given by Dr Emmanuel Nji, who presented approaches that can be used to win the fight against infectious diseases. He stressed the importance of building facilities across the continent that can tackle research related to infectious diseases. Andrew Maloney discussed how the knowledge contained in the Cambridge Structural Database (CSD) can be used in a research setting, with a particular focus on the pharmaceutical industry. Furthermore, he explained how tools that are built upon structural data can help to understand everything from the likely conformation of a new molecule to the properties that underpin drug manufacturing. The second day of the conference started with a plenary lecture from Len Barbour who delivered an excellent talk on *Dynamic Processes in Crystals*. His work demonstrated that it is possible to lose water in porous materials at very low temperatures. This observation makes it possible to design new materials for water harvesting and release. In a related presentation, Patrice Kenfack Tsobnang highlighted the structural dynamics associated with water uptake and release in cobalt and copper coordination complexes.

Just like previous PCCr conferences, presentations on metal–organic frameworks (MOFs) and their applications were a common feature. Maureen Gumbo and Gift Mehlana spoke about MOFs as support materials for chemical and biological catalysts. The presentations highlighted how MOFs can be used in the utilisation of carbon dioxide to produce high-value chemicals. Rufaro Kawondera also showed how chirality can be introduced in already-established MOFs for water-splitting purposes to produce hydrogen, and Mihails Arhangelskis showed how computational calculations can be used to make new MOFs. Other related presentations included *Coordination and Interactions of Transition Metal Werner Complexes* by Merrill Wicht and *Structural Characterization of Coordination Complexes for Catalysis* by Eunice Nyawade. Alessia Bacchi showed how MOFs can be used to transform liquid ingredients into crystalline materials. This work is useful in the food industry, where such ingredients can be used to preserve food.

Elspeth Garman gave an inspiring plenary lecture about her experience and adventures in crystallography. Her work explored physics-based thinking to help establish improved methods for macromolecular crystallography, enabling problems that were not previously accessible to be tackled. A

notable example is the development of protocols to cryo-cool protein crystals prior to diffraction data collection at 100 K, reducing the rate of radiation damage by around a factor of 70 compared with holding the crystal at room temperature. Garman also highlighted that even at 100 K radiation damage can still occur, which may impede correct structural determination. However, she has developed software to correct for the damages that are caused by radiation. Other plenary lectures were from Michele Zema, the IUCr Executive Outreach Officer, who talked about the efforts towards building an African Light Source, as well as the XTechLab project in Benin, and from Sylvain Ravy who discussed how synchrotron radiation can shed light on materials.

Workshops

Tom Blanton, the Director of ICDD, facilitated a workshop on powder diffraction data. The focus of this workshop was to introduce early career researchers, students and those in the industry to using different software (such as *TOPAS* and *Eva*) to analyse diffraction data. An introduction to the PDF4 file was also covered. Another highly successful workshop was organized by the CCDC, which focused on how to use the CSD. This workshop was mainly attended by young scientists and early career researchers.



The CCDC exhibition stand at PCCr3 (photo credit: Susan Bourne).



The CCDC workshop at PCCr3.



A glimpse into the CCDC workshop at PCCr3 (photo credit: Susan Bourne).

Poster session

PCCr3 also had an outdoor poster session. Thanks to generous sponsorship from *CrystEngComm*, *Dalton Transactions* and the IUCr, three poster prizes were awarded to Christelle Ivane Azambou from the University of Dschang, Cameroon; Frederick Okumu from the Jaramogi Oginga Odinga University of Science and Technology, Kenya; and Lavanya Kumar from the University of Warsaw, Poland.

The second Council meeting of AfCA also took place during PCCr3, in hybrid mode. On the final day of the conference, delegates were able to visit Nairobi National Park, the only national park inside a city.

PCCr3 was a great opportunity for crystallographers from around the world to interact in a lovely setting. After the isolation of the pandemic, being able to meet friends and colleagues face-to-face was wonderful. The conference showcased the excellent crystallographic research on the African continent, as well as the growth of the African crystallography community. We are already looking forward to PCCr4!



Mihails Arhangelskis posing for a picture with a regular conference visitor! (Photo credit: Susan Bourne.)

MEETING REPORT

2022 Meeting of the Crystallographic Society of Japan



Kwansei Gakuin University, the venue for CrSJ2022.

Tatsuhiro Kojima, Hiroyoshi Matsumura

The 2022 Annual Meeting and General Assembly of the Crystallographic Society of Japan (CrSJ2022) was held at Kwansei Gakuin University during 26–27 November. The meeting was held face-to-face for the first time in three years. About 215 crystallographers participated in the meeting. There were 215 presentations covering all aspects of crystallography, and four award lectures.

At the CrSJ Awards Ceremony, the Research Award was given to Kunihisa Sugimoto (Kindai University) for his research “Development of advanced X-ray diffractometers for synchrotron radiation and research on functional materials” and Hiroyoshi Matsumura (Ritsumeikan University) for his research “Structural biology of carbon assimilation in photosynthesis”. The Young Crystallographer Award was given to Satoshi Hiroi (Japan Synchrotron Radiation Research Institute) for his research “Development of structural analysis method for crystalline/amorphous phases mixture by X-ray total scattering measurements” and Yoshihiko Furuike (Institute for Molecular Science) for his research “Allostery in Cyanobacterial Clock Protein Orchestrating Circadian Rhythm”.



The recipients of the 2022 CrSJ Awards with the President of CrSJ. From left: K. Sugimoto, S. Hiroi, A. Nakagawa (President), Y. Furuike and H. Matsumura.

Five young scientists were honored with Student Presentation Awards: Y. Nakagawa (Ryukoku University), I. Kurauchi (Osaka University), Y. Zhu (Tokyo Insitute of Technoogy), H. Ito (University of Tokyo) and K. Endo (Tottori University).



The Poster Awardees with the President of CrSJ. From left: A. Nakagawa (President), Y. Nakagawa, I. Kurauchi, Y. Zhu, H. Ito and K. Endo.

The Young Crystallographers' Meeting 2022 was held online on 25 November, and 33 researchers/students participated. This meeting is held every year to give young researchers and graduate students the opportunity to communicate and network with each other, especially beyond the barriers between physics, mineralogy, chemistry and biology, in an informal environment. This year, four lectures by Kentaro Kadota (Kyoto University), Shiori Sugiura (Tohoku University), Rei Matsuoka (Stockholm University) and Yusuke Ishigaki (Hokkaido University) were given, and the participants entered into lively discussions.



Speakers and participants in the Young Crystallographers' Meeting 2022.

The chair of the organization committee was H. Yamaguchi (Kwansei Gakuin University) and the program committee was chaired by I. Takahashi (Kwansei Gakuin University).

The next annual meeting will be held during 27–29 October 2023 at Yamaguchi University in Yamaguchi, Japan. The chair of the organization committee is A. Nakatsuka (Yamaguchi University) and the program committee is chaired by K. Komatsu (University of Tokyo).

MEETING REPORT (IUCR SUPPORTED)

Latin American Crystallographic Association activities in 2022: V Meeting and School in Costa Rica



Andrea Araya-Sibaja, Melissa Camacho-Elizondo, Jose Vega-Baudrit

In 2022, the Latin American Crystallography Association (LACA) had its V Meeting and V School run in a hybrid format in Costa Rica. Both events were supported by the IUCr and chaired by Andrea Araya, a researcher at the National Nanotechnology Laboratory (LANOTEC), Costa Rica. The IUCr President, Dr Hanna Dabkowska, participated in these events and said a few words and gave a short talk in the opening ceremonies.

V LACA Meeting

The meeting was organized and ran concurrently with the Costa Rican Chemistry Congress 2022, which took place from 28 to 30 November at the University of Costa Rica. The V LACA Meeting and Congress sessions occurred in parallel, with the V LACA Meeting sessions being held in the Auditorium of the Plaza de la Autonomía, and the Congress sessions in the Aula Magna, just in front of the Auditorium.

The V LACA Meeting included plenary lectures from recognized crystallographers participating in person and virtually: Hanna Dabkowska (Canada, in person), Jennifer Swift (USA, virtual), Abel Moreno (Mexico, virtual), James Kaduk (USA, in person) and Tom Blanton (USA, in person). In addition, the meeting included semi-plenaries, oral presentations and short oral presentations instead of posters, considering the virtual component of the meeting, mainly for participants who attended remotely. From the sessions of oral and short oral presentations, four prizes by IUCr Journals and one by the Cambridge Crystallographic Data Centre (CCDC) were awarded. The IUCr Applied Crystallography prize went to Teresa García Mendoza (Institute of Technology of Oaxaca, Mexico), the Structural Chemistry prizes went to Eduardo Gutiérrez (Institute of Chemistry of San Luis, Argentina) and Analio José Dugarte (University of Los Andes, Venezuela), and an Honorary Mention went to Cristian Giusseppe Albarracin (Industrial University of Santander, Colombia). Finally, the CCDC prize was awarded to Julian Ticona Chambi (Federal University of São Paulo, Brazil).



IUCr and CCDC prize awardees: (*a*) Eduardo Gutiérrez (left) and Teresa García Mendoza, (*b*) Analio José Dugarte (on screen), (*c*) Cristian Giusseppe Albarracin (on screen) and (*d*) Julian Ticona.

A total of 40 participants, 26 in person and 14 virtual from 13 countries, attended the meeting. The countries included Costa Rica, Guatemala, El Salvador, Mexico, Argentina, Bolivia, Brazil, Colombia, Ecuador, Uruguay, the USA and Venezuela. Thirteen students and young scientists received travel and subsistence support from the IUCr to attend the meeting in person. Unfortunately, the gender balance was similar to past events, with a nearly 40:60 female:male ratio.



Official photo of the V LACA Meeting.

During the meeting, the Costa Rican Union of Crystallographers Assembly took place with the new authorities elected to the national committee by Andrea Araya and José Roberto Vega Baudrit (LANOTEC), Cristian Campos and Jenny Calderón (UCR), Bryan Moncada and José Saavedra (UNA), Jeimy González (ITCR) and Javier Rodríguez Yañez (UNED). The discussion focused on forthcoming activities and the commitments needed to strengthen collaboration between laboratories to grow the Costa Rican crystallography community.

The LACA Assembly also took place during the meeting. The LACA President, José Reyes-Gasga (Mexico), reported on activities carried out in 2020–2022, and one representative per country presented the specific activities in each country. Professor Moreno discussed the proposal to host the 2032 IUCr Congress and General Assembly in Mexico, previously approved by the LACA Assembly. The LACA Assembly ratified the VI LACA Meeting, which will be hosted in Uruguay in 2024, and the 2026 event was also discussed.

V LACA School

The school, named “Polymorphism: applications in industry”, was held from 1 to 3 December at the Costa Rica National Center for High Technology (CeNAT) facilities and hosted by LANOTEC. The program included lectures from Introduction to Polymorphism to Polymorphism in the Courtroom, including polymorphism in pharmaceuticals, nanomaterials, minerals, metals and inorganics, and characterization techniques using single-crystal and powder X-ray diffraction and complementary techniques taught by 13 international instructors. In addition, the International Centre for Diffraction Data (ICDD) and CCDC databases provided workshops. These workshops were possible because of the licenses provided by the ICDD and the CCDC, respectively.



Dr Hanna Dabkowska talking in the opening ceremony (left) and students working at the CCDC workshop, both at CeNAT facilities.

A total of 28 students and young scientists from 13 Latin American countries – Guatemala, El Salvador, Mexico, Ecuador, Bolivia, Brazil, Argentina, Uruguay, Colombia, Venezuela, Chile, USA and Costa Rica – attended the school. Regarding the type of participation, it was very equilibrated, with 15 participants attending in person and 13 attending the school virtually. Participation in person was possible for 13 participants thanks to IUCr funding, which was used to cover their travel and lodging expenses. Finally, the female-to-male ratio for the participants was 40 to 60 in the school.



Official photo of the V LACA School.

MEETING REPORT

SCANZ Crystal 34



Part of the La Trobe University campus and the conference venue.

Christopher Sumby



Back in person for the first time since a joint meeting with the Asian Crystallographic Association conference in 2018, the Society of Crystallographers in Australia and New Zealand (SCANZ) met in Bendigo, a regional city northwest of Melbourne, for a local meeting of the crystallographic community. As we were reminded late in the conference, SCANZ traces its routes back to the group known as the 'Bush Crystallographers' who met around Australia in regional locations. The 2022 meeting in Bendigo was an excellent example of that legacy, being held on the campus of La Trobe University, in a regional city in the heart of the Victorian goldfields.

The meeting was organised by the outgoing SCANZ president, Professor Megan Maher, and a program committee led by Associate Professor Sheena McGowan from Monash University. The meeting was an excellent size for networking and scientific discussions, being attended by around 130 attendees, and was a fantastic opportunity to catch up with much of the Australian crystallographic community. Unfortunately, the higher-than-normal cost and limited availability of trans-Tasman flights lowered attendance from the Kiwis. The program committee developed a vibrant and diverse program with 19 invited speakers and a series of concurrent sessions with speakers selected from abstracts.

Highlights of the program included the 1987 Fund Lecture by Professor Elspeth Garman (Oxford, UK) and the awarding of the 2022 Sandy Mathieson Medal to Professor Stephanie Gras (La Trobe) and the 2023 Lawrence Bragg Medal to Professor Richard Welberry (ANU). Professor Garman gave a wonderful talk covering her work on radiation damage in crystals and approaches to identifying metals in proteins unambiguously. Her candid discussion of and anecdotes about this work made for a lively session and an active Q&A. Professor Gras was the 2022 recipient of the Sandy Mathieson Medal, awarded for distinguished contributions to science involving X-ray, neutron or electron diffraction and/or imaging by a researcher within 15 years of the award of their PhD. Professor Gras, an immunologist and structural biologist, told us about her work on T-cell responses to COVID-19 vaccinations. The final named lecture was the Bragg Medal award for distinguished contributions to science involving X-ray, neutron or electron diffraction and/or imaging to Professor Richard Welberry. Professor Welberry was a pioneer of the development of approaches to understand and utilise diffuse X-ray scattering, and he took us through an

engaging history of that work and many of the interesting developments and results throughout his career.

A diverse group of keynote lecturers provided excellent coverage of redox-active coordination polymers (Professor Brendan Abrahams, University of Melbourne), hydrogen storage in porous materials (Professor Valeska Ting, University of Bristol, UK, but moving to the Australian National University), structure determination and the interplay between the Stanford Synchrotron Radiation Lightsource (SSRL) beamlines and Linac Coherent Light Source (LCLS) (Dr Aina Cohen, SLAC National Accelerator Laboratory) and novel approaches to treat Gram-negative bacterial infections (Dr Steven Rutherford, Genetech).

Other highlights included the Rising Stars session, a lunchtime session hosted by beamline scientists from the Australian Synchrotron on the new capabilities coming online over the next year or two, and updates on the neutron diffraction facilities and the upcoming IUCr 2023 meeting (including the Bragg Your Pattern activities). The Rising Stars of the conference were Eleanor Kearns (University of Sydney), Katrina Black (WEHI), Dr Qingbo Xia (University of Sydney), Andrea Nguyen (La Trobe University), Dr Chathura Suraweera (Monash University) and Dr Curtis Ho (University of Tasmania), who delivered an invited lecture the day before.



Rising Star awardees. Left to right: Dr Qingbo Xia, Andrea Nguyen, Eleanor Kearns, Katrina Black, Dr Chathura Suraweera and Dr Curtis Ho.

Another interesting talk was a peek into the long history of the ‘Bush Crystallographers’, known today as SCANZ, by Dr Rod Hill. Dr Hill approached SCANZ with the idea of a book about the history of SCANZ and was then commissioned to research and write that history. Rod gave a very interesting synopsis of some of the highlights of the society, a little bit of the controversy (about its logo) and some rich social history of the meetings and the community. Later that morning the conference closed out with the awarding of the poster prizes, including the award of an IUCr Journals Poster Prize to Lani Davies (Australian National University).



Lani Davies receiving her IUCr Journals Poster Prize.

Crystal 34 also provided an opportunity to hold a SCANZ business meeting. High on the agenda was the upcoming IUCr meeting in Melbourne in August 2023 but the business meeting also marked the changeover of the SCANZ committee. The reins of SCANZ now pass to the new president Professor Charlie Bond from the University of Western Australia, with the new vice-president being Professor Chris Sumby and a committee comprising Professor Megan Maher (past president), Associate Professor David Turner (secretary), Professor Jack Clegg (treasurer), Dr Michelle Miller (newsletter editor) and committee members Dr Lauren Macreadie, Dr James Hester and Professor Emily Parker. Further representation also comes *via* the National Committee for Crystallography representatives in Australia and New Zealand, Professor Michael Parker and Professor Kurt Krause, respectively.

FEATURE ARTICLE

Structural helix



Istvan Hargittai, Magdolna Hargittai

The authors place the discovery of helicity of biological macromolecules in a historical context and enhance the visibility of the role of the mathematician Harry Bateman and the physicist Horace R. Crane in it.

When J. Desmond Bernal, for the first time, produced a diffraction pattern in an experiment by shining X-rays onto a protein sample in the 1930s, he wandered for hours at night in the streets of Cambridge. The thought kept him sleepless that one day it would be possible to determine the structure of proteins and get closer to uncovering the secret of life. Some of the world's best crystallographers, among them Linus Pauling in Pasadena and W. Lawrence Bragg, Max Perutz and John Kendrew in Cambridge, UK, worked toward this goal.

Already in the early 1930s, William T. Astbury and his group found two forms of the polypeptide chain, the extended β-pleated sheet and the coiled alpha-keratin. Pauling chose to work on alpha-keratin. His strategy was first to predict the dimensions of the polypeptide chain using his knowledge of structural chemistry. Then, he planned to examine the possible conformations of the chain to identify those that agreed with the X-ray diffraction data. The principal information, which was possible to obtain from the rather fuzzy diffraction patterns of alpha-keratin, was that the structural unit repeated every 5.1 Å along the axis of the chain. This would require at least two amino acid residues for this repeat distance.

Pauling had an advantage in narrowing down the problem because he knew that the C–N bond was much shorter than a single bond, that it had a considerably double-bond character and that the peptide bond configuration, that is, the C–N bond and the four adjacent atoms, was planar or nearly planar. This knowledge came from the determination of the geometry of simple molecules and the application of the theory of resonance. Still, he was unable to find a satisfactory solution in the late 1930s. He decided that he needed still more information on the geometry of the individual building blocks of the polypeptide chain. Accordingly, he initiated a series of structure determinations for simple molecules. For a while, he was engaged in other studies during World War II.

Pauling had excellent graduate students, and for some time, each was supposed to determine the structure of a simple molecule either by X-ray crystallography or by gas-phase electron diffraction. He did not order them to choose such a project, but he had his ways of making them prefer it.

Matthew Meselson, the future Harvard professor, was one of Pauling's graduate students already after the war, but his description of choosing his graduate project may characterize the general situation. We quote him on this story [1]:

I became his [Pauling's] graduate student. The first time he gave me a problem, he took a rock and he put it on my desk, and we had a conversation, which went something like this:

Matt, do you know about tellurium?

Yes, Professor Pauling.

It's under selenium and sulfur in the periodic chart of the elements.

Yes, Professor Pauling.

Have you ever smelled hydrogen sulfide?

Yes, Professor Pauling.

It smells bad, doesn't it?

Yes, Professor Pauling.

Have you ever smelled hydrogen selenide?

No, Professor Pauling.

Well, it's much worse.

I see, Professor Pauling.

Now, Matt, have you ever smelled hydrogen telluride? You probably have not.

No, Professor Pauling.

It's much worse than hydrogen selenide as hydrogen selenide is much worse than hydrogen sulfide.

I see, Professor Pauling.

The reason I'm telling you this, Matt, is that I want you to work with the crystal structures of some salts of tellurium, but I want you to be very careful because some chemists have gotten tellurium into their system, and they acquired something called tellurium breath. It'd isolate you from society because it's so bad. Some of these people have committed suicide. But I know you'd be very careful. So, what do you think?

I'd like to go home and think about it.

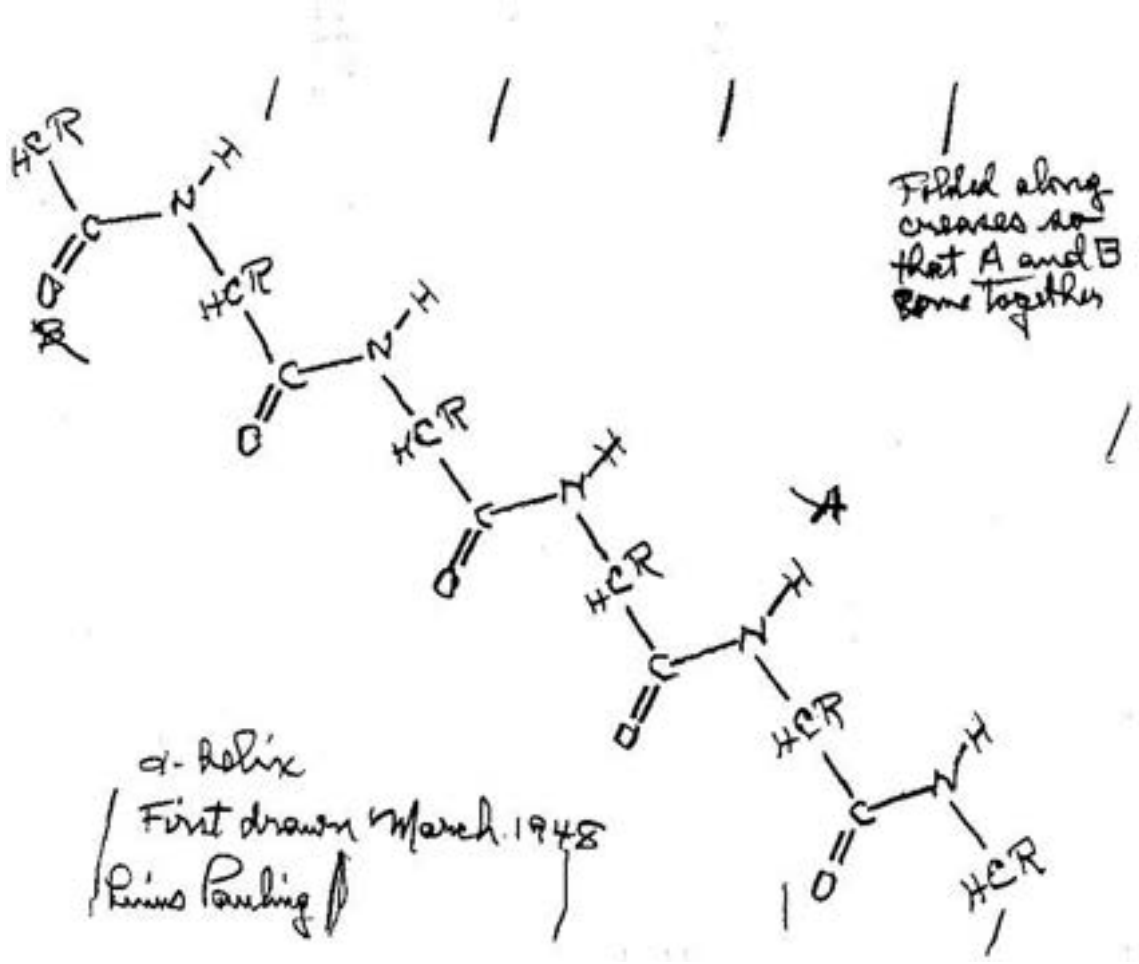
When I came back, I told him that I was really interested in biology, and I asked him to give me a molecule with some carbons and hydrogens and nitrogens. He laughed. I think he may have pulled this trick on other students too. I don't think he was serious, but I don't really know. So, I did a crystal structure with two amide groups to prove what he'd already proven, that the peptide bond is planar because of resonance. He was a wonderful teacher.

Pauling returned to the structure of the peptide chain a decade later, in 1948, while he was on sabbatical in Oxford. He introduced some simplifying assumptions for the chain in order to facilitate the elucidation of its structure. He disregarded the differences in the amino acids building up the polypeptide chain; instead, he considered them structurally equivalent with respect of folding the chain, thereby introducing a helpful symmetry approach in his analysis.



Ava and Linus Pauling. Photograph by and courtesy of the late Karl Maramorosch.

The next step was when he remembered a mathematics course by the English mathematician Harry Bateman (1882–1946) that he had attended 25 years before in Pasadena. Bateman studied in Manchester and earned higher qualifications in Cambridge. He also studied in Göttingen and Paris, taught in Liverpool and Manchester in England, and at Bryn Mawr College and Johns Hopkins University in the United States. He joined what then was Throop Polytechnic Institute in 1917, which changed its name in 1920 to California Institute of Technology. According to Pauling [2], he learned from Bateman that the most general operation that converts an asymmetric element, for example, an amino acid, into an equivalent asymmetric element is a rotation–translation, that is, a rotation around an axis combined with a translation along the axis, and that such an operation produces a *helix*. Accordingly, Pauling took the polypeptide chain and rotated it around the two single bonds to the alpha carbon atom, with the amount of rotation being the same from one peptide group to the next, and on and on and on. He kept the peptide groups planar with the proper dimensions and searched for a structure in which each NH group formed a hydrogen bond with a carbonyl group.

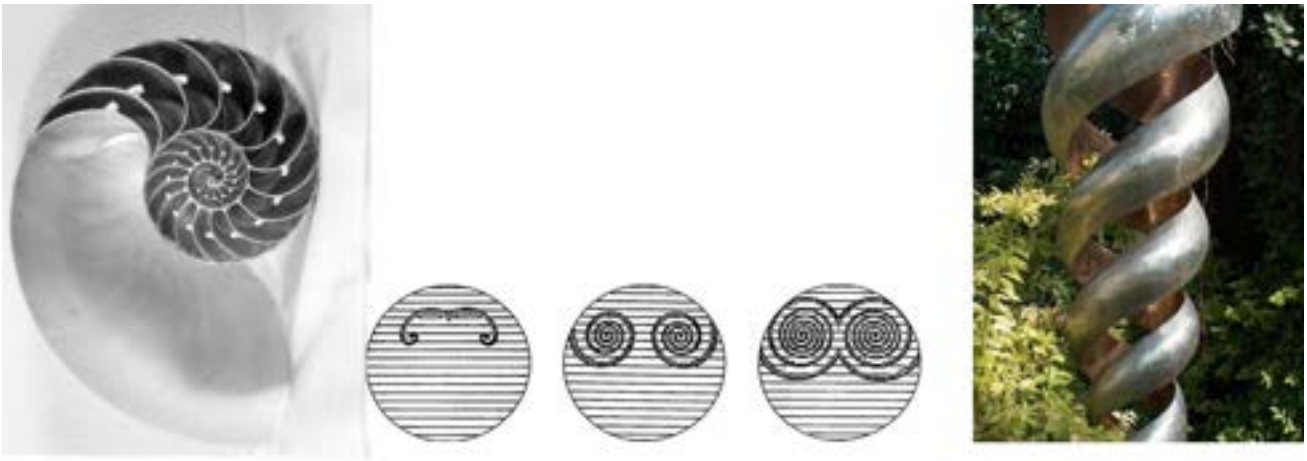


Linus Pauling's drawing of the stretched α-helix structure, March 1948 [2].

Pauling sketched a polypeptide chain on a piece of paper and folded it along parallel lines. Two structures satisfied his assumptions. One of them he named α-helix with 4.6 residues per turn. There was only one disturbing observation that the corresponding repeat distance was 5.4 Å rather than 5.1 (mentioned above). However, this discrepancy did not deter Pauling from proceeding because he believed that his model was right. Eventually, he, and independently Francis Crick, interpreted this discrepancy by some slight additional coiling of the helices, which facilitated it to achieve closest packing. Crick considered the discrepancy and its interpretation a nice example of symmetry-breaking by a weak interaction [3]. Pauling and his associates published the α-helix structure in two papers [4 and 5]. In the meantime, Bragg, Kendrew and Perutz also published their paper on the structure of alpha-keratin [6]. They described about 20 structures, but none of them was correct. They did not utilize the chemical knowledge of the planarity of the peptide group.

At this point, we interrupt our description of events to comment on reference 2. It is a paper by Pauling published posthumously. The gist of its story, following Dorothy Munro's narrative [2], is this: In 1982, Pauling produced a manuscript titled "The Discovery of the Alpha Helix" at the request of W.H. Freeman and Company as a chapter for a book by Donald Voet (it must have been the biochemistry textbook, which has been in print ever since). Pauling died in 1994, and as his long-time former secretary/assistant, Dorothy Munro found out in 1995 that the chapter had not been included in the book. Munro was looking for a venue to bring out the paper. Robert Paradowski, Pauling's authorized biographer, suggested to her the *Chemical Intelligencer*, the recently launched magazine about the culture of chemistry. One of us (IH) was the founding editor of the magazine, which was happy to publish the manuscript [2]. We have asked Donald Voet whether he might add anything to this story. He remembered that the book editor asked Pauling to write the chapter, but as far as he knew, nothing further happened — he responded to our query [7].

Coming back to the discovery of the α-helix, there was a noteworthy difference in the titles of the two Pauling papers in 1950 [4] and 1951 [5]. The first used the word “spiral” and the second, “helix.” Even 70 years later, these two words appear interchangeably, although, strictly speaking, only “helix” is correct for these structures.



Examples of spirals. Left: Nautilus shell. Photograph by and courtesy of Lloyd Kahn [8]. Reproduced with permission. Middle: The evolution of a spiral ring pattern in time, from left to right, in a Belousov–Zhabotinsky oscillating reaction [9]. Right: Double spiral (detail), “The Inner Light” by Gidon Graetz, in the garden of the Weizmann Institute in Rehovot, Israel. Photograph by the authors.

Spirals have changing diameters, whereas the diameter of a helix is constant. Hence, the structure of biological macromolecules is properly described as helical. In everyday speech, helical constructions are often referred to as spiral; examples include the spiral notebook and the spiral staircase. For the latter, we present two examples. We would not suggest trying to change the everyday usage of spiral notebook or staircase, but in technical texts, it is proper to stick to helix for describing the structure of large biological molecules.



Helical structures of “spiral” staircases, both photographs by the authors. The one on the right, the spiral staircase and its shadow, make it a *doubled* helix (though not a *double* helix). It is outside the wall of the former (until 2013) headquarters of the MRC Laboratory of Molecular Biology.

As is seen in the titles of references 4 and 5, Pauling also had to learn the difference between spiral and helix. Jack D. Dunitz first met Pauling in the winter of 1947–1948 during Pauling’s visiting professorship in Oxford. Then, Dunitz stayed in Pauling’s group at Caltech, 1948–1951, so he could closely follow the discovery of the α-helix structure. When Pauling talked to Dunitz about his models, he used the term “spiral.” At one point, Dunitz pointed out to Pauling that “helix” would be the correct term in this case. According to Dunitz, henceforth, Pauling used the term “helix” consistently. Dunitz liked to think that he helped to give the α-helix its name — he considered this to be his personal contribution to molecular biology [10].



Horace R. Crane (National Science and Technology Medals Foundation).

We learned from Donald Caspar [11] that the nuclear physicist Horace R. Crane (1907–2007) was the first to suggest the idea that assemblies of identical units build helical structures [12]. Crane spent his long career as a Professor of Physics at the University of Michigan. In 1986, he received the National Medal of Science “For the first measurement of the magnetic moment and spin of free electrons and positrons.” In World War II, he helped to develop radar at MIT and worked on the proximity fuse at the Carnegie Institution and at the University of Michigan. Less well known is that he also worked on problems of assembly line operation. After the war, this experience led him to recognize the analogy of assembling biological structures to a subassembly manufacturing process [13].

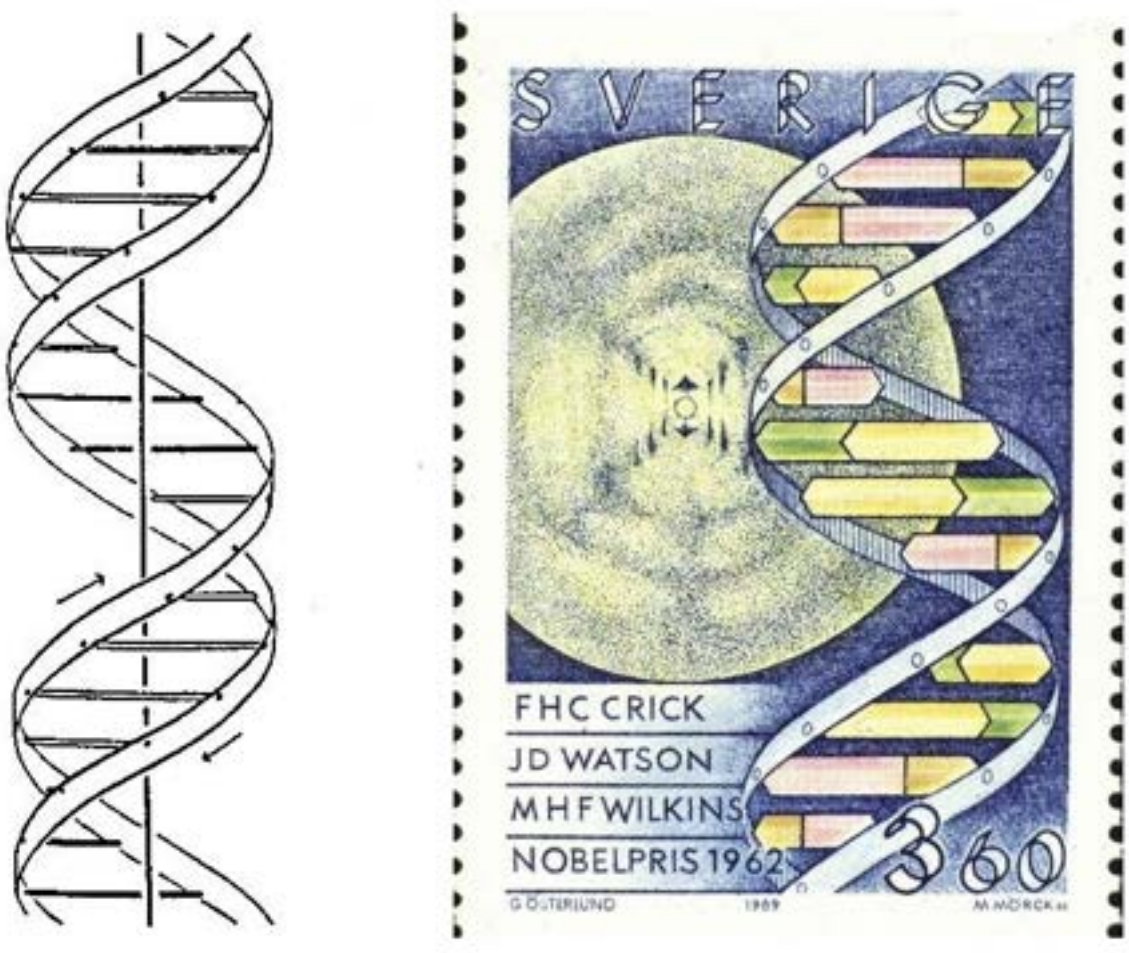
Here we quote Caspar about what Crane did: “He built simple models out of matchboxes, for example, sticking matchboxes together in the same way, arriving at a helix naturally by using the same pair-wise connections repeatedly. He recognized that there is no requirement for the screw symmetry to be rational, that is, that the helix has an integral number of units in some integral number of turns. Such an arrangement in which the unit axial translation is not rationally related to the helix pitch is nowadays called incommensurate periodicity by physicists.” [13]

W. Cochran, Francis Crick and V. Vand worked out the theory of diffraction of helical structures [14]. Initially, they considered a thin helical wire, then a set of identical point atoms spaced at regular intervals on a helix, and finally, the polypeptide helix based on the Pauling α-helix model.



Entrance to 19–20 Portugal Place, the former home of Francis and Odile Crick in Cambridge, UK. Photograph by the authors.

Crick had the single helix (rather than a double helix) in mind when he accorded the name “Golden Helix” his Cambridge home. He erected a simple metallic helix above its entrance, painted yellow. The Nobel laureate Arthur Kornberg published a book about biotechnology ventures and he titled it *The Golden Helix*. He used this expression for the double helix, and the meaning of the title was made unambiguous when he wrote in the preface of the book: “Turning the DNA helix into gold seemed another alchemist dream” [15].



Schematic representations of the DNA double helix in the original *Nature* paper (left) and on a Swedish postage stamp (right). The model on the postage stamp hints at the linked bases somewhat more in detail than the more schematic drawing on the left. The backdrop on the postage stamp represents the famous photograph No. 51 of the DNA diffraction patterns recorded by Rosalind Franklin and her student, Raymond Gosling, without displaying their names.



Left: Odile and Francis Crick, 2004, in their home in La Jolla (photograph by the authors). Right: James D. Watson, 2000, in the Hargittais' home in Budapest (photograph by the authors).

Our mention of Kornberg's book already brings us to the double-helix structure of DNA. Initially, James D. Watson and Francis Crick suggested the double-helix structure for DNA in their one-page seminal *Nature* paper in 1953 [16]. This brief report was illustrated by a schematic drawing of the double helix majestic in its simplicity (see above). For a long time, we supposed that Odile Crick had drawn it, perhaps stemming from our romanticizing the story and the knowledge of her artistic inclination. In 2004, when we visited the Cricks, we asked them about the origin of the drawing. We were taken aback when we

learned that Odile Crick did not play any role in producing this illustration; it was prepared after some other cartoon simply by tracing its contour lines.

The first seminal paper containing the suggestion for the double-helix structure was soon followed by a second, somewhat longer note. This elaborated the genetic implications of the double-helix structure [17]. Watson and Crick must have liked the purely diagrammatic figure quoted above because they reproduced it in this second paper. From the two Watson–Crick papers, it is not obvious that there were four antecedents to their discovery [18]: “One was the discovery of Oswald Avery and his two co-workers that DNA is the substance of heredity [19]. The second was Erwin Chargaff’s observation that the purine and pyrimidine bases occur in a 1:1 ratio in the DNA of all organisms [20], which came to be expressed as base-pairing in the Watson–Crick model. The third was Linus Pauling’s discovery of the α-helix [5] of protein structure, in which he showed the helicity of a biological macromolecule. The fourth was Rosalind Franklin’s careful X-ray diffraction measurements of DNA [21], which, among others, pointed to the C_2 symmetry of the structure.”



Left: Photograph 51 of the X-ray diffraction pattern of DNA by Rosalind Franklin and Raymond Gosling on the mural by Larry Kirkland in the lobby of the Keck Center, 500 5th Street NW in Washington, D.C. The center serves as the offices of the three U.S. national academies: the National Academy of Sciences, the National Academy of Engineering and the National Academy of Medicine. Photograph by the authors. Right: Rosalind Franklin’s portrait in a window display at King’s College, London. Photograph by the authors.

The C_2 symmetry has a special importance in the double-helix structure of DNA [18]: “The importance of the knowledge of C_2 symmetry, which came from the X-ray patterns, was not explicitly acknowledged in Watson and Crick’s communications, which is the more curious because the double-helix structure could have been described in a simplified way stressing the presence of this symmetry. … Of Watson and Crick, Watson gave much less importance to C_2 symmetry than Crick, perhaps because Watson had no background in crystallography. Furthermore, knowing that Watson had very little faith in the importance of Chargaff’s observations, it is remarkable how far he advanced in his intuitive model-building. Crick, on the other hand, understood the implications of C_2 symmetry, and when they arrived at the concept of base-pairing, he pointed out that the base pair implied a twofold axis in the planes of the bases, perpendicular to the axis of the helices. In other words, the two chains were anti-parallel [22].”



Horizontal double helix as part of the fence at a pub near the Cricks' former home, "The Maypole", 20A Portugal Place. Photographed in 2000 by the authors.

The Golden Helix at the Cricks' former residence is right-handed (see above), as is DNA, but the double helix of the fence outside the pub is left-handed [23]. The handedness of the helix in the fence was a mistake by the landlord of the pub, who commissioned it after receiving the dimensions from Crick, who was a regular visitor to the pub. The double-helix model has become a popular icon so widespread that today it is one of the best-known, if not *the* best-known symbol of science. It is a winner, especially if contrasted with another icon, the mushroom cloud of nuclear explosions. Not everybody was pleased, though, by the success of this model. Erwin Chargaff, whose discovery of base-pairing in DNA was a crucial ingredient in making the discovery of the double helix [18], wrote disparagingly about what he considered to be a propaganda campaign for the model [24].

Erecting a sculpture is not a trivial matter, yet double-helix memorials abound. We have selected four examples for presentation.



Left: Sculpture of the double helix by Bror Marklund, 1997, in front of the medical school of Uppsala University. Photograph by the authors. Right: “Temple of Wisdom” by Marino Di Prospero, 2002, on the campus of the University of L’Aquila. Photograph by the authors.

The Uppsala sculpture is large and beautiful. At the top end, it splits as if getting ready for reproduction. At closer scrutiny, what might be the bases appear outside of the backbone. This erroneous arrangement was also in one of Pauling’s models when he somewhat belatedly joined the race for the DNA structure. But on the artist’s part, this may have been an expression of artistic freedom or the consequence of a misunderstanding. The elegance of the L’Aquila sculpture comes from its material being white Carrara marble. Here, also, the top end splits.



Double-helix sculpture by Tom Otterness, 2001, in the sculpture garden at Battery Park City in Lower Manhattan, New York. Photograph by the authors.



Matthew Meselson and Franklin Stahl, many years after their seminal experiment performed at Caltech. Photo courtesy of Franklin Stahl.

The Manhattan double-helix sculpture not only splits at the top end; the split threads are already forming new double helices. To us, it also meant the representation of the beautiful Meselson–Stahl experiment in which Matthew Meselson and Franklin Stahl demonstrated the semiconservative mechanism of DNA replication [25]. It has been called “the most beautiful experiment in biology” [26].



“Spirals Time–Time Spirals” by Charles A. Jencks at the Cold Spring Harbor Laboratory with the residence of James D. and Elizabeth L. Watson in the background. Photograph by the authors. The top end of the Cold Spring Harbor Laboratory sculpture may have caused a problem to the sculptor, hence the awkward solution.



George Gamow with a model of the double helix. Photo courtesy of the late Igor Gamow, George Gamow's son.

Model making was an indispensable component of the discoveries of the α-helix by Pauling and of the double helix by Watson and Crick. It was a finely choreographed spectacle when Pauling introduced his model in a public presentation in Pasadena. The α-helix model was hiding under a cover until the right moment when Pauling, like a magician, removed the cover, and the audience gasped at its magnificence. Soon after the publications on the DNA structure in *Nature*, the great physicist George Gamow turned to Watson and Crick, raising the question of information transfer from nucleic acids to proteins. He was one of the initiators of the search for the genetic code. However, molecular biologists like to stress the factual errors in his ideas rather than recognizing their fruitfulness. He was also a model builder.



James D. Watson with the double-helix model in his left hand at the Cold Spring Harbor Laboratory, June 1953. Photograph by and courtesy of the late Karl Maramorosch.

Watson presented his double-helix model of modest size to a June 1953 meeting at the Cold Spring Harbor Laboratory, that is, soon after the discovery was published in *Nature* in April. There was an impact, and the consequences reverberate to this date. The MRC Laboratory of Molecular Biology developed the art of model-making following Pauling's example, and soon it had a full room of models. During the search for the structure of DNA, it was not yet obvious that they were dealing with a model of historical importance. Eventually, it was not easy to assemble the parts of the original model to be exhibited in the Science Museum in London [27], but it is there today as a milestone in science history.

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AWARDS AND PRIZES

Wayne Hendrickson awarded 13th Ewald Prize



Professor Hendrickson at a 75th birthday celebration for Herbert Hauptman and Jerome Karle in Buffalo, NY, USA, in October 1992 (photo contributed to the IUCr gallery by Bill Duax).

The 13th Ewald Prize has been awarded to Wayne A. Hendrickson (Columbia University, NY, USA) *for his exceptional contribution to structural biology including the development of MAD/SAD methods and crystallographic theory. No-one else is so singularly and formatively identified with the explosive growth in biological crystallography and the consequent benefits to chemistry and biology*.

Wayne Hendrickson transformed structural biology when he discovered and perfected resonant diffraction methods for determining the atomic-level structures of biological molecules, namely the methods of MAD (multiwavelength anomalous diffraction) and its single-wavelength variation SAD, which are now “household” terms in the field of crystallography. MAD and SAD derive from a marriage of chemistry with physics and biology and are the methods of choice for *de novo* X-ray determinations where there is no structural precedent. The ease with which macromolecular structures are determined by these methods served in founding the field of structural genomics, and has led to a flood of atomic-level molecular hypotheses, including many from Hendrickson himself, to inform biochemistry, physiology and genomics.

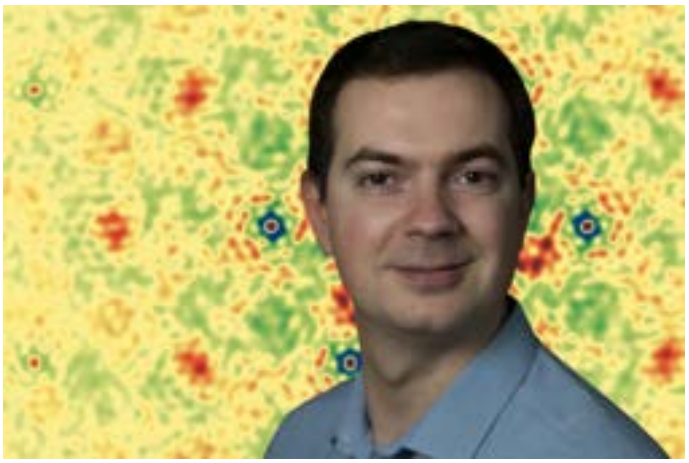
Like the late Professor Ewald, Hendrickson advanced the foundations of crystallography; his essential contributions include not only MAD and SAD but also his phase-encoding coefficients (Hendrickson–Lattman coefficients) and stereochemically restrained refinement.

Professor Hendrickson will deliver the Ewald Prize Lecture during the Opening Ceremony of the 26th IUCr Congress on 22 August 2023.

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

AWARDS AND PRIZES

Second W. H. and W. L. Bragg Prize awarded to Arkadiy Simonov



The 2023 W. H. and W. L. Bragg Prize for outstanding early-career crystallographers has been awarded to Arkadiy Simonov (ETH Zürich, Switzerland) *for his development of the three-dimensional difference pair distribution function (3D-ΔPDF) approach and its transformative effect on the field of materials.*

Over the past decade, Arkadiy has established himself as the single most talented young researcher in the interpretation of diffuse scattering from single crystals. Not only is he the author of the foremost codes for data reduction (*MEERKAT*) and 3D-ΔPDF refinement (*YELL*) but also he is applying his 3D-ΔPDF methods to solve crucially important problems in materials science.

Professor Simonov started his academic career under the tutelage of Dr Thomas Weber and Professor Walter Steurer at ETH Zürich. The *YELL* code was a key outcome of his Doctorate; this software enabled the fitting of the 3D-ΔPDF in terms of pairwise correlation parameters. In this way, Arkadiy established the first general approach for refinement of the diffuse scattering contribution to single-crystal diffraction patterns. He applied his methodology to a range of systems, and in doing so both established a series of proofs-of-concept and solved a number of important outstanding problems in the field of complex materials.

Professor Simonov will present a Keynote Lecture during the 26th IUCr Congress in Melbourne, Australia, in August 2023.

For a list of papers by Arkadiy Simonov appearing in IUCr journals click here.

AWARDS AND PRIZES

Struchkov Prize awarded to Robert R. Fayzullin



Robert R. Fayzullin (Laboratory of Diffraction Research Methods, Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russian Academy of Sciences, Kazan, Russia) has won the 2023 Struchkov Prize *for his work on real-space interpretation of chemical bonding by combining one-electron potentials and associated force fields derived from high-resolution X-ray diffraction data*.

Dr Fayzullin is a specialist in the field of high-resolution X-ray diffraction crystal structure determination, and experimental and theoretical charge-density studies, co-author of about 100 publications. He managed to successfully describe chemical bonding, interatomic charge transfer, electron exchange effects in crystals using novel physically grounded descriptors based on electronic potentials and corresponding vector fields measurable by diffraction techniques. The selection committee appreciated his quite general scientific contribution and its novelty.

The Struchkov Prize was established in 1997 to commemorate the life achievements of Professor Yuri T. Struchkov (1926–1995), an outstanding Russian crystallographer who made substantial contributions to the structural chemistry of organic and organometallic compounds. Now administered by the IUCr, the Prize is awarded every triennium at the IUCr Congress to up to three winners (under 35 years of age at the time of the submission deadline) for outstanding achievements in small-molecule X-ray diffraction methods application in the fields of chemistry, crystal chemistry or materials science.

AWARDS AND PRIZES

Jian-Min Zuo wins 2023 Gjønnes Medal



2023 Gjønnes Medal winner Jian-Min Zuo

Members of the 2023 Gjønnes Medal Committee

After reviewing the nominations and candidates, the selection committee agreed to propose Professor Jian-Min Zuo (University of Illinois at Urbana-Champaign) as the recipient of the 2023 Gjønnes Medal *for his outstanding contributions to the development and application of quantitative electron diffraction.*

For more than 35 years, Jian-Min Zou has been at the frontline of the development of innovative methods based on electron diffraction. At the beginning of his career, he developed quantitative convergent electron beam diffraction and was one of the pioneers of establishing the technique for the determination of low-order structure factors, which allowed the study of charge density and bonding [(*e.g.* in Cu_2O (Zuo *et al.*, 1999)]. He was the first to demonstrate the use of coherent electron diffraction to retrieve atomic resolution images [*e.g.* carbon nanotubes (Zuo *et al.*, 2003) and surfaces of Au nanocrystals (Huang *et al.*, 2008)] by diffractive imaging, an intuition with pivotal importance also for X-ray crystallography. Later, he focused on the study of surfaces and defects, and demonstrated that both convergent and parallel electron diffraction can be efficiently used for studying local structures, defects, lattice strains and crystal orientations.

In addition, Jian-Min Zou is an active disseminator. Together with John Spence he wrote *Electron Microdiffraction*, one of the most studied textbooks on TEM and microdiffraction (Spence & Zuo, 1993). This book has become a key resource for an entire generation of young researchers entering the field of electron diffraction. He has been active in the promotion and maintenance of Web-EMAPS, cloudEMAPS and pyEMAPS tools, used for the accurate simulation of TEM images and diffraction patterns. This contribution has democratised the use of these detailed theoretical tools for non-experts in quantitative modelling of scattering in a TEM, and enlarged the scientific community that is working with TEM.

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This award is managed by the Awards Sub-committee of the IUCr Commission on Electron Crystallography.

AWARDS AND PRIZES

SARS-CoV-2 spike protein work earns rising star award for Jason McLellan



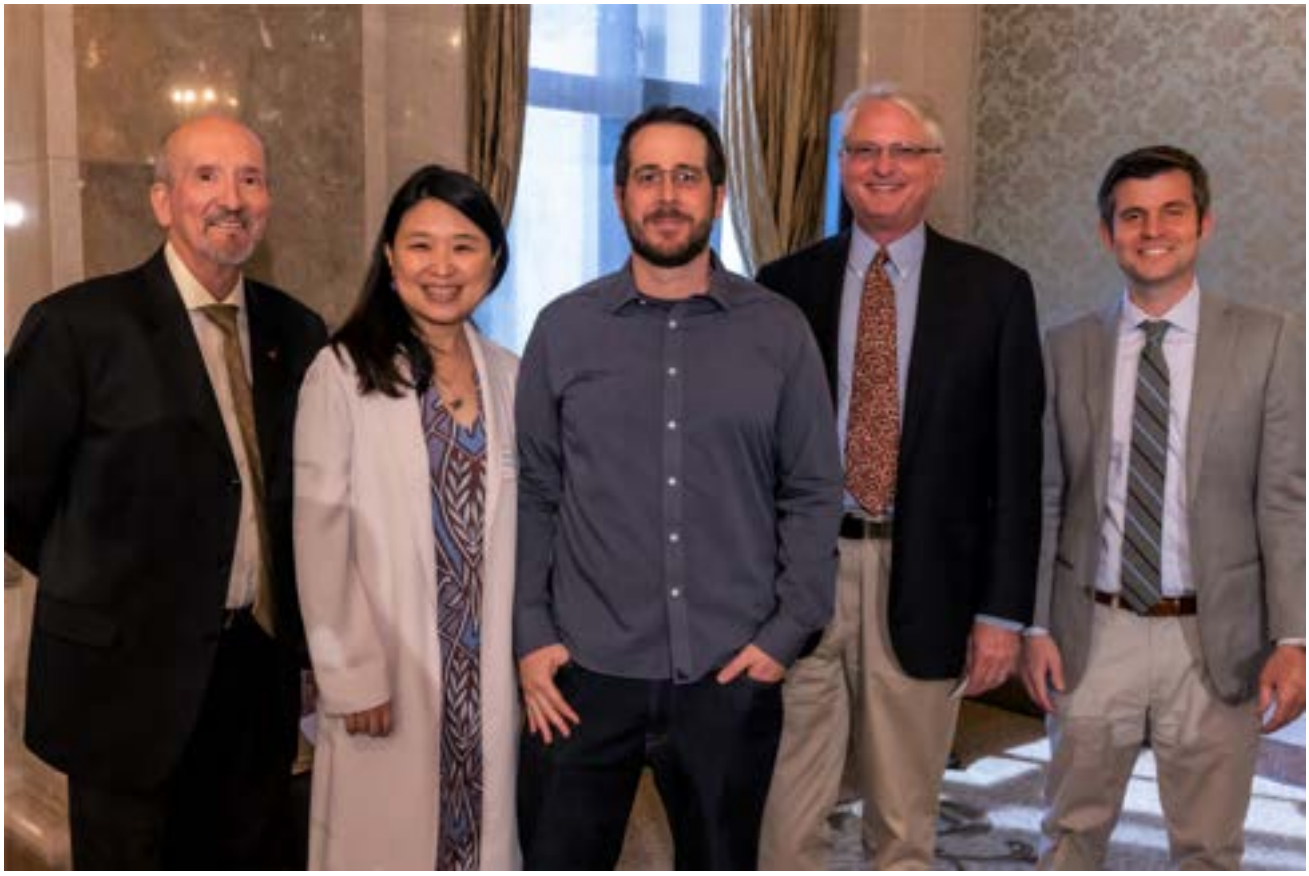
The Hackerman award consists of a framed certificate, a bronze sculpture of a rising star and a check for USD100,000.

Marvin L. Hackert

Professor Jason McLellan was recognized as a “rising star” in structural biology when presented with the Welch Foundation’s Norman Hackerman Award in Chemical Research for having made significant scientific contributions in chemistry and biochemistry. The award was presented at a reception at the University of Texas at Austin (UT Austin) campus on 22 February 2023.

A professor in the Molecular Biosciences Department and Welch Chair in Chemistry at UT Austin, Jason McLellan has distinguished himself as a pioneer in structure-based vaccine design. The award recognizes the accomplishments of chemical scientists in Texas who are early in their careers. McLellan and collaborators determined the structures of coronavirus spike proteins and used that information to design stabilized forms of the spike proteins with enhanced ability to elicit neutralizing antibodies. His stabilized form of the SARS-CoV-2 spike protein forms the basis for all SARS-CoV-2 vaccines approved in the US, including those from Pfizer/BioNTech, Moderna, Johnson & Johnson and Novavax, thus helping save the lives of millions of Americans and others around the world.

The event was attended by the President, Provost and VP Research of UT, plus many of Jason’s students and colleagues as well as representatives from the Welch Foundation. Catherine Murphy, Chair of the Welch Foundation Scientific Advisory Board, stated that “*Every American that has been vaccinated against COVID-19 has directly benefitted from Jason McLellan’s work*.”



Congratulating Jason on his award were some of his structural biology colleagues from UT Austin (l to r): Marv Hackert, Jessie Zhang, Jason McLellan, Dan Leahy and David Taylor.

Jason will also receive the 2023 NAS Award in Molecular Biology for his exceptional contributions to public health and medicine through his groundbreaking work on the molecular biology and structure of viral glycoproteins as applied to vaccine antigen design. That award will be presented at the 160th NAS Annual Meeting on 30 April 2023.

AWARDS AND PRIZES

Sekazi Mtingwa awarded 2023 AAAS Abelson Prize



The American Association for the Advancement of Science (AAAS) has announced the 2023 winners of eight longstanding awards for outstanding achievements, and we are delighted to report that Sekazi Mtingwa has won this year's AAAS Philip Hauge Abelson Prize. This award recognizes someone who has made significant contributions to the scientific community — whether through research, policy or civil service — in the US. The awardee can be a public servant, scientist or individual in any field who has made sustained, exceptional contributions and other notable services to the scientific community. Dr Mtingwa exemplifies a commitment to service and dedication to the scientific community, research workforce and society. His contributions have shaped research, public policy and the next generation of scientific leaders, according to the award’s selection committee.

As a theoretical physicist, Mtingwa pioneered work on intrabeam scattering that is foundational to particle accelerator research. Today a principal partner at Triangle Science, Education and Economic Development, where he consults on STEM education and economic development, Mtingwa has been affiliated during his scientific career with North Carolina A&T State University, Harvard University, the Massachusetts Institute of Technology and several national laboratories.



Sekazi Mtingwa (second from right) at the World Science Forum in Jordan in November 2017 with fellow speakers in the Thematic Session "Light Sources and Crystallographic Sciences for Sustainable Development" (from left): Juste Jean-Paul Ngome Abiaga (UNESCO), Michele Zema (IUCr), Giorgio Paolucci (SESAME), Maciej Nalecz (UNESCO) and Simon Connell (African Lightsource initiative).

His contributions to the scientific community have included a focus on diversity, equity and inclusion in physics. He co-founded the National Society of Black Physicists, the National Society of Hispanic Physicists, the African Physical Society and the African Lightsource Foundation. He is also co-founder and chair of *LAAAMP*, the IUPAP/IUCr/ICTP Lightsources for Africa, the Americas, Asia, Middle East and Pacific project. His work has also contributed to rejuvenating university nuclear science and engineering programs and paving the way for the next generation of nuclear scientists and engineers. Mtingwa served as the chair of a 2008 American Physical Society study on the readiness of the U.S. nuclear workforce, the results of which played a key role in the U.S. Department of Energy allocating 20% of its nuclear fuel cycle R&D budget to university programmes.

“I have devoted myself to being an apostle for science for those both at home and abroad who face limited research and training opportunities,” said Mtingwa. “Receiving the highly prestigious Philip Hauge Abelson Prize affirms that I have been successful in this mission. Moreover, it provides me with the armor to press onward to even greater contributions.”

Mtingwa was honoured with a tribute video at the 2023 AAAS Annual Meeting, held in Washington, DC, in March 2023. The prize includes a commemorative plaque and USD 5000.

AWARDS AND PRIZES

IUCr Poster Prizes at BCA 2023



John R. Helliwell

Three IUCr Journal Poster Prizes were awarded at the annual conference of the British Crystallographic Association (BCA), held at the University of Sheffield, UK, just before Easter 2023. The criteria guidelines were that “The IUCr is pleased to offer a prize for each of the three best posters from an undergraduate, postgraduate or postdoctoral researcher with up to 3 years' experience in distinct areas of crystallography such as structural biology, structural chemistry and applied crystallography”. The judges were Dr Petra Bombicz (Hungary), Professor Bo Brummerstedt Iversen (Denmark), Dr Charlie McMonagle (France) and myself as Chair. There were 58 chemistry posters, 9 in biology, 20 in physics and 1 industrial. The standard of the posters and their science was very high. The prize winners were as follows, in alphabetical order:

Nicholas Funnell of the ISIS Neutron and Muon Facility, Rutherford Appleton Laboratory, Didcot, UK, whose poster was entitled “LMX – a new single-crystal, neutron time-of-flight diffractometer for large-molecule crystallography”.

Lavanya Kumar of the Faculty of Chemistry, University of Warsaw, Poland, whose poster was entitled “Correlating experimental and calculated charge density of halogen-bonded materials”.

Joshua Levinsky of the School of Chemistry, University of Edinburgh, UK, whose poster was entitled “The barocaloric and structural properties of choline-based plastic crystals”. [Barocaloric materials are characterized by strong, reversible thermic responses to changes in pressure and have potential use as refrigerants in cooling systems instead of gases such as hydrofluorocarbons.]



IUCr Poster Prize Awardees, from left: Nick Funnell, Lavanya Kumar and Joshua Levinsky. John Helliwell making the presentations at the conference dinner, held in the University of Sheffield Students' Union building, to Nick and Joshua. Presentation photographs courtesy of Dr Iain Oswald of the University of Strathclyde.

The prize comprised a copy each of the IUCr's *Little Dictionary of Crystallography* 3rd edition and a complimentary three-year membership of the IUCr Associates Programme.

OBITUARY

Olga Kennard OBE FRS (1924–2023)



Dr Olga Kennard giving opening remarks at the CSD's 50th anniversary celebration. From the CCDC.

Michael Francis

It is with great sadness that we learn of the passing of Dr Olga Kennard. Her long, successful life was full of many achievements, including founding the Cambridge Structural Database (CSD) which is now a fundamental resource that supports the global development of new drugs and materials that benefit us all, is used in chemistry education and contributes to the advancement of science. In this obituary for Dr Kennard we celebrate and recognize her many achievements in the scientific community.

Born in Hungary, Dr Kennard moved to the UK in 1939 just before the outbreak of the Second World War. After graduating from the University of Cambridge in 1944, she joined the Cavendish Laboratory under Lawrence Bragg as an assistant to Max Perutz in the Department of Physics.

After completing the first X-ray structure at the Laboratory (albeit on a very small structure), Dr Kennard moved to London in 1948 and then to the Chemistry Department at Cambridge University in 1962. At this point it was difficult to solve larger structures with crystallography and very unusual for crystallographers to be in a chemistry department. Crystallographers often experienced suspicion from more traditional chemists who thought this ‘upstart subject’ was taking over their territory.

Dr Kennard persevered and persuaded the department to purchase a diffractometer, the first to be used for small-molecule studies. With a small but gradually increasing group, supported by the Medical Research Council, Dr Kennard and colleagues worked on a variety of medical compounds including antibiotics and (excitingly) the structure of adenosine triphosphate.

As the volume of structural data increased, Dr Kennard along with Dr J. D. Bernal had a vision that the collective use of data would lead to new knowledge and generate insights:

‘We [J. D. Bernal and I] had a passionate belief that the collective use of data would lead to the discovery of new knowledge which transcends the results of individual experiments’ (Dr Olga Kennard).

This vision led to the founding of the CSD in 1965. From its humble beginnings, the CSD now contains over 1.2 million small-molecule organic and metal–organic crystal structures and is continually growing. Big-data learnings from the collective results are used globally to advance scientific research into pharmaceuticals, functional materials, catalysts and more in both commercial and academic research.

During her 1995 J. D. Bernal lecture, Dr Kennard had no doubt as to the future value of the database:

‘I think that the great ocean of truth is still in front of us and we will continue to discover new aspects of this truth’ (Dr Olga Kennard).

Dr Kennard went on to lead the CCDC until 1997 and authored over 140 structures during her career. One of her first structures with coordinates was published back in 1963 and was a chlorobenzoate salt (CSD refcode MSCBZO). Her more recent examples include a uridine structure, which was published in 1991 (CSD refcode JOSCAV).

Dr Kennard's huge contribution to crystallography was recognized by many prestigious awards, prizes and elections to learned societies.

In 1987 she was elected a Fellow of the Royal Society and, in recognition of her work, there is the Royal Society Olga Kennard Research Fellowship in crystallography.

An OBE for 'Services to Scientific Research on the Structure of Biological Molecules' followed in 1988.

In 1993 Dr Kennard was elected a member of the Academia Europaea, and a Doctor of Law *honoris causa* was awarded to her by the University of Cambridge in 2003.

She won the Gmelin–Beilstein Memorial Medal in 2007, awarded by the German Chemical Society for scientists and scholars who have made an outstanding contribution to the history of chemistry, chemistry literature or chemical information.

In 2020 Dr Kennard was awarded the twelfth Ewald Prize by the International Union of Crystallography (IUCr) 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'.

Recognition for Dr Kennard's huge contribution to structural science continued right up to the end of her life with the award by the Royal Swedish Academy of Sciences of the Gregori Aminoff Prize for 2023 for establishing a crystallographic database. Dr Kennard was due to receive the award at the Aminoff Prize Symposium at the end of March.

This obituary is an edited version of that originally published by the Cambridge Crystallographic Data Centre (https://www.ccdc.cam.ac.uk/discover/news/celebrating-dr-olgakennard-1924-2023/).

OBITUARY

Christer E. Nordman (1925–2022)



Christer Nordman at his desk in 1988.

The Nordman family

Christer E. Nordman, Professor Emeritus of Chemistry at the University of Michigan, Ann Arbor, MI, USA, died peacefully at home on 6 July 2022 at the age of 97.

Christer was born on 23 January 1925 in Helsinki, Finland, to Eric and Gertrud Nordman, the eldest of five children.

He attended Gymnasiet Lärkan secondary school and spent summers in the countryside, fishing, exploring and searching for unusual plants and butterflies. He enjoyed collecting stamps and matchbox covers, chess, building model airplanes and conducting chemical experiments.

As a teenager during wartime, he helped watch for Russian planes overnight from an observation tower and worked at an ammunition factory. At 16, he joined the junior branch of the Finnish volunteer guard. For several months, he rode rural nighttime patrols by bicycle, until stricter age limits were enacted and he returned home.

In 1943, he was drafted into the Finnish Army and sent to the Artillery Training Center in Riihimäki, joining the 17th Heavy Artillery “Tiger” Battalion, 2nd Division, as a radio operator. He was deployed to the front line on the Karelian Isthmus, where he served until the war’s end.

Christer earned a chemical engineering degree from Helsinki University of Technology in 1949, then received a scholarship to attend graduate school at the University of Minnesota, where he studied crystallography under future Nobel laureate William Lipscomb. During this time, he co-authored several publications, including his thesis, *The Crystal and Molecular Structure of Tetraborane*.

After completing his PhD in 1953, he and his new wife, Barbara, moved to Philadelphia, where he was a postdoctoral research associate at the Institute for Cancer Research. In 1955, he joined the chemistry faculty at the University of Michigan, becoming a full professor of chemistry in 1964.

In 1971, he received a National Institutes of Health fellowship for sabbatical study at the University of Oxford, UK, with Nobel laureate Dorothy Hodgkin, and at Uppsala University in Sweden.

Christer’s research focused on X-ray crystallography and computational methods for solving the structure of macromolecules, including viruses, proteins and cholesterol.

He served as a Co-editor (1983–1988) and reviewer for *Acta Crystallographica Sections A*, *B* and *C*; attended IUCr Congresses and ACA meetings; and was a fellow of the American Association for the

Advancement of Science and the Finnish Society of Science and Letters. Students knew him as an enthusiastic crystallography and physical chemistry teacher.

In 1995, Christer retired as professor emeritus, and in 1997 he was honored with the Patterson Award of the ACA for lifetime achievement in his field. Post-retirement, Christer still could often be found in his office on campus working on research. He enjoyed summers in the Finnish countryside, fall apple-picking in orchards near Ann Arbor, and winter cruises with Outi, whom he married in 1994.



Christer Nordman receiving the A.L. Patterson Award from ACA Vice President Penny Codding during the 1997 ACA Annual Meeting. This award is given “to recognize and encourage outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination ...”. Photo contributed to the IUCr gallery by Bill Duax.

Christer is survived by his wife, Outi Marttila-Nordman, and her children Antti Laukkanen (Susanna Melkas), Mari Laukkanen (Kai Schleutker) and Hannu Laukkanen; his sisters Carin Nordman and Bodil Soderberg (Milton); his former wife, Barbara Nordman, and their children Christina Nordman (Gary Dewey), Aleta Adams, Eric Nordman and Carl Nordman (Luisa); grandchildren Andrew Nordman-Kasko (Michele Sedlak), Catherine Bleta (Andy), Ian Adams, Anthony-Emil Nordman, Jacob Nordman and Aaron Nordman; and great-grandchildren Ethan, Avalon, Owen and Brysen.

Christer was predeceased by his father, Eric Johan Nordman; mother, Gertrud (Nordgren) Nordman; sisters Gunilla Nordman and Inger Genberg; and granddaughter Anika Nordman.

This obituary was originally published in The University Record of the University of Michigan.

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

OBITUARY

Alexei Vagin (1944–2023)



Alexei Vagin against a background of a protein structure solved using *BALBES*. Two papers co-authored by Dr Vagin are in the top 10 most cited articles in *Acta Cryst. D*.

Eleanor Dodson

Doctor Alexei Vagin, who died on 25 March 2023, contributed greatly to the practice of X-ray crystallography for over 50 years. He organized the (sparse) computing services of the protein group at the Moscow Institute of Crystallography during the 1970s and 1980s, then after his move to Western Europe in 1994, made major software contributions for macromolecular structure solution, all now distributed through CCP4.

Alexei was born in 1944 in Perm, the most easterly city in Europe, located in the Urals near the natural borderline between Europe and Asia. His family had been evacuated there during the war, but they returned to Moscow for his education. For his degree he studied applied physics at the prestigious Moscow Engineering Physics Institute, specializing in mathematical techniques and computer programming. He started his scientific career in material science – his first publication in 1966 was concerned with the design of blast furnaces, but soon he became more interested in crystallographic method development and moved to the protein group of the Moscow Institute of Crystallography. He was part of the team that solved the structures of bacterial ribonuclease in 1977, catalase in 1979 and was the key player behind the computational part of the latter project where he applied non-crystallographic symmetry (NCS) for phase improvement. From then on, he was involved in almost all the protein structure analyses in the laboratory, developing and implementing many tools. Unfortunately, most of these developments were never written up as Alexei always considered this part of science too boring, a sentiment to which he was loyal for the most part of his life. His PhD thesis, awarded in 1982, described an improved and faster translation function for use in molecular replacement calculations. He organized the software into *BLANC*, a comprehensive package with almost all necessary programs and libraries for crystallographic calculations, from experimental phasing to molecular replacement and map calculations. Considering that there was an embargo on computing resources for all of the Soviet Union, and those available to the institute were scarce, he had to come up with and implement clever algorithms that were both fast and used limited amount of RAM.

In 1990 the scientific scene in Moscow changed dramatically. Funding there became tighter and as the Iron Curtain dissolved it was possible for Russian scientists to move to laboratories in the West with better funding and equipment for science. Many laboratories worldwide benefitted greatly from this influx of well trained, motivated young people from the Moscow Institute (especially the York Structural Biology Laboratory!) but it meant Alexei was witnessing the decline of a great institute. In 1994 he joined the exodus, taking an EU-funded position in Brussels as a member of the team working on *CRITQUAL*. The

Biotech contract he joined was entitled: ‘Integrated procedures for recording and validating results of 3D structural studies of biological macromolecules’. It brought together in a complementary manner several established European laboratories working in the field of macromolecular 3D coordinate provision and analysis. The insights provided into each other’s practices, working approaches and problems proved invaluable. This contract was a delight – all the participants were excited by the challenge and the six-monthly face-to-face meetings positively ‘fizzed’. Atomic resolution structures solved in Hamburg revealed that some of the underlying assumptions about protein conformation derived from the existing databases developed in the EBI and Uppsala were sometimes too restrictive, and Alexei in Brussels was able to quickly recast the new insights into a well designed computer readable form to be used within the refinement program framework being developed in York. He found an elegant solution to the problem of describing ‘LINKS’ – between peptides, nucleic acids, and to covalently linked ligands. The restraint formats (mmCIF) he helped design are now accepted as standard.

In 1998 when the Brussels funding was exhausted, he moved to York and re-joined an active crystallographic laboratory, where he stayed until his retirement in 2010. This was a wonderfully productive period for him, and the community of structural biologists continue to benefit from his work. The program *SFCHECK* developed in Brussels to assess the quality of the agreement between model and experimental data was modified for inclusion in the *CCP*4 suite. He contributed to further developments of *REFMAC*, advised laboratory members on programming problems, structure solution and partying. He was a highly sought-after tutor for training workshops, guaranteeing excellent teaching and good fun for all. But his life-long passion was for improving the methodology of molecular replacement. At one period when both Alexei and Jorge Navaza, the author of the *AMoRe* package, were working in York, it was tremendous fun to hear their on-going debates ranging from ‘what are the best scoring functions?’, to ‘why my fast Fourier routine is faster than yours... ’. In 1997 he published a description of a ‘new’ package, *MOLREP*, in the *Journal of Applied Crystallography* before releasing it through *CCP*4. It was in fact partly a reissue of much work he had done in Moscow, dating back to his 1982 PhD thesis, and partly described in the Russian journal, *Kristallografiya*.

MOLREP contained many innovative features that exploited information easily obtained from the experiment. For example, the package was able to analyse the model-free Patterson maps to consider non-crystallographic symmetry (NCS) and pseudo-translation if present. Once a search model was selected, *MOLREP* then analysed its shape and modified the search procedures to take this into account. In this package, Alexei introduced a translation function which considered all possible symmetry equivalents together. He also improved methods for searching for multiple copies and checked any solutions against the known NCS. Once a possible solution was found, the program checked whether it would pack, and positioned the symmetry copies to give optimal contacts for an assembly. One distinctive feature of Alexei’s approach to software development was a user-centred perspective and he took pains to report results and data analyses with informative graphs and extensive text. *MOLREP* was an instant hit and is still widely used by crystallographers and electron microscopists. Searching the Protein Data Bank (PDB) for references to it yields the amazing score of 36 223 entries.

Once Alexei was reasonably satisfied with the software, he turned his attention to model selection. A search to match a new sequence against the many structures available in the PDB will often produce many closely related hits. Alexei designed a database, distributed first in the package *BALBES*, and later as *MorDa*. This weeded the hits to include only the best model, and then catalogued whether the model structure existed as an oligomer, whether it could be split into flexible domains, and then used this information to design an optimal search strategy.

Alexei will be remembered for his innovative science, and for his interest in and kindness to his many colleagues, both in Moscow and Europe. But of course, he was not just a scientist and the many friends who mourn him remember his humour, his generosity both at work and play, and his wide-ranging conversations. While still in Moscow, he was one of the very few laboratory members with a car, and he was the one who took his colleagues to the airport for their departure to join various crystallographic laboratories in Europe, USA and Australia. He had no children of his own but was very good with those of

his friends – one of whom, a grown up artist now, designed the *MorDa* icon, a wise friendly cat face. He loved Russian culture and his Russian friends, but never Russian politics. He was rather a citizen of the world with a passion for French chanson and movies, and deeply in tune with British black humour which matched his own. He was also profoundly grateful to the NHS which cared for him until his last moments. But his real homeland was the international community of protein crystallography, and that is where he will be remembered with love and gratitude.

This obituary was originally published in *Acta Cryst*. (2023). D**79**.

For a list of papers by Dr Vagin appearing in IUCr journals click here.

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