INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

Volume 32 · Issue 2

Collected archival edition
Original article text and available illustrations

Contents

Letter from the President

President's Letter – Summer 2024 4

Editorial

Editorial 8

IUCr activities

Introducing the new IUCr logo 11

International Tables Volume I - Foreword 13

International Tables Volume I - Preface 15

Crystallography in Africa

The AfCA collection: Celebrating work published by African researchers in IUCr journals 17

Outreach

LAAAMP news 20

Special report

Adding Open Science to the modern discovery and applications toolbox in crystallography 22

Feature article

“Aperiodic crystal” 26

IUCr journals news

IUCr and ResearchGate announce new partnership for complete journals portfolio 28

Editorial

Beyond publishing: introducing Interviews with authors 29

The importance of international collaborations in science and structural biology 31

Chemistry and crystal engineering 33

Commentary

3D ED/MicroED entering a new era 36

A solid solution to computational challenges presented by crystal structures exhibiting disorder 39

3D electron diffraction goes multipolar 41

Perspectives for infrared beamlines in fourth-generation synchrotron facilities 43

Crystallography in Africa

Bridging continents through crystallography: how AFRAMED is revolutionizing scientific collaboration in Africa 45

Bringing crystallography to the classroom: Kenyan teachers learn to engage students in the wonders of crystals 53

Regional news

Women in Crystallography project 56

Meeting report

25th Heart of Europe Bio-Crystallography meeting 57

SEA COAST 2024: Comprehensive training course in macromolecular structure determination in Thailand 60

Meeting report (IUCr supported)

First Senegalese Day of Crystallography 67

15th Biennial Conference on High Resolution X-Ray Diffraction and Imaging (XTOP 2024) 77

Hot Topics in Contemporary Crystallography 6 (HTCC6) 80

Meeting report

FEBS practical crystallization course "Advanced methods in macromolecular crystallization X" 86

Meeting report (IUCr supported)

11th Zürich School of Crystallography: Bring Your Own Crystals 89

Meeting report

CCDC Science Day 96

History of crystallography

Mineralogists and crystallographers at the Berlin Natural History (Naturkunde) Museum 99

Obituary

Dieter Schwarzenbach (1936–2024) 108

Larry W. Finger (1940–2024) 112

Richard Alexander Pauptit (1954–2024) 115

Stephen Edward Tarling (1960–2023) 118

IUCr supported events

IUCr supported meetings 121

Meetings calendar

Meetings calendar 122

LETTER FROM THE PRESIDENT

President's Letter – Summer 2024



The IUCr Executive Committee in Denver, CO, USA, in July 2024. Front row (l-r): Graciela Díaz de Delgado (Vice President), Santiago García-Granda (President) and Hanna Dabkowska (Immediate Past President). Back row (l-r): Atsushi Nakagawa, Susan Bourne, Trevor Forsyth (General Secretary and Treasurer), Maria Cristina Nonato, Thomas Proffen and Manfred Weiss. Angela Altomare was not present.

Santiago García-Granda

It has been a year since the successful IUCr Congress and General Assembly in Melbourne and we are looking forward to the 2026 event in Calgary. This past year has been one of contemplation of our future as an association, a year of change and renewal.

Our Union is based on the significant personal contributions that have graciously built our organization since 1948. Our Chester office is a key part of our functioning, maintaining our activity and planning our future, our resources and optimizing our funding sources to carry out the good works aimed at promoting and defending structural science globally. At the end of May, our Outreach Officer since 2014, Michele Zema, concluded his contract after 10 years of excellent contributions to the IUCr. These contributions have marked a new era in the collaboration and promotion of structural science mainly in Africa, Latin America and Asia, bringing in a substantial amount of funding and creating successful initiatives such as the 'OpenLabs', new labs with modern equipment for structural science in less-developed countries and the light sources within the *LAAAMP* project.

The impending retirements of Peter Strickland and Andrea Sharpe will have a great impact on our activity in Chester and bring an extraordinary emotional burden. Peter will retire from his post as Executive Managing Editor in September after 38 years of the highest responsibilities, not only in our editorial team but also in a position of leadership at Chester and at the IUCr. Peter will be impossible to replace and his generosity will surely allow us to continue to count on his advice and help in the time that his new occupations allow him, especially when the tasks in his garden become less intense.

It will be difficult to imagine the IUCr booth at the different congresses without Andrea or without her contribution to the publication of the four issues of the *Newsletter* that we publish every year. Andrea joined the IUCr in 1980 as an Editorial Assistant, left in 1990 and returned in 1998 as the Promotions Officer; her retirement completes a career of nearly 36 years of service.

We will always be indebted to Peter and Andrea (seen below with Michele during preparations for the 2017 Hyderabad Congress), who are part of our brilliant history, and to whom we are deeply grateful for having dedicated such an important part of their lives to the service of the community of structural scientists.



L-r: Mike Dacombe (former IUCr Executive Secretary), Peter Strickland, Gautam Desiraju (former IUCr President), Jonathan Agbenyega (former IUCr Business Development Manager), Andrea Sharpe and Michele Zema outside the IUCr offices in Chester, UK, in October 2016.

In this first year between Congresses the scientific protagonism lies with our Regional Associates (RAs). The American Crystallographic Association gathered in Denver, CO, USA, in July; the European Crystallographic Association will meet in Padova, Italy, in August; the Latin American Crystallographic Association will meet in Montevideo, Uruguay, in September; and the Asian Crystallographic Association will meet at the beginning of December in Kuala Lumpur, Malaysia. The African Crystallographic Association will meet in Algeria in April 2025.

It is pleasing to note that the 18th European Powder Diffraction Conference (EPDIC18) is being organized jointly with ECM34 in Padova. This arrangement is very satisfying for both organizations as they have common interests, and worked well when EPDIC12 overlapped with ECM26 in Darmstadt in 2010. The attendance will benefit from the joint organization.

Although the Executive Committee (EC) will be represented at all regional meetings at the highest level, this year the EC and the Finance Committee (FC) met in Denver at the 74th ACA Annual Meeting. Given the importance of the upcoming IUCr Congress and General Assembly to be held in Calgary, Canada, in August 2026, this visit and the meetings with the ACA Council and the IUCr2026 Organizing Committees were essential. In particular, it was important to discuss the plans for the formation and the work plan of the International Program Committee and other organizational and financial issues.



IUCr EC/ACA Council/IUCr2026 Organizing Committees meeting in Denver, CO, USA, in July 2024.

All the discussions took place in a splendid atmosphere and at a high scientific level, and the participation of the young generation of structural scientists was excellent. Learning about the many initiatives that the ACA is putting in place was also extremely satisfying for the IUCr EC. A closer collaboration between the RAs and the transfer of good practices between the different regional and national associations was found to be desirable.

In parallel, the FC analysed the Union's financial situation and adopted cost containment measures for 2024 and 2025, pending growth of our publishing revenues. Decisions were also taken on the investment of our funds and the desirability of augmenting the FC with new advisors to complement the current profiles and contribute to the diversity and rejuvenation of the committee.



The IUCr Finance Committee in Denver, CO, USA, in July 2024. L-r: Joe Ferrara (adviser on investments), Hanna Dabkowska, Malcolm Cooper (Convener), Santiago Garcia-Granda (President), Alex Stanley (present in her capacity as IUCr CEO), Andrew Allen (Editor-in-Chief of IUCr Journals) and Trevor Forsyth (General Secretary and Treasurer). Bo Brummerstedt Iversen and Mike Glazer were not present.

At the moment, 55 National Committees make up the IUCr General Assembly. Until the goal of incorporating all countries where there are structural scientists is achieved, the Associates Programme is an excellent way to become an individual member of the IUCr and enjoy the benefits associated with publishing in the 10 IUCr journals and other advantages that will be progressively increased, especially for younger Associates.

Now that the statutes of the International Science Council (ISC) have been approved and the election of the Elections Committee has taken place, the election process for the renewal of the ISC Governing

Board has started. The IUCr, together with the other ISC member unions, is promoting a candidacy that defends the philosophy of rigorous and global science that the scientific unions promote.

Once again, many thanks to all those who form and make our organization work: the RAs, the IUCr Commissions and Committees, Editors, Co-editors, referees and authors of our journals, our Chester staff and all individual crystallographers, women and men.

Thanks to *IUCr Newsletter* Editor Mike Glazer, his team, with one special mention to Andrea, and all contributors for making possible, as every quarter, a new quarterly issue and for continuing to be the communication reference for our community.

Many thanks to all for helping to sustain and reinvent the IUCr from wherever you are in the world.

Enjoy your summer holidays!

EDITORIAL

Editorial



Mike Glazer

The *IUCr Newsletter* has developed its personality over the last few years, starting as a paper journal distributed to crystallographers and others worldwide and becoming the current online journal. As editor of the *Newsletter*, I have been lucky to receive enormous help from the IUCr staff at Chester (UK), especially from Andrea Sharpe, the Promotions Officer. Without her hard work, the *Newsletter* would never have become the success it is today. But time marches on, and Andrea is now retiring from the IUCr, and I shall be sorry to see her go. Let me take this opportunity to express my personal gratitude and thanks for her support over the last few years.

Another loss to the IUCr is Michele Zema, who left at the end of May. Michele performed the task as a kind of ambassador for the IUCr and worked tirelessly to spread crystallography worldwide. For example, in this issue, we have several articles in the Crystallography in Africa category, for which Michele played a significant role:

Bridging continents through crystallography: how AFRAMED is revolutionising scientific collaboration in Africa by Rim Benali-Cherif and Eric Ziki

Bringing crystallography to the classroom: Kenyan teachers learn to engage students in the wonders of crystals by Patricia W. Gitari and Martin N. Mbugua

First Senegalese Day of Crystallography by Magatte Camara, Ibrahima Elhadji Thiam, Rokhaya Sylla Gueye, Mbossé Ndiaye Gueye, Adama Sy, Farba Bouyagui Tamboura, Emmanuel Wenger and Claude Lecomte

Foreword to the AfCA collection: Celebrating work published by African researchers in IUCr journals by Susan A. Bourne, Delia A. Haynes and Michele Zema



Michele Zema (in orange on the left) jumping for joy at the 2017 OpenLab Senegal.

And then there is Peter Strickland, Executive Managing Editor of the IUCr, who is about to retire. I have known Peter ever since he joined and have always been impressed by his knowledge, devotion to the IUCr and his profound ability in managing the production of our journals. I think it will be difficult to find a replacement, and I am sorry to see him go.

I am also grateful to the Hargittais, who have constantly supplied us with fascinating articles for each issue. This time, there are two articles: one on aperiodic crystals and the other on the Berlin Natural History Museum, and the scientists and crystallographers celebrated there. I have a personal interest in the history of crystallography, and I welcome these contributions. I hope you too find them interesting.

In this issue, several reports from around the world illustrate how vibrant our subject is after such a long history. This history goes back hundreds of years, possibly thousands (see https://www.iucr.org/news/newsletter/volume-26/number-2/wrestling-with-questions-at-the-edge-of-science-methods). Crystallography can be seen to be developing well in Africa (see above) and in places like Thailand.

One of my sad tasks in each issue is the need to publish obituaries, often of people I have known for years. This time, Stephen Tarling and Larry Finger were both well known within the crystallography community. Larry was a genius who revolutionised the use of computers in our subject. Crystallographic research relies heavily on the use of software and computer-aided equipment. Today, such tools have become commonplace, so much so that many crystallographers are unaware of the science behind their automatic machines. Larry worked before such automation existed and built a computer that became the mainstay for many crystallographic laboratories worldwide. He even built the PDP11 and Microvax computers used for the beamlines at the Brookhaven synchrotron light source from spare parts.

Stephen Tarling was a clever researcher with an engaging and somewhat eccentric sense of humour. As such, he was always a pleasure to work with. My interactions with him were mainly through working with him as expert witnesses in patent litigations (in one case, we came up on opposite sides!). These were court cases, mainly in the USA, in which the financial stakes were very high, and, as a result, arguments in court could often be fraught and bad-tempered. When confronted by some of the most highly paid and artful lawyers, one had to develop a thick skin to stand up to aggressive examination. The first of these cases was on an antibiotic called cephadroxyl monohydrate. The main item of contention related to the argument that the crystal structure of this material, prepared initially under a lapsed patent, was no longer possible to obtain. Instead, a new form was developed and covered by a new patent. The

argument was exceedingly complex, and I can't provide details here. But, this was, I believe, one of the first cases where the subject of "disappearing polymorphs" was raised. This is where the crystal structure of a pharmaceutical, for some reason, changes, and one is subsequently not able to recover the original structure. There were many anecdotes of such peculiar behaviour in the literature, but none had been proven. Below, for your entertainment, I attach a screen image of a paper published in 1975 in the *Journal of Applied Crystallography* by Woodard and McCrone, in which many unusual and intriguing examples are described.



342 LETTER TO THE EDITOR

Letter to the Editor

J. Appl. Cryst. (1975). **8**, 342

Unusual crystallization behaviour

Sir,

There are many instances, some reported in the literature, and many others not, of crystalline compounds behaving respectably for many months or years until nucleation of a more stable form. After this occurs, the previously obtained crystal form cannot be made to crystallize often even in laboratories many miles away. We have recently encountered such an event and became interested in the prevalence of such behaviour. The results were so interesting to us we felt your readers might be equally interested.

The compound that started us on this search is ampicillin, 6-[D(−)-α-aminophenylacetamido]penicillanic acid. It is readily crystallized as a trihydrate or anhydrous (two polymorphs). Early workers (Doyle, Foster, Naylor & Smith, 1962; Grant & Albuin, 1965) obtained a monohydrate. Later the trihydrate was obtained and the later workers then disputed the earlier existence of a monohydrate (Austin, Marshall & Smith, 1965). Certainly no one has reported crystallization of the monohydrate despite persistent efforts since the trihydrate appeared. This seems to us to be a case of nucleation of a more stable form (trihydrate), ubiquitous nuclei of which preclude subsequent formation of the monohydrate. We have been able to find a large number of parallel cases. It seems to us important that crystallographers recognize this phenomenon as an important and relatively common behaviour. We would like to cite a few examples.

Ethylenediamine tartrate was recrystallized routinely on a large scale as a commercial piezoelectric (anhydrous) crystal (Weiden & Singer, 1960). After four years of research and production a monohydrate nucleated and grew preferentially. Soon the affliction spread to a second plant many miles away.

D-galactono-γ-lactone apparently crystallized only in an anhydrous form until a monohydrate nucleated (Richtmeyer, Hann & Hudson, 1938) and since that time the anhydrous form has not been reported. Xylitol, first prepared in 1891, was considered a liquid until 1941 or 1942, when a form melting at 61°C crystallized (Wolfrom & Kohn, 1942). These experiments were successfully repeated by Carson, Waisbrot & Jones (1943) and in the course of further recrystallizations a new form, melting at 94°C, crystallized. Subsequent attempts to prepare the lower melting form were unsuccessful (Kim & Jeffrey, 1960).

A number of additional examples are known among the sugars. β-D-Mannose was prepared without difficulty (Hudson & Yanovsky, 1917), but in 1934 the α-form was prepared (Lavene, 1936) and subsequent crystallization by the normal route for the β-form gave instead the α-form. Melibiose was first isolated in the β form as a dihydrate (Bertholet, 1902), melting at 83°C. This preparative method was repeated and an α-form monohydrate crystallized (*Ind. Eng. Chem.* 1953), melting at 178–181°C. Similar results were reported later (Wolinsky & Smith, 1958).

Turanose was officially described as a liquid but eventually it crystallized and has done so ever since (Powers, 1971). Benzosphenone behaved similarly to turanose. Levulose existed for years as a viscous liquid until Jackson crystallized it and it has readily crystallized everywhere in the world since the first nucleation. α-D-lyxopyranose tetrabenzoate was crystallized as a form melting at 151–151°C. Later, a form melting at 138–139°C was isolated and spontaneously appeared in subsequent crystallizations (Fletcher, Moss & Hudson, 1951).

Bavin (1959) reported a 115–116°C m.p. for 10 methylbenzochrysene but after seeding with a 150°C melting form obtained elsewhere (Bradshaw & Rapoport, 1944) he was never able to obtain the lower melting form.

Many other examples could be cited – glycerin, gossypol, pentaerythritol etc. The phenomenon is apparently widespread. Most interesting to us is the fact that once one laboratory has serendipitized a compound, either for the first time or in a more stable form, other laboratories were able to do so. As Seyler picturesquely commented, 'as though the seeds of crystallization, as dust, had been carried upon the winds from end to end of the earth'.

We wish to acknowledge the help of M. Bavin, W. M. D. Bryant, H. G. Fletcher, B. H. Harbottome, F. T. Jones, C. W. Mason, H. Powers, N. Richtmeyer and C. P. Seyler in compiling these examples.

GODFREY D. WOODARD
McCrone Research Associates Ltd
2 McCrone Mews
Ballsbridge Lane
London NW3 5BG
England

WALTER C. MCCRONE
Walter C. McCrone Associates, Inc
2820 South Michigan Avenue
Chicago
IL 60616
U.S.A.

(*Received* 31 January 1974; *accepted* 27 December 1974)

References

Austin, K. W. S., Marshall, A. C. & Smith, H. (1965). *Nature, Lond.* **206**, 999–1000.
Bavin, M. (1959). *Canad. J. Res.* **37**, 2029.
Bertholet, M. (1902). *Z. Ver. Zuckerind.* **39**, 1078.
Bradshaw, C. K. & L. Rapoport, (1944). *J. Amer. Chem. Soc.* **66**, 1261.
Carson, J. F., Waisbrot, S. W. & Jones, P. T. (1943). *J. Amer. Chem. Soc.* **65**, 1773–1778.
Doyle, P. F., Foster, G. R., Naylor, J. H. C. & Smith, H. (1962). *J. Chem. Soc.* pp. 1440–1444.
Fletcher, H. G. Jr, Moss, R. K. & Hudson, C. S. (1951). *J. Amer. Chem. Soc.* **73**, 3698–3699.
Grant, N. H. & Albuin, H. E. (1965). *Nature, Lond.* **207**, 645–646.
Holden, A. & Singer, P. (1960). *Crystals and Crystal Growing*, pp. 79–83. New York: Doubleday.
Hudson, C. S. & Yanovsky, E. (1917). *J. Amer. Chem. Soc.* **39**, 1032–1026.
Ind. Eng. Chem. (1953). **45**, (December), 11A–12A.
Kim, H. S. & Jeffrey, G. A. (1960). *Acta Cryst.* **13**, 2607–2611.
Levene, P. A. (1936). *J. Biol. Chem.* **114**, 419–420.
Powers, H. (1971). *Z. Zuckerind.* **21**, 272–277.
Richtmeyer, W. L., Hann, R. M. & Hudson, C. S. (1938). *J. Amer. Chem. Soc.* **61**, 340–343.
Wiegerly, P. & Smith, F. (1958). *J. Org. Chem.* **24**, 124–125.
Wolfrom, M. L. & Kohn, E. J. (1942). *J. Amer. Chem. Soc.* **65**, 1739.

When Stephen and I first became involved, the idea seemed so unlikely, but as the case evolved, the evidence for it became firmer. At one stage, I recall a long discussion in court and with lawyers about the so-called seeding hypothesis, in which seeds of crystallisation are spread around the world: I recall a discussion on the last breath of Henry VIII! I also was grilled for roughly an hour by a particularly aggressive and feared lawyer about whether two powder diffraction experiments could result in an exact match in the diffraction patterns. I maintained that it was impossible to be exactly the same, but this meant holding out under an intense barrage of questioning. Funnily enough, this same lawyer approached me at the end of the day, shook my hand and told me how much he had enjoyed the argument. At a later stage, I received a phial from the Organic Chemistry Department in Oxford containing a liquid with crystals at the bottom. X-ray diffraction suggested that the material was of the old form. But also very quickly, new crystals formed on the surface of the liquid, which were of the new form. This established that such weird phenomena can and do occur, and today, the idea of the so-called "disappearing polymorphs" is now more accepted. Stephen and I flew back and forth (sometimes on Concorde!) to the USA, and we had a great time together. I am sorry to hear of his demise.

News has reached us of the recent deaths of two other stalwarts of the crystallography community, Richard Pauptit and Dieter Schwarzenbach. Their obituaries are included in this issue.

IUCR ACTIVITIES

Introducing the new IUCr logo

After the celebrations of the 75th anniversary of the IUCr in 2023, it was time to acknowledge our past, celebrate our achievements and plan for our future. As such, it was decided that the IUCr should re-visit not only our brand but also our purpose, vision and value statements. Members across the world contributed to this exercise via two surveys and a well-attended workshop during the 2023 Congress, held in Melbourne, Australia. The new purpose and vision statements have been formally adopted as follows:

Purpose Statement: To advance structural science globally

Vision Statement: To empower a thriving structural science community

And, in support of our vision and purpose statements, the **IUCr Values** have been prioritised as follows:

We exemplify scientific excellence and rigour

We operate responsibly, sustainably, ethically and with integrity

We are diverse, inclusive and welcoming to all

We are future-focused and innovative

We collaborate widely and champion the next generation

These statements and values were developed to reflect the organisation’s commitment to its members and its role in advancing crystallography and sharing knowledge globally. In practice, these aspects are delivered through our ethical publishing strategies, outreach commitments and the organisation and support of meetings, workshops and schools.

The new logo and branding

It is intended that this refreshed logo and branding reflect a modern-day scientific union that has a wide appeal to a variety of audiences beyond the traditional idea of pure crystallography. The logo does not shy away from our name and incorporates facets of a crystal or polyhedral shapes observed in crystal packing. The strong connecting lines between these facets symbolise the strong network and community that has been the foundation of our Union and is inherent in our vision and value statements.

This logo was designed by a professional graphic designer, with input and guidance from the IUCr Executive Committee, IUCr Chester staff and members of the Journals Management Board. After several iterations and reviews, we are proud to present this new logo in 2024, giving the IUCr an updated identity alongside the purpose, vision and value statements.

Over the coming weeks and months, we will be updating our online presence with this new logo, and we encourage you to support this by downloading the logo pack and updating the IUCr logo your own webpages where necessary.

As we embark on this exciting new chapter with our refreshed logo and branding, we remain steadfast in our dedication to serving you, our valued members, in every endeavour we undertake to advance the field of structural science. Your ongoing support and collaboration are the driving force behind our mission, and we look forward to continuing this journey together towards new discoveries and innovations in crystallography.

Download the logo pack from here. Please direct any questions or feedback to marketing@iucr.org.

IUCR ACTIVITIES

International Tables Volume I - Foreword



Sofia Diaz-Moreno

The following article appears as the Foreword to Volume I of International Tables for Crystallography, X-ray Absorption Spectroscopy and Related Techniques.

Volume I of *International Tables for Crystallography*, *X-ray Absorption Spectroscopy and Related Techniques*, is a welcome and very timely addition to this encyclopaedic series of volumes, fitting well with the statement of purpose of the International Union of Crystallography (IUCr), 'Advancing structural science globally', that was revisited as part of the 75th anniversary of the organization in 2023. X-ray absorption spectroscopy (XAS) and related techniques such as X-ray emission spectroscopy (XES) complement other structural techniques that are the subject of previous volumes well, expanding the reach and coverage of *International Tables*.

Although there are many excellent books and manuals describing XAS and related techniques, including both practice and theory, there are none as complete or comprehensive as Volume I. The range of topics covered by the present volume is extremely extensive, from the instrumentation needed to perform the experiments, describing the data reduction and analysis, discussing important considerations when preparing samples, presenting theoretical approaches and the statistical significance of the results, and highlighting applications. Each of the nine parts in the volume addresses a specific aspect that is relevant to those who regularly use XAS and related techniques, but also to those who are novices and who would like to understand the potential of using spectroscopy for detailed structure determination. The three Editors have done an exceptional job in attracting many contributions from world experts on the topics covered by the volume, and this is shown in the quality of the final product. The overall result is a very coherent and self-contained volume.

I believe the contents of Volume I will attract interest from a wide variety of researchers. Scientists working on synchrotron beamlines will find that the *Experimental methods* part (Part 3) is an excellent manual describing the instrumentation needed to perform X-ray spectroscopy measurements, and the detectors needed for optimal experiments. It will also serve as a guide for experimentalists interested in improving data quality by optimizing sample preparation and data-collection methods. For those more interested in the fundamentals of the technique, I would recommend Part 2, *Theory*, which includes the theoretical approaches and approximations most often used for the interpretation of XAS and other techniques such as diffraction anomalous fine structure and X-ray magnetic circular/linear dichroism. In my opinion, researchers interested in using XAS for the first time will enjoy Part 5 (*Analysis of experimental data*), which is an excellent compendium of the many steps required for XAS data reduction and analysis. Personally, as a spectroscopist and expert XAS and XES user, I have found Part 6, *Packages*

and approaches for data collection and data reduction, very useful. Descriptions of many of the most frequently used software packages for XAS and XES data analysis and simulations are included, with most of the chapters written by the developers of the codes, and openly discussing their strengths and their limitations. This is a unique feature of the volume, and no other publication exists where all this information can be found in one place. The *Applications* part (Part 8), which focuses on examples showing the applicability of the techniques, will attract the interest of scientists working in many different scientific areas, from catalysis to battery materials, environmental science, bioscience, cultural heritage and many more.

Volume I is consequently a very comprehensive compilation of the fundamentals, state of the art and future directions of XAS and related techniques. I have every expectation that it will become a classic reference text for any expert in the field, but also as a starting manual for those who would like to learn more about the techniques and use them in their research.

Volume I of *International Tables for Crystallography*, *X-ray Absorption Spectroscopy and Related Techniques* is available in print and online. Authors, IUCr Associates and individuals are eligible for a discount on the price of print copies. Please see ordering information here.

IUCR ACTIVITIES

International Tables Volume I - Preface



Chris Chantler holds a collection of sample chapters at the IUCr Congress in Melbourne, Australia, in August 2023.

Christopher T. Chantler, Federico Boscherini, Bruce Bunker

The following article appears as the Preface to Volume I of International Tables for Crystallography, X-ray Absorption Spectroscopy and Related Techniques.

In May 2010, during a meeting of the International Programme Committee for the Twenty-Second Congress and General Assembly of the International Union of Crystallography (IUCr), discussions started between C. J. Gilmore and Isabella Ascone (then Chair of the IUCr's Commission on XAFS) about the possibility of including XAFS-related information in a new volume of *International Tables for Crystallography* that would cover mainly powder-diffraction techniques. After the IUCr decided to dedicate one volume to powder diffraction (subsequently published in 2019 as Volume H of the series) and a separate one to the XAFS technique, the Commission on XAFS submitted a detailed document with suggestions for the content of this Volume I to the IUCr Editorial Office at the beginning of December 2010.

This first proposal was composed primarily by I. Ascone with assistance from C. T. Chantler (then Secretary of the Commission). As Chair of the Commission, I. Ascone started many challenging projects, including looking at XAFS data formats, the standardization of XAFS experimental procedures, contributing XAFS-related definitions to the IUCr's Online Dictionary of Crystallography at https://dictionary.iucr.org ('the XAFS dictionary'), work towards this volume of *International Tables*, and fostering close cooperation with other IUCr commissions and with the International XAFS Society (IXAS) at IUCr Congresses and in the organization of workshops. These projects progressed well as the XAFS Commission was a highly functioning team. The data-format work led to the inauguration of a series of Q2XAFS (Quality and Quantity in XAFS Spectroscopy) conferences as a joint project with IXAS, then led by Hiroyuki Oyanagi, resulting in many publications in IUCr journals as an outcome of the meetings.

Great support for the *International Tables* project was provided by the IUCr Executive Committee, including Sine Larsen and M. L. Hackert; Michael Dacombe; Samar Hasnain; and indeed the Chair of the Commission on *International Tables*, Carol Brock. From early on, it was planned that, as far as possible, different experimental and theoretical backgrounds and regional approaches should be presented, in particular to bring the whole international XAFS community together to share their amassed knowledge. In 2013, three editors for the volume were appointed: Professor Christopher Chantler (Australia), Professor Bruce Bunker (USA) and Professor Federico Boscherini (Italy). The final version of the proposal

for the volume was approved by the IUCr's Executive Committee in 2014. The first submissions started to arrive in 2015 and were subsequently fully reviewed and revised before acceptance.

Many chemists, bioscientists and crystallographers often need the supporting evidence and investigations afforded by XAS and XES. Our deliberate purpose is that this volume should be self-contained and, as far as possible with any developing live technique, we intend it to be complete. It has been written for the worldwide XAS community of thousands of practitioners, user communities, beamline scientists, experts and academics, and for the neophyte user who wishes to know what XAS and XES can do for them and how they may use these techniques for their particular purposes. The volume is therefore intended to be an authoritative resource that can be used for training, learning or teaching, providing practical guidance for readers of all levels of experience. It also provides full discussions of the many questions and practical issues that can arise at all stages of XAS or XES experiments and data processing. In addition, it can simply be used as a reference work like a normal *Handbuch* or encyclopaedia, and dipped into for insightful discussion of or solutions to problems or questions.

There are smaller-scale works, including textbooks and books, that have provided much insight into XAS and XES, but there is certainly a need for an authoritative and more comprehensive summary such as the present volume. Several authors of these valuable smaller or focused works are also authors of chapters in this volume, which has thus benefitted from their expertise.

The Editors would like to express particular thanks:

To all the expert authors and referees who have contributed outstandingly to so much of this work, and in some cases have not lived to see the fruition of their extensive efforts.

To our fellow Editors, without whom this would not have been possible. We have worked collaboratively and collegially on all aspects of the project.

To the team at the IUCr's Editorial Office (Simon Glynn, Nicola Ashcroft and Peter Strickland) for their many hours, months and years of work. We are amazed at their continued energy, enthusiasm and the level of care they have shown for the project.

To Isabella Ascone, whose drive and initiative inspired the Commission, IXAS and the push towards producing this volume.

To Ted Maslen, who guided many of us within and outside crystallography towards the path of accuracy and insight in science.

To the close and warm relations between crystallography, X-ray spectroscopy and all techniques, that we may understand one another better!

Volume I of *International Tables for Crystallography*, *X-ray Absorption Spectroscopy and Related Techniques* is available in print and online. Authors, IUCr Associates and individuals are eligible for a discount on the price of print copies. Please see ordering information here.

CRYSTALLOGRAPHY IN AFRICA

The AfCA collection: Celebrating work published by African researchers in IUCr journals



Susan A. Bourne, Delia A. Haynes, Michele Zema

The AfCA–IUCr Virtual Collection is a celebration. It is a celebration of crystallography in Africa, and a celebration of the international crystallography community. It commemorates the founding of the African Crystallographic Association (AfCA), which was accepted as the newest Regional Associate of the International Union of Crystallography (IUCr) in 2023, the year of the 75th anniversary of the first IUCr Congress and General Assembly. The collection contains research articles authored by scientists across the African continent, as well as a selection of articles giving context to crystallography in Africa. These discuss history, collaboration between scientists and between associations, and various educational and outreach initiatives.

Africa is a fascinating and diverse continent. It has the world's youngest population, more than 50 countries, well over 1000 languages and a wealth of natural resources. Despite this huge potential, Africa is the least wealthy continent *per capita*, and science remains underdeveloped on the continent as a whole. There are many complex reasons for this. For example, it is interesting to note that in 1947, when the IUCr was founded, only five African countries were not colonies. Recent years have shown great developments in science in Africa, often driven by African scientists who want to develop African solutions to African and global problems.

As all crystallographers know, crystallography is a key science, underpinning developments in a variety of diverse fields from biology to mineralogy and materials science. The potential of crystallography to make key contributions to addressing a variety of challenges is undisputed. There is therefore great value in developing crystallography as a science in Africa.

Through the support of crystallographers worldwide, particularly under the auspices of the IUCr and its Crystallography in Africa initiative (Lecomte, 2017), and of the European Crystallographic Association (ECA), the teaching and use of crystallography on the African continent is growing and developing at a rapidly increasing rate, which is evidenced by the articles in this collection. There are regular schools and workshops across the continent, and the IUCr–UNESCO OpenLabs (Zema & Lecomte, 2015; Zema *et al.*, 2017) continue to be extremely successful. Through this initiative, crystallographic educational and research centres are being implemented at existing centres of competency. Building on the expertise gained through these actions, brand new developments are being established promoting regional research excellence and capacity building in multidisciplinary research based around a new well-equipped X-ray laboratory. These new facilities become a hub for regional excellence. This is the

case for the X-TechLab project at Sèmè City in Benin (Agbahoungbata *et al*., 2021), which is an outgrowth of the IUPAP–IUCr–ICTP Lightsources for Africa, the Americas, Asia, Middle East and Pacific (*LAAAMP*) initiative (Scandolo *et al.*, 2017) in collaboration with the government of Benin.

Four new crystallographic associations have been inaugurated in Africa in recent years (Senegal, Gabon, Republic of Congo and Ivory Coast). There are also regular scientific meetings and conferences involving crystallography around Africa. The Pan African Conference on Crystallography (PCCr) series is now well established, with PCCr4 set to take place in Algeria in 2025. The COVID-19 pandemic actually had some positive outcomes in terms of the development of crystallography in Africa – the increased use of online tools enabled African crystallographers to meet and network much more easily, rapidly advancing the formalisation of a crystallographic association. Thus, AfCA was officially launched in 2021. In 2023, at the General Assembly of the IUCr in Melbourne, AfCA was accepted as the fifth Regional Associate of the IUCr. This is a truly significant milestone for crystallography in Africa.

The history of AfCA has involved a long road and a lot of hard work by many people around the globe. In his article ‘When a dream comes true: birth of the African Crystallographic Association (AfCA)’, Andreas Roodt tracks this history (Roodt, 2024). He begins with the early days of crystallography in northern Africa (Egypt, Tunisia, Algeria and Morocco) and South Africa, highlighting the role played by various individuals, and by the IUCr, particularly through the IUCr Crystallography in Africa initiative and the International Year of Crystallography in 2014.

As pointed out by Roodt, access to infrastructure is a significant challenge to many crystallographers in Africa. Not only is acquiring instrumentation difficult, but stable electricity and water supplies cannot always be taken for granted. In addition, research funding is limited or non-existent in many African countries. There are several approaches that African researchers follow to tackle these challenges. One of these is to foster collaborations with institutes that have the required facilities. The benefits of collaboration are elegantly illustrated in the article co-authored by researchers from the universities of Dakar in Senegal and Southampton in the UK (Orton *et al*., 2023). This highly productive collaboration is an example of what can arise from networking between scientists in Africa and those from around the world, as emphasised in the article.

The importance of collaboration is also highlighted in Simon Billinge’s article about JUAMI, the Joint Undertaking for an African Materials Institute (Billinge, 2024). As described by Billinge, JUAMI is a ‘community-building exercise’, and an exciting example of how training and networking can lead to valuable and productive collaboration. The number of exciting projects that have developed from these schools is inspiring. Another recent approach to solving the infrastructure challenge is the concept of a ‘remote lab’. This has been driven by researchers at the University of Lorraine in Nancy, France, and is described in articles in the *IUCr Newsletter* (Abdel-Aal *et al.*, 2023; Benali-Cherif & Ziki, 2024). This project provides intense crystallographic training to researchers at African institutes, who are then able to access a diffractometer remotely and control their own data collections. This approach has been successfully used for teaching at several workshops and OpenLabs. Most excitingly, the first crystal structure obtained using the remote lab concept has been published as part of this collection (Kenfack Tsobnang *et al.*, 2024).

The development of crystallography in Africa is part of a wider drive to develop science in Africa. This strong drive is exemplified by the African Light Source Foundation (AfLS). The progress of the AfLS is presented in the article by Connell *et al.* (2024) in this collection. The article discusses the significant advances made towards building an advanced lightsource on the African continent and highlights the importance of societies working together and the value of science diplomacy.

The first two objectives of the IUCr, as stated in the statutes, are ‘to promote international cooperation in crystallography’, and ‘to contribute to the advancement of crystallography in all its aspects …’. It is clear from this virtual collection that the work of the IUCr in promoting crystallography in Africa is fulfilling these objectives. Despite many challenges, African crystallographers are producing excellent science. Crystallography in Africa has come of age, and this virtual collection reflects that.

References

Abdel-Aal, S. K., Kenfack Tsobnang, P., Bouraima, A., Djifa Hounsi, A., Wenger, E., Bendeif, E.-E. & Lecomte, C. (2023). *IUCr Newsletter*, **31**(1).

Agbahoungbata, M. Y., Bonou, S. A. S., d'Almeida, T., Zema, M. & Borna, C. (2021). *Acta Cryst.* A**77**, C606.

Benali-Cherif, R. & Ziki, E. (2024). *IUCr Newsletter*, **32**(2).

Billinge, S. J. L. (2024). *Acta Cryst.* E**80**, 102–105.

Connell, S., Dollman, K., Kamel, G., Khan, S. A., Mitchell, E., Mtingwa, S. K., Newton, M. C., Ngabonziza, P., Nji, E., Norris, L. & Zema, M. (2024). *J. Synchrotron Rad.* **31**, 1–9.

Kenfack Tsobnang, P., Ziki, E., Siaka, S., Yoda, J., Kamal, S., Bouraima, A., Djifa Hounsi, A., Wenger, E., Bendeif, E.-E. & Lecomte, C. (2024). *Acta Cryst.* E**80**, 106–109.

Lecomte, C. E. P. (2017). *Acta Cryst.* A**73**, C1394.

Orton, J. B., Diouf, N., Gueye, R. S., Gaye, M., Thiam, I. E. & Coles, S. J. (2023). *Acta Cryst.* E**79**, 1109–1114.

Roodt, A. (2024). *Acta Cryst*. E**80**, 94–101.

Scandolo, S., Mtingwa, S. & Zema, M. (2017). *Acta Cryst*. A**73**, C1069.

Zema, M., Desiraju, G. R., Lecomte, C., Nalecz, M. & Ngome Abiaga, J. J.-P. (2017). *Acta Cryst.* A**73**, C363.

Zema, M. & Lecomte, C. (2015). *Acta Cryst.* A**71**, s177.

Susan A. Bourne, Department of Chemistry, University of Cape Town, Rondebosch, South Africa
Delia A. Haynes, Department of Chemistry & Polymer Science, Stellenbosch University, Matieland, South Africa
Michele Zema, IUCr, Chester, UK/Department of Earth and Geoenvironmental Sciences, University of Bari "Aldo Moro", Bari, Italy
Correspondence should be addressed to Professor Haynes at dhaynes@sun.ac.za.

A version of this article will be published in *Acta Cryst. E* as a Foreword to the collection.

OUTREACH

LAAAMP news



LAAAMP call for 2025 FAST Team applications

The International Union of Pure and Applied Physics (IUPAP), the International Union of Crystallography (IUCr) and Abdus Salam International Centre for Theoretical Physics (ICTP) will award Faculty-Student (FAST) Team grants to enhance advanced light source (AdLS) and crystallography sciences in eight targeted regions of the world: Africa, the Caribbean, Mexico, South America, Central Asia, Southeast Asia, Middle East and the Pacific. The successful applicants will spend two months during 2025 at *LAAAMP*'s AdLS Collaborative Partners to acquire expertise in accelerator technology or AdLS beamline techniques, including those involving crystallography.

For more information, including a link to the application form, please see here. Application deadline: **31 October 2024**.

New member of *LAAAMP* Executive Committee

IUCr Vice President Graciela Diaz de Delgado has been nominated by the IUCr as the new IUCr delegate in the *LAAAMP* Executive Committee (EC).



Professor Diaz de Delgado (Universidad de Los Andes, Mérida, Venezuela) is a member of the American Crystallographic Association (ACA) and the American Chemical Society (ACS), and a founding member of the Venezuelan Society of Crystallography and of the Latin American Crystallographic Association (LACA). She is also a Member of the Liaison Committee of the International Science Council (ISC) Regional Focal Point for the Latin American and Caribbean Region. Currently, she serves in the Board of Directors of the International Centre for Diffraction Data (ICDD), and is Section Editor of *Acta Cryst. E.*

All members of the *LAAAMP* EC welcome Graciela and wish her every success in her new role.

The LAAAMP (Light sources for Africa, the Americas, Asia, Middle East and Pacific) project is an international initiative to broaden and democratise the use of synchrotron radiation around the world. This IUPAP–IUCr–ICTP joint programme was started in 2016 through a grant awarded by the ISC. More details can be found on the LAAAMP website.

SPECIAL REPORT

Adding Open Science to the modern discovery and applications toolbox in crystallography



John R. Helliwell

Introduction

Open Science is a movement for change in research practices. It started with open access to publications and is now being significantly elaborated by UNESCO and the International Science Council (ISC). Their approach was explained in a milestone event held in June 2022 [1]. An overarching principle is that taxpayers have paid for research so it should be open by default as its aims are always ultimately for the public good. Over the past few years, an extensive consultation by UNESCO has led them to conclude that it would be best for both the Global South and the Global North to adopt Open Science. Recently, UNESCO held numerous discussions *via* Zoom, which I have attended on behalf of the IUCr. In my Annual Report for the IUCr Executive Committee submitted in April this year, I summarized these UNESCO discussion forums and quote my report below. As these proposals are momentous in scope, I offer this article in the *IUCr Newsletter* to engender wider discussion.

As further background, I recall that UNESCO's Recommendation on Open Science was adopted by the General Conference of UNESCO at its 41st session on 23 November 2021 [2]. The Recommendation affirmed the importance of open science as a vital tool to improve the quality and accessibility of scientific outputs and scientific process, bridge the science, technology and innovation gaps between and within countries, and fulfil the human right of access to science.

UNESCO Working Groups

UNESCO then convened five *ad hoc* Working Groups focusing on key impact areas:

Open Science Capacity Building

Open Science Policies and Policy Instruments

Open Science Funding and Incentives

Open Science Infrastructures

Open Science Monitoring Framework

bringing together experts and open-science entities, organizations and institutions according to their field of activity and expertise.

These Working Groups each had at least three virtual events, some now four, and the recordings are available [3]. A key output is a helpful toolkit [4], which includes a checklist for publishers [5].

A linked event to the UNESCO efforts was a three-day hybrid event on Open Science in February 2023 organized by the UN Library [6]. This event focused on accelerating the UN Sustainable Development Goals (SDGs) and democratizing the record of science.

On behalf of the IUCr, I made specific inputs into these various events on (i) the importance of global collaborative sharing of instrumentation [7] and (ii) a fine example of open science in practice: the ESRF (European Synchrotron Radiation Facility) heritage database for palaeontology, evolutionary biology and archaeology [8]. Basically, so much of these data can be measured quickly at ESRF that Europe's palaeontologists decided to share all their data with the world's palaeontologists to allow analysis of the data as promptly as possible.

Reform of publishing

A specific conclusion from the UN/UNESCO deliberations features the growing importance of, and seeking of funds for, prioritizing diamond (sometimes called platinum) open access for publications. Diamond open access refers to a scholarly publication model in which journals and platforms do not charge fees to either authors or readers, for example see [9]. This approach addresses the challenge perceived by UNESCO for the Global South of article processing charges (APCs) for authors. A group disadvantaged by APCs are researchers from low-to-middle income countries. Fluctuating currency exchange rates can significantly reduce purchasing power. Others disadvantaged by APCs, around the whole world, include retired or out-of-work scientists or even researchers from institutions on restricted budgets. In mid-December 2023, all the above work by UNESCO on open science led to the launch event [10].

Linked with this UNESCO effort is that of the ISC in calling for feedback on the reform of scientific publishing [11], again emphasizing openness. I provided detailed input in consultation with the Editor-in-Chief of IUCr Journals, Andrew Allen, and the Executive Managing Editor, Peter Strickland. This emphasized the importance of pre-publication peer review of articles with a data and checking report, such as the IUCr's *checkCIF* and the Protein Data Bank's Validation Reports, which both ensure trust in our scientific publications. This can still allow for post-publication peer review where necessary *via* refereed critique articles, the process consistently adopted in IUCr Journals. These are, however, a very rare occurrence. Probably the most well known were the space group corrections in crystal structure publications reported by Dick Marsh in the pre-2000s decades.

Industry and the UN SDG 9

UNESCO's work involving industry's needs is not explicitly covered so far. This is important, as recognized by the UN SDG 9 [12]. Indeed, there are aspects of industry's work that can be open, notably at the pre-competitive phase. An example of such collaborative work among companies is the Industrial Macromolecular Crystallography Association (IMCA) Collaborative Access Team at the Advanced Photon Source in Argonne [13].

My critique of some assumptions

Besides not consulting industry, there are also implicit assumptions made by the ISC and UNESCO that are incorrect. Firstly, there is a confusion that FAIR data always equals Open Science. Secondly, there is an assumption that uncertainty estimates on data are somehow unnecessary. Thirdly, they assert that pre-publication peer review is not where proper peer review is done but happens only post-publication. Thus, they confuse reproducibility with replicability, terms that are very well described by the US National Academies report [14]. They even advocate doing away with journals in favour of preprints.

The ISC does realize, though, that different areas of science may vary in their approach [1]. For us crystallographers, the very basis of the crystallographic tradition of careful validation of data underpinning our journal articles, as exemplified by our excellent databases [15], can be argued as the best approach. In other areas of science, such as cognitive neuroscience and the behavioural and social

sciences, pre-registered reports have been introduced [16]. These allow researchers to be open by default because the methods and proposed analyses are pre-registered and peer-reviewed before the research is conducted.

Conclusions

I would stress the following positives that commend adding or expanding Open Science in our research toolbox beyond that already achieved, such as with the IUCr's open-access journals (**IUCrJ**, *Journal of Synchrotron Radiation*, *Acta Cryst. E* and *IUCrData*). I would firstly mention the need to improve how society tackles neglected diseases, such as the Drugs for Neglected Diseases projects [17], where industry is much less interested, if at all, but where a fully open global collaborative approach could deliver hugely. UNESCO, as well as the World Health Organization, is aware that global funding schemes could really help here. Secondly, measured raw data that have not led to eventual publication need opening to wider sharing and exploitation, as led by the EU's PaNOSC project [18]. So, I agree with the funding agencies' push on this front, certainly in Europe and most recently in the USA. Our *IUCrData* Raw Data Letters initiative offers one such route [19].

Also, it is noteworthy that in an extensive 'scoping review', the most impactful domain for Open Science thus far is Citizen Science [20]. So, we can be encouraged to continue and even expand our crystal growth competitions as one of our citizen science project themes and maybe initiate new themes for Open Crystallographic Science. A range of ideas is provided by the Center for Open Science in Charlottesville, VA, USA, *via* their Open Science Framework (OSF). This is a free open-source software project that facilitates open collaboration in science research. It is neatly explained in a 14-minute ‘basics’ video [21]. An easy win in my view of an OSF would be to openly report negative results or outcomes, rather than the generally always positive outcomes in our peer-reviewed publications.

Acknowledgements

I am very grateful to Andrew Allen, Editor in Chief of IUCr Journals; Peter Strickland, Executive Managing Editor of IUCr Journals; Mike Glazer, *IUCr Newsletter* Editor; and Alice Brink, IUCr Committee on Data (CommDat) member, for detailed discussions and comments.

References

1. https://council.science/events/isc-members-session-on-the-unesco-open-science-recommendation/

2. https://www.unesco.org/en/open-science?hub=686

3. https://www.unesco.org/en/open-science/implementation

4. https://www.unesco.org/en/open-science/toolkit

5. https://unesdoc.unesco.org/ark:/48223/pf0000383327

6. https://www.un.org/en/library/OS23

7. Warren, J. E., Diakun, G., Bushnell-Wye, G., Fisher, S., Thalal, A., Helliwell, M. & Helliwell, J. R. (2008). Science experiments *via* telepresence at a synchrotron radiation source facility. *J. Synchrotron Rad.* **15**, 191–194.

8. http://paleo.esrf.eu/

9. *Action Plan for Diamond Open Access*, March 2022. Brussels: Science Europe.

10. https://www.unesco.org/en/articles/open-science-outlook-1-status-and-trends-around-world-0

11. https://council.science/publications/reform-of-scientific-publishing/

12. https://www.un.org/sustainabledevelopment/infrastructure-industrialization/

13. https://www.aps.anl.gov/

14. https://www.nationalacademies.org/news/2019/05/new-report-examines-reproducibility-and-replicability-in-science-recommends-ways-to-improve-transparency-and-rigor-in-research

15. Bruno, I., Gražulis, S., Helliwell, J. R., Kabekkodu, S. N., McMahon, B. & Westbrook, J. (2017). Crystallography and Databases. *Data Sci. J.* **16**, 38.

16. https://www.nature.com/nature/for-authors/registered-reports

17. https://dndi.org/

18. https://www.panosc.eu/

19. Kroon-Batenburg, L. M. J., Helliwell, J. R. & Hester, J. R. (2022). *IUCrData* launches Raw Data Letters. *IUCrData*, **7**, x220821.

20. Cole, N. L., Kormann, E., Klebel, T., Apartis, S. & Ross-Hellauer, T. (2024). The societal impact of Open Science: a scoping review. *R. Soc. Open Sci.* **11**, 240286.

21. Getting to Know the OSF: The Basics.

Emeritus Professor John R. Helliwell, DSc, is IUCr Representative to UNESCO's Open Science Working Groups. E-mail: john.helliwell@manchester.ac.uk

FEATURE ARTICLE

“Aperiodic crystal”



Aaron Klug’s tutorial to Istvan Hargittai in Klug’s office at the MRC Laboratory of Molecular Biology, Cambridge, UK, on 18 February 2000 (taken by unknown photographer).

Istvan Hargittai

'An *aperiodic crystal* is a structure with sharp diffraction peaks, but without lattice periodicity' [1].[1] This is a modern definition thanks to crystallography having become a science of structures, *i.e.* more than what classical crystallography is. As far as I know, the theoretical physicist Erwin Schrödinger (1887–1961) was the first to use the term 'aperiodic crystal' in his most influential book *What is Life?* published in 1944, *i.e.* 80 years ago [2]. The book appeared at a time when the nature of the gene was not yet known but there was intensifying interest and research effort to identify it. Schrödinger’s book pointed to the possibility that the gene may be molecular. In a remarkable coincidence, also in 1944, Oswald T. Avery (1877−1955) and his two associates provided experimental evidence that DNA was the substance of heredity [3].

Schrödinger’s book hinted at the intriguing possibility that, for understanding life, heretofore unknown physical laws might have to be uncovered. This possibility added to the recent lure of biological research, and both established scientists and budding researchers joined in (see *e.g.* [4]). Schrödinger’s ideas have earned much appreciation, but also criticism. Forty-three years after the publication of the book, Max Perutz noted ungenerously that 'what was true in his book was not original, and most of what was original was known not to be true even when it was written' ([5], p. 558).

To Schrödinger, a small molecule would be an initial seed for the gene. Its extension by mere repetition – the way a crystal is formed – could not lead to the gene because periodicity would exclude carrying information. The other way to extend the initial seed molecule would be to build up a complex organic molecule – proteins could be such systems, or DNA as we know it today. DNA, as it was known in Schrödinger’s time, could not be considered the substance of genes as it had been hypothesized to be uniformly repetitive (see *e.g.* [6]).

Curiously but understandably, Schrödinger’s aperiodic crystal has not been related to the aperiodic structures in modern crystallography, *i.e.* quasicrystals and various classes of incommensurate structures. The reason is that the relationship is not functional, merely semantic. However, an interesting analogy may be drawn between Schrödinger’s aperiodic crystal and Aaron Klug’s (1926−2018) idea of the fundamental difference between ordinary polymer molecules and biopolymers. The ordinary polymer consists of periodic repetition of the basic motif whereas the biopolymer has variability. From this, Klug recognized that identifying nucleation, *i.e.* the initial seed, was necessary for understanding the structure of a biopolymer. There was a further lesson in Klug’s discovery. When he put together his Nobel lecture

for publication, the editor wanted him to delete the picture depicting Klug's original idea of nucleation [7]. Klug admitted that it was wrong in detail, but its inclusion demonstrated a process in science of establishing the truth. Klug referred to the philosopher Alfred N. Whitehead (1861−1947), coauthor with Bertrand Russell of the famous *Principia Mathematica*, who said 'It is more important that an idea be fruitful than that it be correct' ([7], p. 313). This may also apply to Schrödinger's aperiodic crystal.

References

[1] International Union of Crystallography (1992). *Acta Cryst.* A**48**, 922–946.

[2] Schrödinger, E. (1944). *What is Life?* Cambridge University Press.

[3] Avery, O. T., MacLeod, C. M. & McCarty, C. (1944). *J. Exp. Med.* **79**, 137–158.

[4] Hargittai, I. (2024). *What is Life?* – 80 years: from Erwin Schrödinger to Paul Nurse. *Struct. Chem.* **35**, 1039–1047.

[5] Perutz, M. (1987). Physics and the riddle of life. *Nature*, **326**, 555–558.

[6] Hargittai, I. (2009). The tetranucleotide hypothesis: a Centennial. *Struct. Chem.* **20**, 753–756.

[7] Hargittai, I. (2002). *Candid Science II: Conversations with Famous Biomedical Scientists*, edited by M. Hargittai, pp. 306–329. London: Imperial College Press. (Conversations with Aaron Klug on 9 October 1998, and in February and March 2000, at the MRC Laboratory of Molecular Biology, Cambridge, UK.)

1For a more recent statement, see the IUCr Online Dictionary of Crystallography: 'In aperiodic crystals (incommensurate and quasicrystals) the arrangement is not periodic in three dimensions but is nevertheless still fully ordered, where the ordering follows particular mathematical rules.'

IUCR JOURNALS NEWS

IUCr and ResearchGate announce new partnership for complete journals portfolio



The IUCr and ResearchGate have announced a new partnership that will drive readership and authorship for the IUCr's full journal portfolio through ResearchGate's innovative Journal Home offering.

This new agreement covers all 10 IUCr journals, both fully open access and hybrid open access. The version-of-record of all content published since 2000 and all newly published articles, encompassing approximately 80,000 articles, will be available through ResearchGate, boosting visibility and readership for structural science research, as well as enabling easier access to subscription content for entitled ResearchGate members.

Through Journal Home, all these journals will gain enhanced global brand visibility through the ResearchGate platform. This increased discoverability and accessibility will grow readership and enable crystallography researchers to more easily find high quality journals for their research. Dedicated journal profiles providing key information and content from the journals will enable ResearchGate members to uniquely explore how their community is connected to a journal. Journal branding will also feature prominently on all associated article pages, and other relevant touch points with members across the platform.

Authors publishing in IUCr journals additionally benefit from having their articles automatically added to their ResearchGate profiles – gaining valuable insights, and deepening their understanding of who is reading and citing their work.

"We're very pleased to be partnering with ResearchGate for IUCr's complete portfolio of journals, supporting our goals to ensure high-quality peer-reviewed structural science research reaches the widest possible community," said Alex Stanley, CEO at the IUCr. "Work published with the IUCr has applications spanning a wide range of scientific research areas. ResearchGate's unique network-based discovery enables these findings to reach new readers and authors and build global reach for our authors and their content."

"ResearchGate is very proud to work with the full portfolio of a publisher that has such high data standards and a long history of high quality publishing," said Sören Hofmayer, co-founder and Chief Strategy Officer at ResearchGate. "Journal Home provides these journals with a unique and innovative way to grow the engagement and community around their authors and content. I look forward to seeing the results from our collaboration!"

For more information about Journal Home, please visit researchgate.net/journal-home.

EDITORIAL

Beyond publishing: introducing Interviews with authors



Maria Cristina Nonato, Mark J. van Raaij, Jon Agirre

What lies beyond publication in the life cycle of a successful scientific article? Were there any struggles that led the authors to alter their preferred course of action? Was the motivation for the research project personal or societal?

Frustratingly, we rarely get any answers to these kinds of questions when we read an article. On the one hand, conferences might provide a rare opportunity to satisfy our curiosity – should we be so lucky to meet the authors in person. But with the frequency and dynamics of personal interactions radically changing at the start of the present decade, it is now possible to have a friendly chat with authors online without having to wait for a summer fixture.

Making effective use of these new means of communication, we have decided to start meeting willing authors online after their research has been published in our journal. Why? Fundamentally, because we care about the answers. We edit a journal of the International Union of Crystallography (IUCr), which is a body that was created by scientists, including structural biologists like ourselves, for the common good. And there are so many ways in which these – completely voluntary – interviews will serve the community.

First, there is improved visibility. A list of names on an article does not necessarily reflect the wonderful diversity of the structural biology scene; also, social inequality, affinity bias, groupthink, deeply ingrained hierarchies, time and space constraints, and associated ills can make it difficult for conferences to showcase the obvious diversity of an International Union. In interviewing first authors, we aim to amplify the voice of early career researchers across the world, boosting their profiles and sharing their experiences with the community.

Second, because interviews provide an opportunity to engage the public. Interview videos are attached to articles in the journal so they are easily findable, but importantly our videos are published on the IUCr's YouTube channel (https://www.youtube.com/@theIUCr) and publicized on social media. Anyone can tune in and listen. And so that anyone can also understand, all interviews will commence with a lay summary of the presented research. Because it is not just the general public who might be interested in the results: policymakers have communicated time and again that it can be hard to distil the findings of a study from either an overly technical article or a potentially overblown press release. Lest we forget that science has a strong social role to fulfil.

Finally, in a world dominated by the media, bringing these interviews to as many authors as possible will help propagate interview experiences and skills worldwide. We do hope the initiative will be well received by the community. The series has recently started, with the first episode of *Structural Biology*

Communications: Interviews with authors featuring Sintayehu Manaye Shenkutie (Hawassa University, Ethiopia) and Jon Hughes (Justus-Liebig University Giessen, Germany) discussing their article on the photosensory module of phytochrome B from *Sorghum bicolor* (Shenkutie *et al.*, 2024).

Want to have a chance to talk to the community about your research, let them get to know you and share advice with them? Submit your articles to *Acta Crystallographica F – Structural Biology Communications* and get your own episode of *Interviews with authors*!

References

Shenkutie, S. M., Nagano, S. & Hughes, J. (2024). *Acta Cryst.* F**80**, 59–66.

This article was originally published in *Acta Cryst.* (2024). F**80**, 73.

EDITORIAL

The importance of international collaborations in science and structural biology



Maria Cristina Nonato, Mark J. van Raaij, Jon Agirre

International collaborations have been a fundamental pillar for the advancement of modern science. In particular, in structural biology, joining forces with researchers from different parts of the world not only enriches research but also accelerates discoveries that can benefit humanity. *Acta Crystallographica F – Structural Biology Communications* is proud to support this union, as shown by the global contributions to the journal. Structural biology, dedicated to studying molecular structures and their functions, is a very inclusive area of research that greatly benefits from the diversity of thoughts and techniques. Different specific expertises, whether in X-ray crystallography, cryo-electron microscopy, nuclear magnetic resonance spectroscopy, or computational methods, when combined, result in a more holistic and innovative approach to solving complex problems. In the last two years, *Acta Cryst. F* has received submissions from a wide array of countries, highlighting the global nature of scientific research. These countries include the following. North America: USA, Canada; Europe: Germany, France, United Kingdom, Belgium, Czechia, Denmark, Estonia, Finland, Italy, Netherlands, Portugal, Spain, Sweden; Asia: China, India, Indonesia, Israel, Japan, South Korea, Taiwan; Oceania: Australia, New Zealand; Africa: Egypt; and South America: Argentina.

This diversity of contributing regions emphasizes the widespread commitment to structural biology and the collective effort to advance scientific knowledge across borders. However, it is important to note that the majority of the papers, more than 50%, are led by scientists from developed countries, particularly from North America, Europe and Japan.

To foster a more heterogeneous distribution, leading laboratories in structural biology could take on the responsibility and privilege of hosting researchers from developing regions. These collaborations are vital for addressing specific problems in those countries, which are often neglected. For example, endemic diseases affecting millions in tropical regions can receive the necessary attention and resources when scientists from different parts of the world join efforts.

Moreover, these partnerships promote the transfer of technology and knowledge, empowering developing laboratories to conduct cutting-edge research and become more self-sufficient in the future. This is an investment that benefits both developing countries and the global scientific community.

This regional diversity underscores the importance of cross-border cooperation in advancing scientific understanding and tackling global challenges. *Acta Cryst. F* is committed to fostering these collaborations, starting from the international team of Main Editors, Co-editors and reviewers. The journal

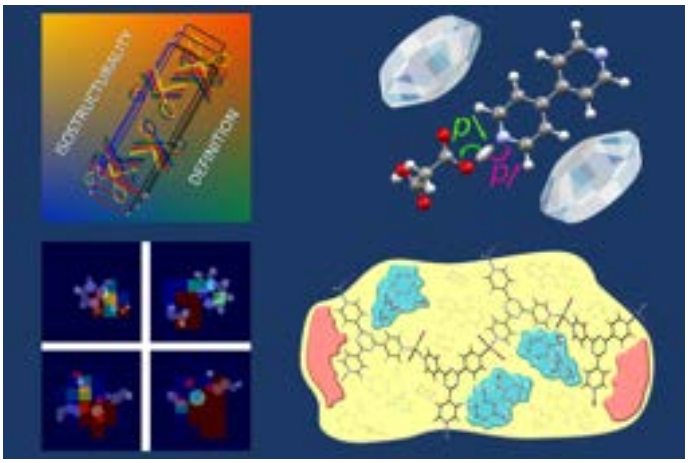
not only publishes research that is the product of international partnerships but also encourages the submission of articles that highlight the importance of global cooperation.

Science knows no boundaries, and international collaborations are the heart of scientific progress. In structural biology, joining forces enables advances that no single laboratory could achieve alone. Supporting partnerships between laboratories from different regions, especially those in developing countries, is crucial for solving global problems and democratizing scientific knowledge. *Acta Cryst. F* will continue to be a catalyst for these collaborations, promoting inclusive and globally connected science.

This article was originally published in *Acta Cryst*. (2024). F**80**, 116.

EDITORIAL

Chemistry and crystal engineering



Susan A. Bourne

The **IUCrJ** theme of *Chemistry and crystal engineering* covers a broad range of topics and this is reflected in the articles published in **IUCrJ**. In 2022, Desiraju suggested that 'the Holy Grail of crystal engineering is to answer the question: *Given the molecular structure of a compound what are all the possible crystal structures?*' (Desiraju, 2022). It is interesting and instructive therefore to reflect on advances made towards this goal in recent years. While there is still a focus in crystal engineering to deepen our understanding of the influence of intermolecular interactions on crystal packing, increasingly the focus has moved to practical applications such as devices and materials with useful physical and chemical properties (Braga, 2023; Xiong *et al.*, 2024; Kasuya *et al.*, 2024; Xu *et al.*, 2024). Recent articles in the journal highlight developments both in methodology and techniques as well as a diverse range of classes of compounds being studied and of problems being tackled.

Studies on the nature of non-covalent interactions are highly topical (Biot & Bonifazi, 2020; Rajapaksha *et al.*, 2023) and are well represented in recent publications in the journal. These include the nature of π-hole interactions between iodide anions and quinoid rings which have been shown to be predominantly electrostatic (Milašinović *et al.*, 2023) while Carroll and co-workers used a crystalline sponge to isolate and characterize a family of biaryl alcohol guest molecules, showing that the orientation and molecular conformation adopted by the guest molecules is controlled by the intermolecular interactions (hydrogen-bonding, halogen-bonding and/or aromatic interactions) available at the guest exchange site (Carroll *et al.*, 2023).

Interesting questions remain, such as how far can a packing motif change while still being considered the same? This is the subject of a re-evaluation of the definition of isostructurality (Bombicz, 2024) which argues that consideration of symmetry and supramolecular interactions and their influence on the resulting crystal structure is required. The concept of similarity and isostructurality is key to the study of polymorphism (Subanbekova *et al.*, 2024; Jeziorna *et al.*, 2023) and even of the disappearance and reappearance of polymorphs (Sacchi *et al.*, 2024). A recent example of the value of such considerations is the study of the mechanism and kinetics of transforming polymorph C of the pharmaceutical ingredient ibrutinib to its halogen benzene solvates using a flow-through capillary mounted directly on a powder X-ray diffractometer (Jirát *et al.*, 2023). Four different transformation mechanisms were determined despite the isostructurality of three of the four solvated crystal structures. The influence of environmental factors on molecular packing is another area of ongoing interest. The increasing availability of diamond-anvil cells has promoted an interest in the effect of pressure on molecular packing. High pressure promotes some interactions over others and can force the molecules to adopt a particular conformation (Sacharczuk *et al.*, 2024) while pressure changes can induce migration of a proton to allow interconversion between a cocrystal form to an ionic salt (Patyk-Kaźmierczak *et al.*,

2024).

Crystallography may be said to have reached a mature phase as a science but new techniques and computational approaches are essential to allow researchers to tackle ever more complex problems. Recent developments in quantum crystallography hold great promise for improving the accuracy of key structural parameters. For example, Hirshfeld atom refinement (HAR) uses aspherical structure factors obtained from calculation to produce more accurate structural information such as more accurate hydrogen atom positions even in cases where the hydrogens are close to heavy elements (Capelli *et al.*, 2014; Woińska *et al.*, 2023). Zwolenik *et al.* (2024) applied HAR to a molecular structure at high pressure and compared the result with an analysis of the same structure measured over a temperature range of 90 to 390 K.

Developments in machine learning and artificial intelligence will have an increasing impact on the nature of the questions that can be addressed using crystallography (Ekeberg, 2024; Billinge & Proffen, 2024; Zhu *et al.*, 2024). An intriguing example is recent work by Takiguchi *et al.* who devised a deep learning model to determine which of 20000 metal complexes extracted from the Cambridge Structural Database (CSD) are single-molecule magnets (SMM) with 70% accuracy (Takiguchi *et al.*, 2024). The latter article highlights the enormous value the CSD (Ferrence *et al.*, 2023) and other databases offer so it is encouraging to see the work being done by CODATA to ensure the interoperability of crystallographic data within the FAIR principles (findable, accessible, interoperable and reusable) (Brink *et al.*, 2024).

In conclusion, recent articles in the journal are evidence that crystal engineering concepts are well embedded in many aspects of chemical crystallography. Further advances in these themes are to be expected and will be welcomed in **IUCrJ**.

References

Billinge, S. J. L. & Proffen, Th. (2024). *Acta Cryst.* A**80**, 139–145.

Biot, N. & Bonifazi, D. (2020). *Chem. Eur. J.* **26**, 2904–2913.

Bombicz, P. (2024). *IUCrJ*, **11**, 3–6.

Braga, D. (2023). *Chem. Commun*. **59**, 14052–14062.

Brink, A., Bruno, I., Helliwell, J. R. & McMahon, B. (2024). *IUCrJ*, **11**, 9–15.

Capelli, S. C., Bürgi, H.-B., Dittrich, B., Grabowsky, S. & Jayatilaka, D. (2014). *IUCrJ*, **1**, 361–379.

Carroll, R. C., Harrowven, D. C., Pearce, J. E. & Coles, S. J. (2023). *IUCrJ*, **10**, 497–508.

Desiraju, G. R. (2022). *IUCrJ*, **9**, 329–330.

Ekeberg, T. (2024). *J. Appl. Cryst.* **57**, 1–2.

Ferrence, G. M., Tovee, C. A., Holgate, S. J. W., Johnson, N. T., Lightfoot, M. P., Nowakowska-Orzechowska, K. L. & Ward, S. C. (2023). *IUCrJ*, **10**, 6–15.

Jeziorna, A., Paluch, P., Zając, J., Dolot, R. & Dudek, M. K. (2023). *Cryst. Growth Des.* **23**, 5998–6010.

Jirát, J., Rohlíček, J., Kaminský, J., Jirkal, T., Ridvan, L., Skořepová, E., Zvoníček, V., Dušek, M. & Šoóš, M. (2023). *IUCrJ*, **10**, 210–219.

Kasuya, K., Oketani, R., Matsuda, S., Sato, H., Ishiwari, F., Saeki, A. & Hisaki, I. (2024). *Angew. Chem. Int. Ed.* **63**, e202404700.

Milašinović, V., Vuković, V., Krawczuk, A., Molčanov, K., Hennig, C. & Bodensteiner, M. (2023). *IUCrJ*, **10**, 156–163.

Patyk-Kaźmierczak, E., Izquierdo-Ruiz, F., Lobato, A., Kaźmierczak, M., Moszczyńska, I., Olejniczak, A. & Recio, J. M. (2024). *IUCrJ*, **11**, 168–181.

Rajapaksha, H., Augustine, L. J., Mason, S. E. & Forbes, T. Z. (2023). *Angew. Chem. Int. Ed.* **62**, e202305073.

Sacchi, P., Wright, S. E., Neoptolemou, P., Lampronti, G. I., Rajagopalan, A. K., Kras, W., Evans, C. L., Hodgkinson, P. & Cruz-Cabeza, A. J. (2024). *Proc. Natl Acad. Sci. USA*, **121**, e2319127121.

Sacharczuk, N., Olejniczak, A., Bujak, M., Dziubek, K. F., Katrusiak, A. & Podsiadło, M. (2024). *IUCrJ*, **11**, 57–61.

Subanbekova, A., Bezrukov, A. A., Bon, V., Nikolayenko, V. I., Koupepidou, K., Sensharma, D., Jan Nikkhah, S., Wang, S.-Q., Kaskel, S. & Vandichel, M. (2024). *ACS Appl. Mater. Interfaces*. In the press.

Takiguchi, Y., Nakane, D. & Akitsu, T. (2024). *IUCrJ*, **11**, 182–189.

Woińska, M., Pawlędzio, S., Chodkiewicz, M. L. & Woźniak, K. (2023). *J. Phys. Chem. A*, **127**, 3020–3035.

Xiong, Y.-A., Duan, S.-S., Hu, H.-H., Yao, J., Pan, Q., Sha, T.-T., Wei, X., Ji, H.-R., Wu, J. & You, Y. (2024). *Nat. Commun.* **15**, 4470.

Xu, W., Huang, G., Yang, Z., Deng, Z., Zhou, C., Li, J.-A., Li, M.-D., Hu, T., Tang, B. Z. & Phillips, D. L. (2024). *Nat. Commun.* **15**, 2561.

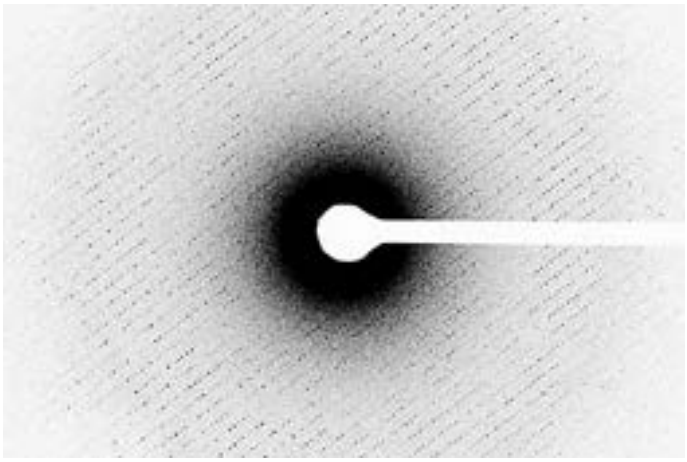
Zhu, Z., Zhang, Y., Wang, Z., Tang, W., Wang, J. & Gong, J. (2024). *Cryst. Growth Des.* **24**, 4245–4270.

Zwolenik, A., Tchoń, D. & Makal, A. (2024). *IUCrJ,* **11**, 519–527.

This article was originally published in *IUCrJ* (2024). **11**, 434–435.

COMMENTARY

3D ED/MicroED entering a new era



Mauro Gemmi

After the development of cryoEM single-particle analysis, the advent of three-dimensional single-crystal electron diffraction (Gemmi *et al.*, 2019), known as 3D ED/MicroED, was one of the major novelties in crystallography (Service, 2018). The possibility of a full single-crystal diffraction analysis on nanocrystals has opened a new area of research in crystal structure determination, that since the discovery of X-ray diffraction has remained quite unexplored. Interestingly, the first 3D ED/MicroED experiments date back to almost 20 years ago (Kolb *et al.*, 2007), but the technique was limited to a few laboratories for almost a decade, until it started to be applied to samples which have an unquestionable value, both commercial and medical, like pharmaceuticals (Jones *et al.*, 2018; Andrusenko *et al.*, 2019) and proteins (Nannenga *et al.*, 2014).

Aragon *et al.* (2024), by reporting the discussion and final conclusions of a round table held during a symposium at the National Center for CryoEM Access and Training, well describe all the advances that have been made for the application of the technique to these sample types. The biggest issue that is still limiting the diffusion of the method is the request of putting together the know-how of an electron microscopist and a crystallographer for setting up procedures that should work on instruments, the TEMs, that are mainly designed for imaging. This issue is partially mitigated by the availability of data collection software packages that can be applied to simplify any 3D ED/MicroED experiment in most TEMs, and also by the appearance on the market of dedicated electron diffractometers, in which the data collection procedure is partially automated (Simoncic *et al.*, 2023; Truong *et al.*, 2023). Both these solutions make 3D ED/MicroED more friendly for crystallographers that are used to X-ray diffraction; however, it is unquestionable that the formation and training of electron crystallographers is of great importance for every laboratory that aims to set up a 3D ED/MicroED facility.

Luckily, as can be seen by the initiative of the National Center for CryoEM, there is a strong tradition among electron crystallographers in organizing teaching events which dates to the nineties of the last century, thanks to the endless effort of Professor Sven Hovmöller. It is therefore common that a lot of schools and workshops are set up every year on different continents. Both the IUCr and ECA strongly support these initiatives: last year an electron crystallography school was organized as a side event of the IUCr Congress in Melbourne, while this year, an electron crystallography school will be held in Padova, Italy, as a side event of ECM34, and finally next year, in Erice, Italy, the International School of Crystallography will be devoted to electron crystallography, as happens every seven years. Finally, thanks to the great effort of Tatiana Gorelik, ELECTRA was founded last year in Europe (https://electraec.wordpress.com/), which is a non-profit educational association with the scope of supporting the organization of schools and workshops related to electron crystallography.

From the experimental point of view, Aragon *et al*. (2024) correctly identify the full automation of the data collection procedure, following the road opened by cryoEM, as one of the major expected developments. If the fast data collection time of 3D ED/MicroED could be coupled with automation, the method will become appealing for sample screening and quality control. At the same time, the crystallization procedures should be adapted to a new crystal size range which is well below one micron. This will require new crystallization recipes, especially in the case of macromolecules, where the search for 'large' crystal size was the only driving force.

Another interesting aspect, still scarcely explored, concerns spatially resolved crystallography, a field where 3D ED/MicroED has a lot to say. In 3D ED/MicroED, the beam size can be reduced to a few nanometres allowing structure variations to be sampled on the same scale (Passuti *et al.*, 2023). If we consider that 3D ED/MicroED can already investigate very fundamental and elusive aspects like absolute structure (Klar *et al*., 2023) and charge–density phenomena (Olech *et al.*, 2024), we can imagine that, once coupled with the spatial resolution of the technique, we will assist in the appearance of a new science.

The success of 3D ED/MicroED is now producing a flow of new structures determined and refined every year, which requires that the Crystallographic Information File (CIF) standard be made compatible with the peculiarities of ED data. Aragon *et al.* (2024) pointed out carefully all the critical issues and the IUCr is working on this problem in collaboration with the standardization committee of the NanED (Electron Nanocrystallography) project (https://naned.eu), a project funded by the EU (grant agreement No. 956099) for training the next generation of electron crystallographers. At the moment, a proposed extension of the CIF dictionary is under revision by NanED scientists and by the Commission on Electron Crystallography of the IUCr. The scientific community must also be aware that 3D ED/MicroED data sets are starting to populate open repositories like Zenodo, where two communities (3DED/MicroED data sets; NanED – Electron nanocrystallography project) are actively depositing their experimental data which are freely available for test and for those who want to practice 3D ED/MicroED data analysis.

As can be seen, 3D ED/MicroED has undergone the first stage of development, with both a theoretical and an experimental solid basis, and it is now entering a new era: an era of growth and expansion in which it will support side-by-side single-crystal and powder X-ray diffraction in most crystal structure determination laboratories.

Acknowledgements

The author would like to thank the European Union for funding under the Marie Skłodowska-Curie grant agreement the project NanED – Electron Nanocrystallography, that is significantly boosting the development of electron crystallography.

Funding information

The following funding is acknowledged: European Union (Marie Skłodowska-Curie grant) (grant No. 956099).

References

Andrusenko, I., Hamilton, V., Mugnaioli, E., Lanza, A., Hall, C., Potticary, J., Hall, S. R. & Gemmi, M. (2019). *Angew. Chem. Int. Ed.* **58**, 10919–10922.

Aragon, M., Bowman, S. E. J., Chen, C., Jason, M., Cruz, D., Decato, D. A., Eng, E. T., Flatt, K. M., Gulati, S., Li, Y., William, J., Lomba, C. J., Mercado, B., Miller, J., Waterman, D. & Zimanyi, C. M. (2024). *Acta Cryst.* C**80**, 179–189.

Gemmi, M., Mugnaioli, E., Gorelik, T. E., Kolb, U., Palatinus, L., Boullay, P., Hovmöller, S. & Abrahams, J. P. (2019). *ACS Cent. Sci.* **5**, 1315–1329.

Jones, C. G., Martynowycz, M. W., Hattne, J., Fulton, T. J., Stoltz, B. M., Rodriguez, J. A., Nelson, H. M. & Gonen, T. (2018). *ACS Cent. Sci.* **4**, 1587–1592.

Klar, P. B., Krysiak, Y., Xu, H., Steciuk, G., Cho, J., Zou, X. & Palatinus, L. (2023). *Nat. Chem.* **15**, 848–855.

Kolb, U., Gorelik, T., Kübel, C., Otten, M. T. & Hubert, D. (2007). *Ultramicroscopy*, **107**, 507–513.

Nannenga, B. L., Shi, D., Leslie, A. G. W. & Gonen, T. (2014). *Nat. Methods*, **11**, 927–930.

Olech, B., Brázda, P., Palatinus, L. & Dominiak, P. M. (2024). *IUCrJ*, **11**, 309–324.

Passuti, S., Varignon, J., David, A. & Boullay, P. (2023). *Symmetry*, **15**, 1459.

Service, R. F. (2018). *Science*, **362**, 1350.

Simoncic, P., Romeijn, E., Hovestreydt, E., Steinfeld, G., Santiso-Quiñones, G. & Merkelbach, J. (2023). *Acta Cryst.* E**79**, 410–422.

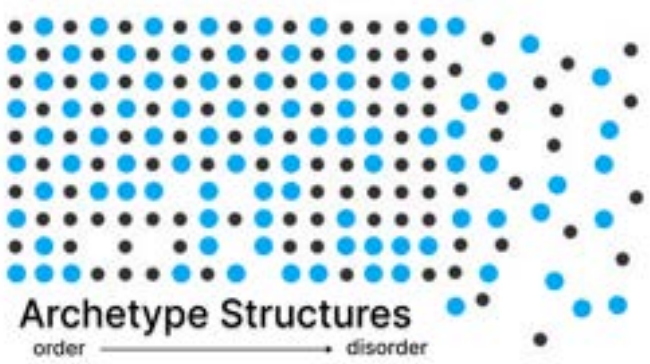
Truong, K. N., Ito, S., Wojciechowski, J. M., Göb, C. R., Schürmann, C. J., Yamano, A., Del Campo, M., Okunishi, E., Aoyama, Y., Mihira, T., Hosogi, N., Benet-Buchholz, J., Escudero-Adán, E. C., White, F. J., Ferrara, J. D. & Bücker, R. (2023). *Symmetry*, **15**, 1555.

This article was originally published in *Acta Cryst*. (2024). C**80**, 177–178.

The article by Aragon *et al.* is part of "Advances in electron diffraction for structural characterization", a growing collection of articles in *Acta Cryst. C* that will attempt to lay groundwork in establishing crystallographically sound standards and best practices for data collection and structural interpretation.

COMMENTARY

A solid solution to computational challenges presented by crystal structures exhibiting disorder



Peter R. Spackman

Crystallography is, in part, an ongoing effort to distil and rationalize interactions and behaviour at the atomic/molecular scale so we may identify their observable impact on macroscopic properties. It is a journey from the invisible world that we can only probe – via poking and prodding with increasingly sophisticated and precise sticks – to the world we perceive around us.

Though it can be very challenging, there is a certain appeal in the endeavour to connect such characteristics of a macroscopic object – a crystal can be held in the hand or examined under a microscope – into a refined, minimalist description characterized by mathematical concepts and constructs like symmetry and infinite lattices. In this manner a real, physical crystal can effectively be encoded into a world of geometric precision and orderly arrangement.

This reduction is not merely a simplification, it is an elegant distillation of natural complexity into comprehensible and manageable terms. It is also more than just a theoretical curiosity; it has implications for the prediction of bulk properties and therefore in praxis. Batteries, pharmaceuticals, an ongoing list of everyday and exotic materials, are all in principle predictable and understandable. The approach is so effective, in fact, that it is routinely applied using surrogate systems to model liquids, amorphous materials and other systems in simulations. The success of computational methods in treating these systems, which are emphatically not periodic, through a periodic lens showcases the fundamental value of reducing a really, really, big, complicated mess to a simple, symmetric and understandable model for analysis and prediction.

Disorder in crystals, then, poses a significant computational challenge; a thorn in the side for those seeking minimalist elegance and a harsh reminder that the reality of the physical world is typically neither elegant nor simple. The challenge is then compounded by further misfortune: crystals often exhibit degrees of disorder, probably even more often than in cases where they do not. Understanding why disorder arises is complex, and the temptation to wave it off with a simple statement like ‘it is entropically favourable’ provides no insight. It can stem from a variety of factors associated with the inherent properties of the materials or the conditions under which the crystals form. In brief, disorder is not just a minor inconvenience; it poses substantial challenges in accurately modelling and predicting the properties of bulk materials, and it is necessary to understand disorder before we can understand the real world. Indeed, many macroscopic properties directly result from the disorder (Welberry & Goossens, 2014), and would not occur in perfect crystals.

Thankfully, even within the realm of disordered structures, there are degrees of order. Sometimes it is as simple as a 50–50 mix of two orientations of a functional group; at other times there is effectively an infinite number of orientations of a solvent or trapped gas molecule, and sometimes we have solid solutions where molecules are effectively interchangeable at specific crystallographic sites. There is also a link to higher *Z*' crystal structures, which have been demonstrated to frequently be symmetry 'near misses' with regard to lower *Z*' *i.e.* higher symmetry structures (Brock, 2016).

Crystallographers, practical as they are, have been tackling disorder for a long time. However, for many computational folks (including myself) if the material is disordered, we would really prefer not to deal with the hassle. It would be unfair to imply that no work has been done at all to resolve the challenges. Indeed, the problem may be circumvented by treating a system as ordered, evaluating local defects in infinite systems or a variety of other approaches. But I believe the most common choice is likely to be simple: just avoid working on systems that exhibit disorder!

It is in this context that providing the community with clear methods to rationalize the order within disordered structures is invaluable for many real-world scientific problems, and that is exactly where Dittrich *et al.* (2024) provide an excellent step in the right direction in the latest issue of **IUCrJ**.

Their concept of 'archetype crystal structures' will no doubt help in wrangling disorder in many computational methods and applications. Further, the authors provide practical advice and concrete examples to help resolve many thermodynamic problems associated with several varieties of disordered crystals, including solid solutions. This is accomplished in a unified manner with analysis of polymorphism in crystals – an area itself once considered niche but increasingly seen as normal. As it turns out, we found different polymorphs almost everywhere once we started really looking for them (Bernstein, 2020).

The above work in particular showcases tangible applications of the concept of archetype structures to high-*Z*' structures, and molecules in special positions which, like disordered systems, many scientists would prefer to avoid. In this manner it serves both as an excellent exposition and showcase of the practical value of the concept.

That is not to say the work is done – there are still various factors associated with free energies which themselves have an impact on the explanation of these phenomena (including entropy, vibrational energies *etc*.) but the work here should find a variety of uses and prove valuable both within the crystallographic community and to the broader chemical, physics and materials communities.

In my view, the particular value of works such as this lies in the simple fact that the use of the concepts presented should reduce the difficulty of analysing many real-world problems. It is wonderful when we, as scientists, can find lower-hanging fruit; it is perhaps even better when others provide us with a ladder to reach up to new heights.

References

Bernstein, J. (2020). *Polymorphism in molecular crystals*, 2nd ed. International Union of Crystallography/Oxford University Press.

Brock, C. P. (2016). *Acta Cryst*. B**72**, 807–821.

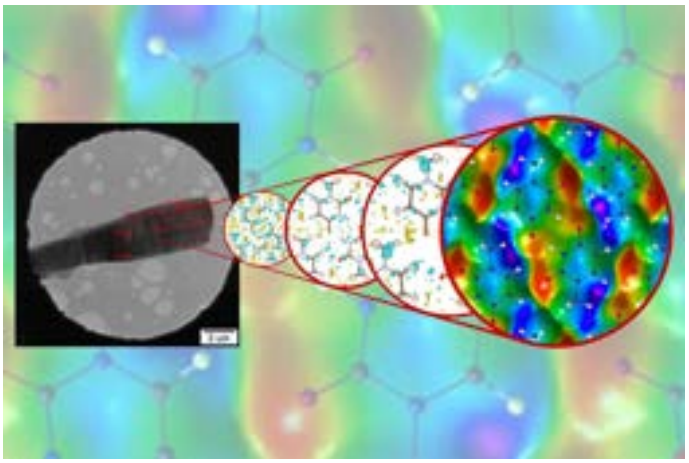
Dittrich, B., Connor, L., Fabbiani, F. & Piechon, P. (2024). *IUCrJ*, **11**, 347–358.

Welberry, T. R. & Goossens, D. J. (2014). *IUCrJ*, **1**, 550–562.

This article was originally published in *IUCrJ* (2024). **11**, 275–276.

COMMENTARY

3D electron diffraction goes multipolar



R. Beanland

The article by Olech *et al.* (2024) in this issue of **IUCrJ** marks an important step forwards in accessing some of the wealth of information that can be obtained from materials using electron diffraction (ED). It brings together an accurate description of electron scattering and quantum crystallography models of bonding between atoms in a crystalline solid. The field of ED is developing rapidly at the moment, as quantitative measurements and computer control of electron microscopes [and indeed dedicated electron diffractometers (White *et al.*, 2021; Merkelbach *et al.*, 2022)] are beginning to give routine access to high-quality data that has for so long been the norm in X-ray diffraction (XRD) and neutron diffraction (ND). Approaches that have been developed over decades in the latter two fields are now being applied to ED, opening up whole new fields of investigation, particularly for nanoscale crystals that can be easily studied by electrons due to their much stronger interaction with matter.

This strong interaction, inherent in electron diffraction – and resultant multiple scattering – brings many benefits that are beyond the reach of measurements where single scattering dominates. Friedel's law, mandating equivalence of the intensity of reflections related by inverting the scattering geometry, does not apply, allowing absolute structure to be determined (Buxton *et al.*, 1976; Brázda *et al.*, 2019). Additionally, low-order structure factors may be measured much more accurately using ED in comparison with XRD or ND, giving the chemical (bonding) information that is the focus of this article. However, access to the rich and deep information available in ED comes with the cost of increased complexity in the models required to give a good description of the data and the desired measurements.

The benefits, and limitations, of ED have been apparent for some time (Spence, 1993) and bonding effects were determined using dynamical scattering theory in combination with convergent beam electron diffraction (CBED) patterns over thirty years ago (Zuo & Spence, 1991). Nevertheless, the measurement was not straightforward, requiring manual control of both the transmission electron microscope (TEM) and the crystal goniometer to select and orient a suitably defect-free region of a thin crystal for the diffracted beam(s) of interest; recording the pattern on film; digitizing the negative; and refining to a solution using the limited computing resources of the time. The result was a handful of low-order electron structure factors that, in combination with higher-order structure factors determined by XRD, could be used to measure deviations from the neutral, spherical atoms of an independent atom model (IAM) (Zuo *et al.*, 1999).

Olech *et al.*'s article clearly shows that the success of CBED can be replicated by the various techniques that fall under the acronym 3DED (Gemmi *et al.*, 2019). Importantly, computer control of both the electron optics and the noise-free detectors of current methods makes them relatively straightforward experimentally. Furthermore, the use of a parallel beam removes the restriction on lattice parameters imposed by CBED, in which the convergence angle must be smaller than the smallest Bragg angle in the

diffraction pattern. These advantages mean that 3DED techniques are relevant to materials that are of interest to a wide range of scientists and crystallographers. Here, the material chosen to demonstrate the approach is an organic, beam-sensitive molecular crystal, which yielded only a few reliable measurements even with specimen cooling. That a refinement performed on this less-than-ideal data using an aspherical multipolar atom model not only gave a significantly better match between model and experiment, but yielded chemically sensible results, demonstrates the strong influence of bonding effects in ED and is very encouraging for future studies. Furthermore, the ability to qualify different versions of transferable aspherical atom model (TAAM) against experimental data as demonstrated in this article will undoubtedly drive improvements in quantum crystallography.

This article is yet another demonstration that improvements in technology, technique and modelling in ED are opening avenues of research that previously have been only partially visible. There is yet some distance to travel.

References

Brázda, P., Palatinus, L. & Babor, M. (2019). *Science*, **364**, 667–669.

Buxton, B., Eades, J., Steeds, J. W. & Rackham, G. (1976). *Philos. Trans. R. Soc. London Ser. A*, **281**(1301), 171–194.

Gemmi, M., Mugnaioli, E., Gorelik, T. E., Kolb, U., Palatinus, L., Boullay, P., Hovmöller, S. & Abrahams, J. P. (2019). *ACS Central Science*, **5**(8), 1315–1329.

Merkelbach, J., Jandl, C., Steinfeld, G., Hovestreydt, E. & Stam, D. (2022). *Acta Cryst.* A**78**, e741.

Olech, B., Brázda, P., Palatinus, L. & Dominiak, P. M. (2024). *IUCrJ*, **11**, 309–324.

Spence, J. C. H. (1993). *Acta Cryst*. A**49**, 231–260.

White, F., Yamano, A., Ito, S., Matsumoto, T., Sato, H., Ferrara, J., Meyer, M., Jasnowski, M., Okunishi, E. & Aoyama, Y. (2021). *Acta Cryst*. A**77**, C941.

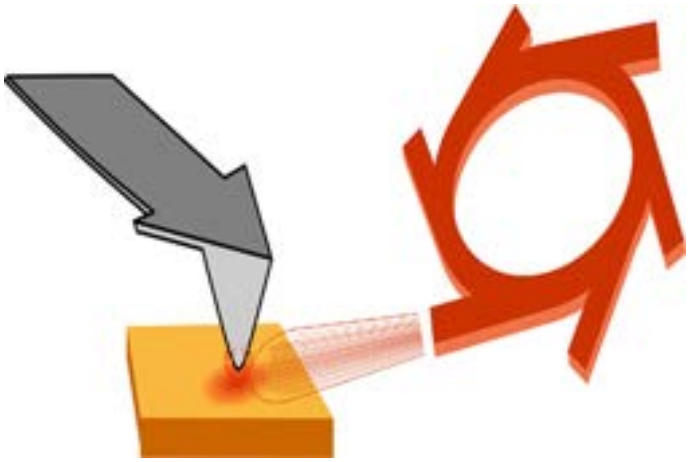
Zuo, J.-M., Kim, M., O'Keeffe, M. & Spence, J. C. H. (1999). *Nature*, **401**, 49–52.

Zuo, J.-M. & Spence, J. (1991). *Ultramicroscopy*, **35**(3–4), 185–196.

This article was originally published in *IUCrJ* (2024). **11**, 277–278.

COMMENTARY

Perspectives for infrared beamlines in fourth-generation synchrotron facilities



Ferenc Borondics

Fourth-generation synchrotron facility upgrades are upon us, and published results are indeed outstanding. With several fourth-generation, or diffraction-limited, storage rings and multiple beamlines in operation, the missing range of the spectrum was infrared ... until recently.

Infrared (IR) beamlines benefit from the accumulated knowledge of more than a century as IR spectroscopy itself is a well accepted and used laboratory-based technique due to its ability to solve scientific problems from a plethora of research fields. Therefore, IR beamlines have been an integral and productive part of the synchrotron world for many decades, are implemented at multiple facilities and have reached a worldwide presence (Miller & Dumas, 2013). Most of these facilities, recognizing the high added value of synchrotron IR techniques, have already committed to or are looking to raise funds for implementing new IR extractions in the upgraded diffraction-limited storage rings.

While third-generation machines already provide diffraction-limited IR beams (Dumas *et al.*, 2006), upcoming upgrades will significantly improve electron beam stability and characteristics, and thus, through a cascade of developments, we can expect higher signal-to-noise ratios in IR experiments.

The first demonstrated implementation of a fourth-generation IR facility is the IMBUIA beamline in SIRIUS, at the Brazilian Synchrotron Light Laboratory in Campinas, Brazil. Here, we highlight the paper published in the May 2024 issue of *Journal of Synchrotron Radiation* by Santos *et al.* (2024) describing the performance of a scattering-type scanning near-field optical microscopy (s-SNOM) endstation at the IMBUIA-nano branch. Synchrotron IR nanospectroscopy is one of the most recent synchrotron IR techniques that greatly benefits from the ultrabroadband spectrum and diffraction-limited focus spot of synchrotron IR radiation (Hermann *et al.*, 2013). At SIRIUS, the current IMBUA extraction is implemented with a relatively small extraction angle, around 6 mrad × 6 mrad (H × V). However, the results shown in the paper underline that a very important parameter with s-SNOM is the quality of the focused IR beam spot under the atomic force microscopy tip. This can be well realized with smaller extraction angles (*i.e.* shorter source depth), and using single focal length optics and very high quality wavefronts. Wavefront simulations and measurements as well as near-field spectra (showcased in Fig. 1), their signal-to-noise and bandwidth, especially towards the high-energy part of the spectrum, highlight the advantage of synchrotron IR beamlines. The plans of the IMBUIA team include the implementation of a wider-angle, higher-flux extraction that will benefit near-field experiments and will be also important when implementing traditional, synchrotron-based diffraction-limited IR spectromicroscopy.

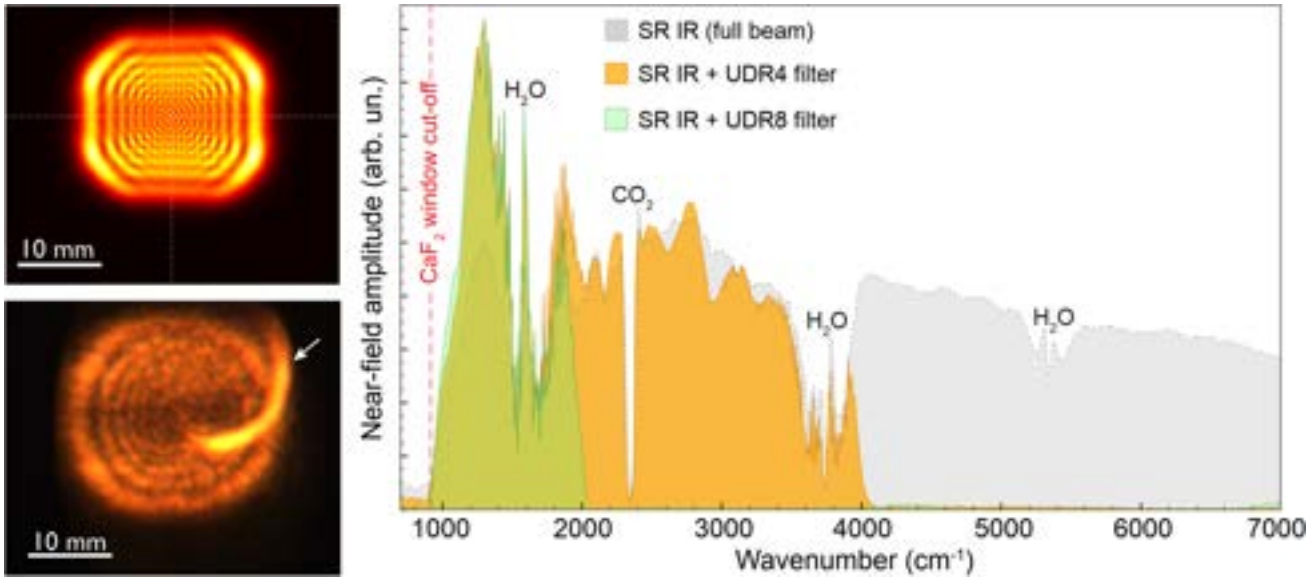


Figure 1. Simulation (top-left) and measurement (bottom-left) of the extraction wavefront of IMBUIA at 633 nm. Broadband near-field nanoFTIR spectrum of the IMBUIA-nano source (right). [Partially reproduced with modifications from Santos *et al.* (2024) with the permission of the authors.]

Large-opening-angle extractions, due to the typically smaller diameter of the fourth-generation storage ring vacuum vessels compared with their third-generation predecessors, will present some challenges. To achieve extraction angles similar to third-generation IR beamlines, in the 30–80 mrad range, extraction mirrors need to be placed in very close proximity to the electron beam. The electromagnetic shielding of the small vacuum vessels at increasingly higher energies needs to be taken into account, as explained in detail by Bosch (2002). Radiation emitted from the complex and densely populated structures of multibend achromat lattices needs to be well understood, and innovative beamline optics will be required to manage wavefronts and recollimate optically deep sources (Moreno *et al.*, 2013). Still, these issues can be overcome and the example of IMBUIA shows that fourth-generation IR beamlines are off to a flying start. With other scheduled upgrades, we are looking at a new era of improved IR spectromicroscopy in both the far- and near-field.

References

Bosch, R. A. (2002). *Nucl. Instrum. Methods Phys. Res. A*, **482**, 789–798.

Dumas, P., Polack, F., Lagarde, B., Chubar, O., Giorgetta, J. L. & Lefrançois, S. (2006). *Infrared Phys. Technol.* **49**, 152–160.

Hermann, P., Hoehl, A., Patoka, P., Huth, F., Rühl, E. & Ulm, G. (2013). *Opt. Express*, **21**, 2913.

Miller, L. M. & Dumas, P. (2013). *Encyclopedia of Biophysics*, pp. 1106–1112. Berlin, Heidelberg: Springer.

Moreno, T., Westfahl, H., Freitas, R. O., Petroff, Y. & Dumas, P. (2013). *J. Phys. Conf. Ser.* **425**, 142003.

Santos, T. M., Lordano, S., Mayer, R. A., Volpe, L., Rodrigues, G. M., Meyer, B., Westfahl, H. Jr & Freitas, R. O. (2024). *J. Synchrotron Rad.* **31**, 547–556.

This article was originally published in *J. Synchrotron Rad.* (2024). **31**, 430–431.

CRYSTALLOGRAPHY IN AFRICA

Bridging continents through crystallography: how AFRAMED is revolutionizing scientific collaboration in Africa



Rim Benali-Cherif, Eric Ziki

A report on the Second Session of AFRAMED Training, from 28 August to 23 September 2023.

The field of crystallography has long stood at the forefront of scientific discovery, offering insights into the atomic structure of materials and paving the way for innovative applications in various industries. The AFRAMED project, spearheaded by Professor Claude Lecomte, stands as a testament to this pioneering spirit. Officially inaugurated on 31 August 2022, AFRAMED (Appui à la Formation et la Recherche en Afrique par des Mesures à Distance) symbolizes a bridge of knowledge and expertise, connecting researchers across continents through the power of remote measurement technology.

AFRAMED goes beyond just providing remote access to equipment. It is about building a sustainable ecosystem for scientific research and education. The project fosters collaboration between African and French researchers, facilitating knowledge exchange and mentorship. This partnership is instrumental in developing local expertise and capacity in crystallography, thereby nurturing the next generation of African scientists.

The AFRAMED journey: from concept to reality

AFRAMED emerged as a vital solution to a pressing challenge: advancing the field of crystallography in Africa. The project's innovative approach lies in its use of remote operation technology. This allows African researchers and students to conduct advanced diffraction experiments using a French diffractometer, all from the comfort of their local laboratories. This innovative methodology not only bridges geographical distances but also opens new horizons in scientific exploration and learning.

Our collective experience in AFRAMED: a journey of discovery and collaboration

Our journey as part of the second AFRAMED training session was a comprehensive and enriching experience that spanned various facets of crystallography. As a group of four, hailing from different African countries (Senegal, Congo, Côte d'Ivoire and Algeria), we delved into an intense month of learning and exploration at the CRM^2 laboratory, University of Lorraine, Nancy, France.



From left to right: CRM^2 Trainers: Emmanuel Wenger, El-Eulmi Bendeif and Claude Lecomte. Trainees: Ibrahima el Hadji Thiam, Ferland Ngoro-Elenga, Eric Ziki and Rim Benali-Cherif.

The training commenced with an in-depth exploration of crystallography's theoretical aspects. We engaged in insightful lectures presented by Dr Emmanuel Wenger that unravelled the complexities of X-ray diffraction and its critical role in material science. This theoretical foundation was crucial as it laid the groundwork for our practical sessions.

The practical aspects represent the most central part of this training course and have been made possible thanks to the availability of equipment on the PMD²X platform at CRM². This practical training was an immersive experience with the state-of-the-art Bruker D8 Venture diffractometer. Under the expert guidance of Dr Emmanuel Wenger, Dr El-Eulmi Bendeif and Professor Claude Lecomte, we delved deep into the nuances of crystallography. We began by learning how to meticulously select and mount single crystals – a task that requires a keen eye for detail and a steady hand. Each crystal was carefully chosen based on its size, shape and quality, ensuring optimal results for our experiments.

Our training also extensively covered the use of advanced crystallographic software. We became adept at using Bruker *APEX4* for data collection and processing. This software's intuitive interface and powerful features allowed us to efficiently navigate through the complexities of X-ray diffraction data. Additionally, we explored the capabilities of *Olex2*, a versatile tool for structure resolution and refinement. Working with *Olex2*, we learned how to interpret the diffraction data, solve crystal structures and refine them to obtain accurate and reliable results.



Practical training on the Bruker D8 Venture diffractometer of the PMD²X@CRM² platform. Upper left: Eric, Ibrahima, Rim and Ferland. Below: Emmanuel after his teaching.

These practical sessions were more than just learning how to operate equipment and software; they were an exercise in translating theoretical knowledge into real-world applications. We not only honed our technical skills but also developed a deeper understanding of the intricate relationship between crystal structure and its properties. This comprehensive approach to training equipped us with a profound skill set, ready to tackle the challenges in the world of crystallography.

Our collaborative efforts led to the identification of several novel structures, which are now set to be detailed in forthcoming publications. These discoveries not only enhance the scientific knowledge base but also symbolize the fruitful collaboration and skill-sharing fostered by the AFRAMED initiative.

Collaboration and diversity: enriching the learning experience

Our diverse backgrounds added significant value to the training. The exchange of ideas, experiences and cultural insights among us enriched the learning environment. This diversity fostered a deeper understanding and appreciation of the scientific community's interconnected nature.

Our experience in the AFRAMED training session was transformative. It went beyond acquiring technical skills; it was about being part of a ground-breaking initiative that is paving the way for advanced scientific collaboration across continents.

Synchrotron visit: a glimpse into advanced research

Our training ended with a two-day visit to the SOLEIL Synchrotron. It was organized by Dr El-Eulmi Bendeif with the scientists of the beamlines that we visited (CRISTAL, DIFFABS, PSICHE, SIXS, ROCK and PROXIMA1). Dr Jean Daillant (Director General of SOLEIL) gave a welcome speech highlighting the applications of synchrotron research to crystallography. This experience provided us with a unique perspective on these applications.



During our visit to the SOLEIL Synchrotron. Back row from left to right: Emmanuel, Jean Daillant, Ferland, Eric and Ibrahima. Front row from left to right: Rim, El-Eulmi and Sameea.

Making a mark: remote sessions and workshops

Post-training, remote sessions and workshops were actualized with notable success, demonstrating the practical application of our training. Remote sessions have been organized in Côte d'Ivoire and Algeria using the Nancy diffractometer. The next sessions are planned for Cameroon, Congo and Senegal.

Remote sessions and workshops in Côte d'Ivoire

After the Nancy training, a remote access tool for X-ray single-crystal measurements was presented to Ivory Coast colleagues by Lecturer Dr Eric Ziki (figures below). The aim of this presentation was to tell them that they should no longer hesitate to involve X-ray single-crystal measurements and associated crystallographic analysis approaches in the development of their research and teaching activities as the equipment is now available "remotely". Physicists, chemists, material scientists, geologists and biologists were involved.



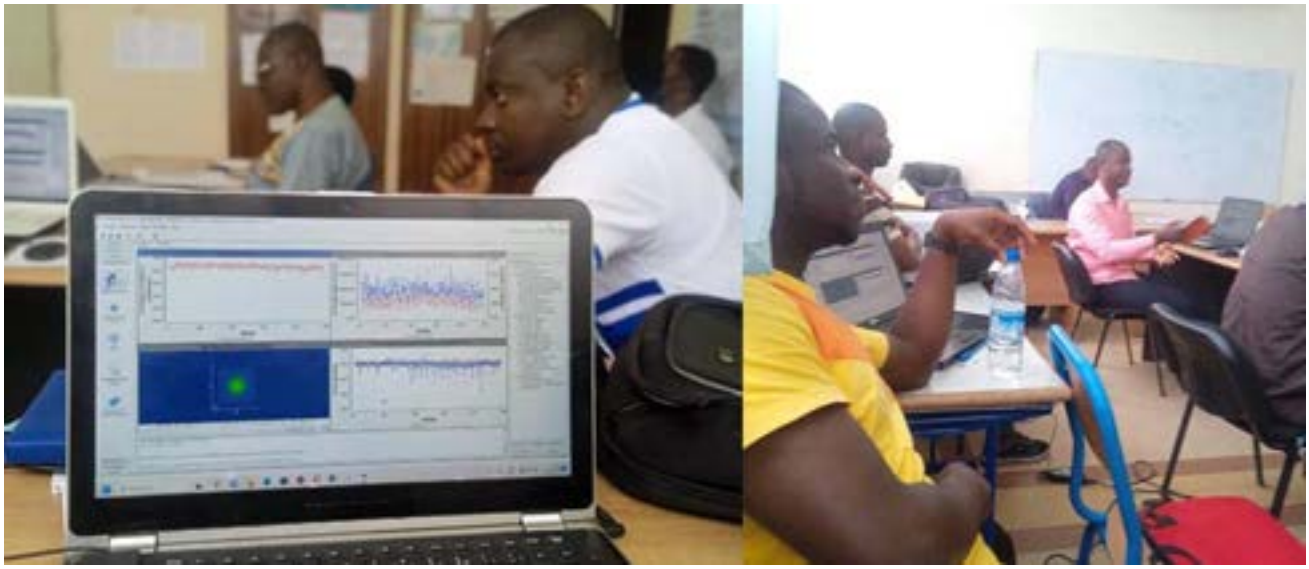
Presentation of the AFRAMED project to researchers of some laboratories in Abidjan.

Two remote sessions were organized at Félix Houphouët-Boigny University, Abidjan, on 20 and 27 October 2023. The crystals were centred by Emmanuel Wenger on the goniometer of the Bruker D8 Venture diffractometer prepared for these remote measurements. The students were then able to follow all the actions needed to select a good crystal and centre it on the diffractometer. This was done under the explanation of Eric Ziki (see figures below). The crystals were then remotely analysed by Dr Ziki at low temperature (100 K) to obtain data of good quality.



Students practising data reduction and structure determination under the supervision of Eric Ziki during the first practical remote session at Félix Houphouët-Boigny University.

A second remote session was organized on 27 October 2023, to reinforce the capacities of the researchers of the Crystallography and Molecular Physics Research Team of the Laboratory of Matter, Environmental and Solar Energy Sciences (LAMES) at Félix Houphouët-Boigny University in the determination of the structure of materials via X-ray single-crystal measurements. These researchers had been well trained to use the diffractometers and software to determine the structure of the materials but due to a lack of activity, the knowledge had been forgotten.



LAMES researchers practising data reduction and structure determination under the supervision of Eric Ziki.

Remote sessions and workshops in Algeria

Additionally, we also successfully organized a remote workshop in Algeria. This event, co-hosted by Rim in Algeria and Emmanuel in France, gathered over 120 participants, both in person and remotely, including a notable representation of 20 attendees from Senegal. The remote participants were students, PhD students and academic researchers from various African countries. Furthermore, the workshop included attendance from trainees of both the first and second AFRAMED sessions, creating a dynamic and interactive learning environment. Covering every aspect of crystallography practice, from crystal selection to structure resolution and refinement, this workshop vividly demonstrated the extensive reach and depth of the AFRAMED training. It was a remarkable display of how effectively remote collaboration can bridge distances, bringing together a diverse group of students, doctoral candidates and teachers to engage in advanced scientific exploration.



Rim during her workshop, held as part of the AFRAMED project.

These remote sessions are just the beginning of an exciting journey ahead. They serve as a foundation for more expansive and innovative collaborations, paving the way for a new era in scientific research and education. As we continue to harness the power of technology, we are not only bridging geographic distances but also creating a vibrant community of shared knowledge and expertise. This is a stepping stone towards a future where remote learning and collaboration become integral parts of advancing scientific discovery and fostering global connection.

Impact and future prospects

AFRAMED is more than just a training programme; it's a catalyst for scientific growth and collaboration across continents. By enabling remote measurements, it has revitalized crystallography in Africa, turning the challenge of distance into an opportunity for shared learning and discovery. The project's success serves as a beacon, promising to extend its reach to other scientific instruments, facilities and disciplines.

Conclusion

AFRAMED is not just a bridge between laboratories; it's a means for transferring knowledge and igniting a passion for science across continents. This project exemplifies the spirit of international collaboration and the relentless pursuit of knowledge, making the seemingly impossible, possible.

The success of AFRAMED serves as a model for future scientific collaborations and capacity building initiatives. It demonstrates the power of international cooperation in advancing science and education. The project is a beacon of hope, showing that with the right resources and collaboration, the challenges of distance and access can be overcome, paving the way for a brighter, more inclusive, scientific future in Africa.

This project is a part of the IUCr Crystallography in Africa initiative. The AFRAMED members warmly thank CNRS, IUCr, UNESCO and the University of Lorraine for providing travel, accommodation and food for all trainees as well as diffractometer costs. A special thanks goes to our enthusiastic teachers Emmanuel Wenger, El-Eulmi Bendeif and Claude Lecomte. We also would like to express our gratitude to Ferland, Ibrahim, El-Eulmi, Emmanuel and Claude for their valuable comments and corrections, which have greatly contributed to the improvement of this report.

Rim Benali-Cherif (benalicherif.rim@univ-khenchela.dz) is at the Laboratoire des Structures, Propriété et Interactions Interatomiques (LASPI2A), Université Abbes Laghrour-Khenchela, Algeria, and Eric Ziki (eric.ziki@gmail.com) is at the Crystallography and Molecular Physics Research Team, Department of Physics, University Félix Houphouët-Boigny, Abidjan, Côte d'Ivoire.

CRYSTALLOGRAPHY IN AFRICA

Bringing crystallography to the classroom: Kenyan teachers learn to engage students in the wonders of crystals



Figure 1. Group photo of participants during the opening of the teachers' training workshop on 29 November 2023 (copyright UoN and CSIC). Front row, left to right: Martin Mbugua (Senior lecturer, UoN), David Kamau (Chairman, Department of Chemistry, UoN), Stephen Kiama (Vice Chancellor, UoN), Ms Natalia Suarez de Puga Canosa (Consul-Spanish Embassy to Kenya), Juan Manuel García-Ruiz (CSIC-University of Granada), Fermín Otálora (CSIC-University of Granada) and Solomon Derese (UoN).

Patricia W. Gitari, Martin N. Mbugua

Over three days in late November 2023, high-school teachers from across Kenya gathered at the University of Nairobi (UoN) for an immersive training workshop on using crystallography to teach science in an engaging, hands-on way.

The workshop, entitled *Learning How Science Works with Crystals*, was led by renowned crystallography experts Professor Juan Manuel García-Ruiz (Donostia International Physics Center and the Instituto Andaluz de Ciencias de la Tierra-CSIC, Spain) and Dr Fermín Otálora (Instituto Andaluz de Ciencias de la Tierra-CSIC, Spain). Through a blend of informative talks, engaging videos, captivating demos and hands-on practical activities, the teachers were immersed in the fascinating world of crystallography, crystallization and the practical applications of crystals and crystallographic techniques in everyday life.

'Crystals provide a visual, tangible way to illustrate core scientific concepts in chemistry, physics, biology, biomedicine, engineering, mathematics and the arts,' said García-Ruiz. 'By giving students the ability to grow and examine crystals themselves, we can spark their curiosity and help abstract principles come to life.'

A highlight was the *crystallization kit* – a simple set of materials teachers can use to guide students through growing crystal structures from solutions and gels. Seeing these crystals take shape allows students to witness the dynamics of molecular interactions first-hand.



Figure 2. Interactive training on crystallography (copyright UoN and CSIC).

The workshop also introduced the *Spanish Crystallography Contest for Schools*, which challenges students to design and conduct crystallization experiments, explore how to grow large and better crystals, or search for crystalline and polycrystalline materials with specific properties. A diversity of Kenyan schools will now have the opportunity to participate in the *Africa Education Program for the Crystallisation Contest in Schools.*

Science teachers commented on the workshop: 'These kinds of immersive, practical learning experiences are invaluable. We cannot wait to set up crystallization activities in our own classrooms and watch students' fascination as they explore the hidden worlds of crystal formation.'

The workshop was organized by Dr Solomon Derese, Dr Patricia Gitari, Dr Joey Kiano, Dr Martin Mbugua, Dr Fermín Otálora and Professor Juan Manuel García-Ruiz under the auspices of the Consejo Superior de Investigaciones Científicas, UoN and the Spanish Embassy.

Students from various public and private schools in Kenya are now hard at work learning the secrets of crystallization, understanding the importance of crystals and enjoying their beauty. The final contest is scheduled for September 2024 after ECM34. A display of an African version of the exhibition *CRISTALES* is also planned. In addition to strengthening science education, the workshop aimed to foster connections between Kenya and Spain in scientific research and knowledge exchange. Representatives from both nations' governments attended and voiced their support for such collaborative initiatives.



Figure 3. Examining crystals grown by the teachers (copyright UoN and CSIC). Left to right: Nyongesa; Martin Mbugua; Fermín Otálora; HE Ambassador Cristina Díaz Fernández-Gil, Ambassador of Spain to Kenya; and Juan Manuel

García-Ruiz.

The crystallography training equipped Kenyan educators with innovative tools and methods to inspire the next generation of scientists and drive STEM learning forward through exploration and inquiry. As we look to the future, there is also a need to address the under-representation of women in many scientific disciplines, especially in physical sciences and engineering. Girls often face biases, lack mentorship and role models, and experience persistent stereotypes that end up discouraging them from pursuing careers in science. By nurturing and empowering the next generation of female scientists, we can unlock vast reserves of human potential and accelerate the pace of scientific discovery.



Figure 4. Organisers of the teachers' training workshop in Nairobi (copyright UoN and CSIC). Left to right: Martin Mbugua, Juan Manuel García-Ruiz, Patricia Gitari, Solomon Derese, Joy Kiano and Fermín Otálora.

Patricia Gitari is a Consultant Chemist at AESA and Martin Mbugua is at the Department of Chemistry, UoN.

REGIONAL NEWS

Women in Crystallography project



Women in Crystallography fundraising project – first awardees announced

The “Women in Crystallography” project, an initiative of the ECA General Interest Group on Education in Crystallography (GIG-03), aims to improve the participation of women, especially young scientists, at events around the world and to create a balanced attendance among participants and speakers.

Funds are raised via donations for limited-edition T shirts, first seen at the launch of the project at ECM31 in Oviedo, Spain in 2018, and then making an appearance at ECM33 in Versailles, France in 2022; down under at the IUCr Congress in Melbourne, Australia in 2023; and across the Atlantic at ACA2024 in Denver, CO, USA in 2024. For the history of the logo, see here.

The first awardees are already benefiting from this fund to attend different crystallographic events:

Lamis Elaa Eldin Refat, from Ireland, attended the 15th International Workshop on Crystal Growth of Organic Materials in Phuket, Thailand in July 2024

Anara Omarova, from Kazakhstan, attended the 9th European Crystallography School in Nancy, France in June 2024

Almudena Inchausti Valles, from Spain, took part in the 2nd High-Pressure Single-Crystal X-Ray Diffraction Summer School in Edinburgh, UK in July 2024

Laura Pacoste, from Sweden, will join ECM34 in Padova, Italy in August 2024.

The fundraising for this project will continue at ECM34, where the 2024 edition of the T shirt will be available from the ECA booth as well as those of co-supporters Dectris, the IUCr and STOE. The promoters of the initiative have created the hashtag #Womenincrystallography to share on X (Twitter).

First video in the “Women in Crystallography” series

GIG-03 has also announced the release of the first video of the project supported by the Royal Society of Chemistry Inclusion and Diversity Fund. The project’s scope is to celebrate the importance of women in the field of crystallography and science while raising awareness about the pitfalls and obstacles on the way to reach gender parity in science, eliminate stereotypes, increase sensitivity and facilitate equal treatment of everyone at all stages of a scientific career. The speaker is Professor Shanti Deemyad from the Department of Physics & Astronomy of the University of Utah, Salt Lake City, UT, USA: “Journey Through the Quantum Realm: My Path as a High-Pressure Physicist”.

Watch the video on the ECA YouTube channel here.

MEETING REPORT

25th Heart of Europe Bio-Crystallography meeting



Group photo.

Przemysław Grudnik

The 25th Heart of Europe Bio-Crystallography meeting (HEC25) took place in September 2023 in Salem, located in the state of Mecklenburg-Vorpommern in Germany. The attendees were able to appreciate the beautiful scenery of Lake Kummerow. The meeting was organized by Professor Michael Lammers' group from Greifswald University. As previously, the organization of HEC was supported by 11 sponsors including IUCr Journals.

The meeting was attended by 113 structural biologists from 23 research groups in central Europe (Austria, the Czech Republic, Germany and Poland), and opened with the introduction of two new HEC groups, the group led by Ingrid Span (FAU, Erlangen-Nurnberg) and that by Johanna Hakanpää (PETRA III, DESY, Hamburg).

Over the course of three days, 27 PhD students and postdocs presented current topics of their research. Several prizes were awarded for outstanding short talks and flash talks, made possible by generous support from the IUCr, Gesellschaft für Biochemie und Molekularbiologie e.V. (GBM) and *Structure*/Cell Press. As typical for HEC presentations, the quality of the talks was remarkable, making it hard for the HEC Prize Committee to reach its decision. Three PhD students — Stephanie Himpich from Markus Wahl's group, Stefan Djukic from Pavlina Rezacova's group, and Paweł Kochanowski from Przemysław Grudnik's group — received awards from *Structure*/Cell Press.



HEC25 Prize recipients: Paweł Kochanowski (second from left), Stefan Djukic (center) and Stephanie Himpich (second from right).

The best flash-talk prizes were awarded to Evangelia Nathanail from Oliver Daumke's group (GBM prize) and Chen-Chiao Yang from Norbert Sträter's group (IUCr prize), presented by Michael Lammers. Dominik Rafalski from Matthias Bochtler's group was awarded the PostDoc prize for the best short-talk (IUCr prize).

The recipients were acknowledged for their well-organized presentations, exceptional clarity in explaining their research and the significant impact of their projects. These projects covered a diverse range of topics, including phage defense systems (S. Himpich), purine nucleoside hydrolase inhibitors (S. Djukic), the DHS-ERK2 complex (P. Kochanowski), the MICOS complex involved in mitochondrial integrity and form (E. Nathanail), crystallographic fragment screening with amino acid derivatives (C.-C. Yang) and CRISPR-associated proteins Csx15 and Csx20 (D. Rafalski), demonstrating the remarkable talent within the crystallography and cryo-EM communities.

The HEC lecture, presented each year by a prominent scientist outside the HEC community, was delivered by Alfred Wittinghofer (MPI of Molecular Physiology/Dortmund). His talk “Nature uses Phosphates” was a summary and celebration of his entire scientific career, highlighting the contributions of structural research to the study of enzymes utilizing phosphates.

The inclusion of brief company-sponsored presentations throughout the program helped introduce new technologies to the participants. The afternoon canoeing experience in the windy weather fulfilled the expectations of adrenaline-seeking participants.

A heartfelt thank you is due to the entire team led by Michael for the excellent organization of this event. Another fantastic meeting celebrating a quarter-century of the HEC community concluded with the traditional group singing of the “HEC song”.

The next Heart of Europe Bio-Crystallography meeting (HEC26), organized by Sebastian Glatt and Przemysław Grudnik of the Jagiellonian University in Krakow, will take place in Krakow, Poland, from 26 to 28 September 2024.

MEETING REPORT

SEA COAST 2024: Comprehensive training course in macromolecular structure determination in Thailand



The organizers treated the participants to an excursion to Mullika old town in Kanchanaburi Province, where they learned about aspects of Thai traditions and farming.

Leela Ruckthong, Ronan Keegan, Garib Murshudov, Ruslan Sanishvili

From 29 January to 7 February 2024, King Mongkut's University of Technology Thonburi (KMUTT) in Bangkok, Thailand, hosted the third macromolecular structure determination training course entitled South East Asian Crystallographic Overview And Systematic Training (SEA COAST). The course was organized jointly by Leela Ruckthong and Ruslan Sanishvili (KMUTT, Thailand), Ronan Keegan (CCP4, STFC Rutherford Appleton Laboratory, UK) and Garib Murshudov (MRC LMB, UK).

Two prior courses at KMUTT were held in 2019 and 2020, but this was the first one after the COVID-19 outbreak. The training course, which covered all aspects of macromolecular crystallography, was designed to benefit researchers at various levels of their expertise. The course comprised the theoretical foundation and general principles of macromolecular crystallography, and of specific software programs, along with software tutorials. A significant portion of the time was dedicated to problem-solving sessions where the participants worked on their own crystallographic projects under the tutelage of the experts.

Applicants

Within the SEA COAST training series, we strive to bring the world's most advanced expertise to the Southeast Asian region, although we do not limit participation to this region. Graduate students, postdoctoral researchers and young scientists, from both academia and industry, who have a background in protein X-ray crystallography or are interested in it were encouraged to apply. For SEA COAST 2024, applications were accepted from Thailand, Malaysia, India, Hong Kong, Japan, UK and Austria.

Topics

Macromolecular crystallographic topics, such as crystallization, diffraction basics, data collection and processing, structure determination with experimental phasing and molecular replacement, AlphaFold-generated models for molecular replacement, molecular graphics, model building, structure refinement, model validation, ligands and bioinformatics were taught by some of the world-leading experts. The course also included introductory lectures on cryo-EM and neutron crystallography.

Software programs such as the *CCP4* suite, *Phenix* suite, *AutoProc*, *DIALS*, *MOSFLM*, *XDS*, *Arp/wARP*, *Coot*, *Phaser*, *ARCIMBOLDO*, *VAIRO*, *BUSTER*, *REFMAC* and *PISA* were taught during the course.

Instructors

Overall, 22 instructors took part in the course: Terese Bergfors, Uppsala University, Sweden; Grzegorz Chojnowski, EMBL, Germany; Kay Diederichs, Universität Konstanz, Germany; Maria Fando, CCP4, UK; Dave Hall, Diamond Light Source, UK; Robbie Joosten, NKI AvL, Netherlands; Ronan Keegan, CCP4, Harwell, UK; Eugene Krissinel, CCP4, Harwell, UK; Andrey Lebedev, CCP4, Harwell, UK; Andrew Leslie, MRC LMB, Cambridge, UK; Dorothee Liebschner, Lawrence Berkeley National Laboratory, USA; Bernhard Lohkamp, Karolinska Institutet, Sweden; Garib Murshudov, MRC LMB, Cambridge, UK; Dean Myles, Oak Ridge National Laboratory, USA; James Parkhurst, Diamond Light Source, UK; Randy Read, Cambridge Institute for Medical Research, UK; Marasri Ruengjitchatchawalya, KMUTT, Thailand; Ruslan Sanishvili, KMUTT, Thailand; Sofia Trampari, Dectris, Switzerland; Isabel Uson, IBMB CSIC, ICREA, Spain; Clemens Vonrhein, Global Phasing Ltd, UK; and Martyn Winn, STFC, UK.



First day of SEA COAST 2024. Some of the speakers arrived later and are not present in this picture.

Daily schedule

Typically, the first half of the day was dedicated to the lectures covering the topics of the day. They were followed by software tutorials and then by interactive problem-solving sessions where the tutors worked with students one-on-one or in small groups. The problem-solving sessions lasted till 22:00 and sometimes later.

The organizers also provided on-site catered coffee breaks, lunch and dinner. These were an integral part of the course as they fostered informal discussions between the participants – both students and instructors.



Randy Read explaining the fundamentals of experimental phasing.



Ronan Keegan talking about molecular replacement.



Garib Murshudov explaining the principles of macromolecular structure refinement.

New additions

There were some exciting new additions to our typical content. For the first time in the SEA COAST series, we added crystallographic data collection from students' crystals, conducted remotely on the I04 beamline of the Diamond Light Source (DLS). We also added introductory lectures in cryo-EM by Martyn Winn, Randy Read and Garib Murshudov.

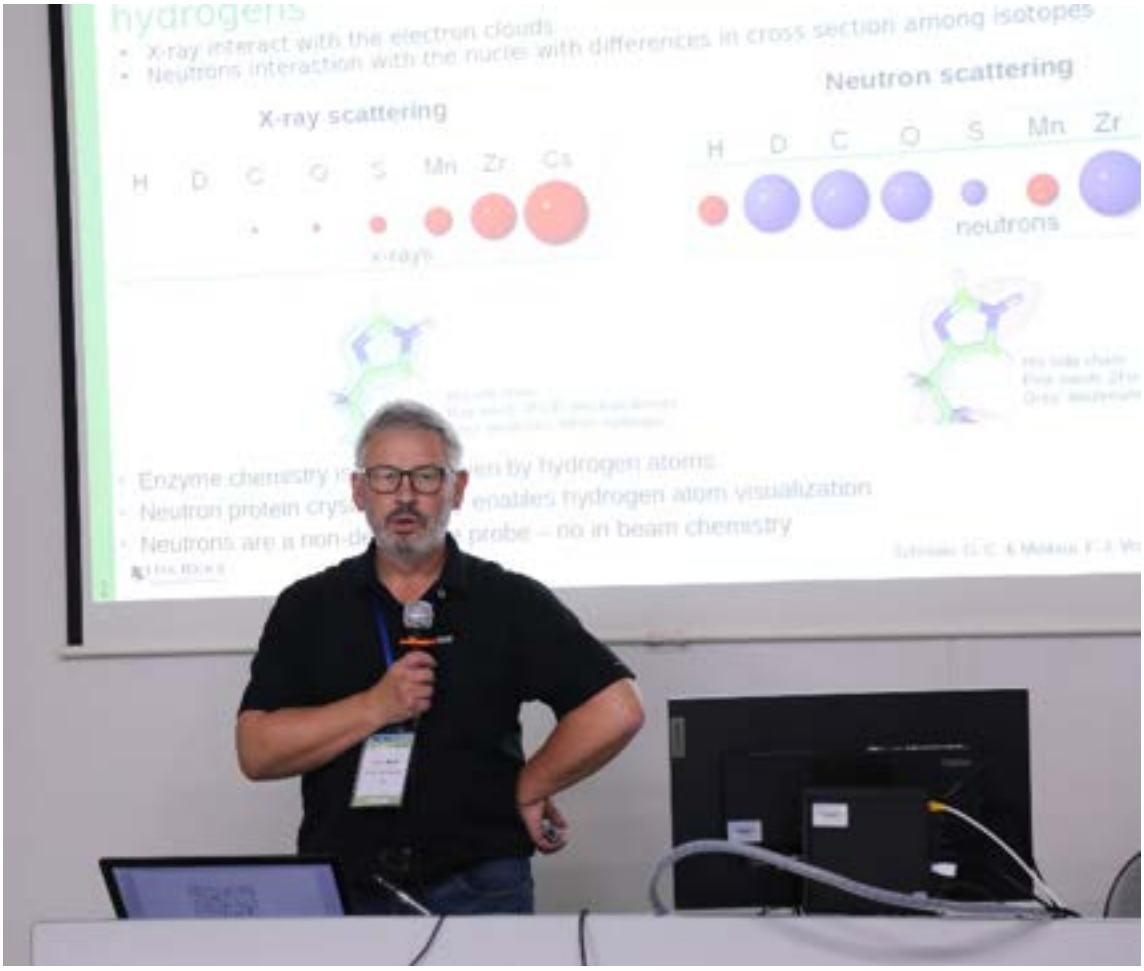
Dean Myles overviewed the method of neutron crystallography and caused quite a buzz when he revealed a new development in the field. Oak Ridge National Laboratory is building a new beamline to take advantage of spin alignment and anti-alignment of neutrons and protons, which should dramatically increase the signal-to-noise ratio, thus reducing the required sample size for data collection. In addition, deuteration of the sample will no longer be needed, significantly improving the accessibility of the method.



Dave Hall and Ruslan Sanishvili helping during remote data collection on the I04 beamline of the DLS.



Martyn Winn introducing all phases of structure determination with cryo-EM.



Dean Myles talking about the basics of neutron crystallography and new developments in the field.



Robbie Joosten (left) and Dorothee Liebschner (second from right) assisting the students from Malaysia.

Results

Twelve students had one or more challenging crystallographic problems to resolve. They had brought either the data (raw or processed), crystals or both to work on. Out of ten participants who tried data collection at DLS, six had diffracting crystals of one or several proteins and their modifications. Data measured during the course typically were of higher quality than prior data (when available). Several challenges could not be overcome as they were related to non-diffracting or very poorly diffracting crystals. In all other cases, students made significant progress in their projects during the course. Several structures of new mutant proteins and/or their complexes with desired ligands were solved and refined. In some cases, the absence of ligands was confirmed. One new structure was solved and refined as well. There was one exception. One set of well-diffracting crystals produced data with a non-trivial anomaly. This was true for data collected during the workshop and data measured previously. This problem could not be resolved during the course, and several experts were spurred to continue investigating the issue after the workshop.

There were a few novice participants with no specific crystallographic problems to work on. The workshop proved very useful for them as well, as they were able to enhance their understanding of the basics and were encouraged to further pursue their efforts to solve structures.

Feedback

A few quotes below, which were edited only for grammar, indicate the overall success of the course:

“All experts were very much involved in problem solving. We had complete guidance from beginning to end of the session”.

“My understanding of fundamentals has improved substantially after the workshop, and I learned a variety of new features of programs that I did not know before”.

“Please keep the workshop going for the coming years. This workshop will help to grow a community of structural biologists in Thailand and South East Asia”.

Future

Encouraged by the response from the students, and the enthusiasm of the speakers, we intend to organize this training course regularly. We will further expand the cryo-EM and neutron crystallography parts of the course. We will continue X-ray diffraction data collection from the students’ crystals and will eventually include data collection for cryo-EM and neutron diffraction as well.

Acknowledgments

We would like to express our gratitude to the Ministry of Higher Education, Science, Research and Innovation (MHESI) of Thailand, and the Science and Technology Facilities Council (STFC) of the UK for their generous funding of SEA COAST 2024. Additional funding was provided by the Faculty of Science of KMUTT, the Chemistry Department of KMUTT, the Protein Society of Thailand and MiTeGen. Computers used in the workshop were supplied by the Department of Mathematics, KMUTT. We are especially grateful to Dectris, whose generous sponsorship made the data collection at the DLS possible. We would also like to thank Dave Hall, Felicity Bertram, Marco Mazzorana and David Aragao for their support in preparation for and during data collection. We are also grateful to the KMUTT management for their overall support of the project.

MEETING REPORT (IUCR SUPPORTED)

First Senegalese Day of Crystallography



Magatte Camara, Ibrahima Elhadji Thiam, Rokhaya Sylla Gueye, Mbossé Ndiaye Gueye, Adama Sy, Farba Bouyagui Tamboura, Emmanuel Wenger, Claude Lecomte

1. Introduction

The aim of this article is to report on the first Senegalese Day of Crystallography organized by the Senegalese Crystallographic Association (ASC, Association Sénégalaise de Cristallographie).

2. Context

The First Senegalese Day of Crystallography (Cristal Ô) organized by the ASC took place on 19 February 2024 at Cheikh Anta DIOP Dakar University in the conference room of the International Center for Research and Training in Applied Genomics and Health Surveillance (CIGASS).

The aim of the event was first and foremost to launch the activities of the ASC and to enable young Senegalese researchers, teacher–researchers and engineers working in the fields of crystallography, material sciences, chemistry and biology to get to know each other through the presentation of the different activities of their home laboratories, and to encourage interactive exchanges between specialists and novices in crystallography. Particular attention was paid to the new CNRS/CRM^2 AFRAMED project (Doctoral Training and Research in Africa through remote X-ray diffraction measurements), a remote laboratory led by Professor Claude Lecomte. Launched on 31 August 2022, this project enables scientists from African laboratories to remotely control the CRM^2 single-crystal X-ray diffractometer located at CRM^2, Université de Lorraine, Nancy, France. This conference day was attended by 81 participants from five Senegalese public universities: Assane Seck University of Ziguinchor (UASZ), Alioune DIOP University of Bambey (UADB), Gaston Berger University of Saint-Louis (UGB), Amadou Mahtar Mbow University of Diamniadio (UAM), Iba Der THIAM University of Thies (UIT) and, of course, Cheikh Anta DIOP University of Dakar (UCAD).

3. The 2024 edition

Course of activities

The scientific day began under the auspices of the university authorities. The opening ceremony was presided over by Professor Bassirou Lô, Dean of the Faculty of Science and Technology at UCAD, representing the Rector, in the presence of the Head of the Chemistry Department, Professor Momar Ndiaye, the Director of Pedagogical Affairs (DAP) and many other leading figures from the Senegalese scientific world.

The event began with an official welcome address by Professor Ibrahima Elhadji Thiam, Chair of the day's organizing committee (UCAD), followed by words from Professor Magatte Camara, ASC President (UASZ);

Professor Emeritus Claude Lecomte; Professor Momar Ndiaye; and Professor Bassirou Lô.



Welcome addresses were given by (from left to right) Magatte Camara, Momar Ndiaye, Bassirou Lô, Claude Lecomte and Ibrahima Elhadji Thiam.

Immediately after the opening ceremony, we moved onto the inaugural lecture by Professor Lecomte entitled "Crystallography in Sub-Saharan Africa: Contribution of AFRAMED to the CNRS-IUCr-UNESCO Africa Initiative".

Why this conference? To understand the importance of developing crystallography and structural sciences in Sub-Saharan Africa. By answering the question: What is crystallography? Prof Lecomte showed that it is an essential science at the crossroads of disciplines such as mineralogy, geology, physics, chemistry, materials and life sciences.

The AFRAMED project was prompted by the emergence of COVID-19, with its widespread travel constraints. In 2022, the CNRS decided to give priority to collaborations with Africa and created the AFRAMED IRN (International Research Network) proposed by Professor Lecomte. AFRAMED is a five-year CNRS project: during one month, three or four young African colleagues are trained intensively to 'drive' single-crystal diffractometers by CRM^2 researchers (Dr Emmanuel Wenger, Dr El-Eulmi Bendeif and Professor Lecomte). Then, back in their home country, these colleagues can collect diffraction data on the CRM^2 diffractometers in remote mode for teaching and research. Since September 2022, Egypt, Togo, Cameroon and Gabon, Senegal, Congo Brazzaville, Ivory Coast and Algeria have been involved; in 2024, Madagascar, Burkina Faso and Mauritania will be the hosts of CRM^2. The trainees are fully funded by the CNRS IRN and the IUCr within its Crystallography in Africa initiative. UNESCO will join in 2024.

During the conference day, a remote session on single-crystal X-ray diffraction was led by Dr Wenger. Emmanuel centered a paracetamol single crystal on the diffractometer and taught all steps of XRD data collection. We noted great enthusiasm from the participants.



Researchers from eight research teams and laboratories in Senegal reviewed their research work in oral presentations, giving a brief overview of the research team, highlighting the use of the diffractometer – an iconic instrument in crystallography –, the contribution of crystallography to their field of research and their prospects.

Laboratory of Chemistry and Physics of Materials, LCPM (UASZ)



The Materials Chemistry and Physics Laboratory (LCPM) was established in 2010 and recognized by a Rector's decree in 2017. It is attached to the Sciences and Technologies UFR and Science, Technology and Engineering (STI) Doctoral School. Its current Director is Professor Magatte Camara, assisted by Professor Lat Grand Ndiaye. The LCPM has published over 300 publications and patents, and collaborates with 22 partner laboratories worldwide. Its research themes involve rare-earth-based inorganic materials, microporous and nanoporous materials, switchable materials, crystallography, materials engineering (ceramics, single crystals, thin films, nanostructures, waste recovery, biomass, biogas *etc*.), the chemistry of natural substances (extraction, isolation, characterization, fine chemical recovery) and synthesis methods for innovative molecules and molecular materials.

Organic Coordination Chemistry Laboratory, LCCOB (UCAD)



The Laboratoire de Chimie de Coordination Organique et des Biomolécules (LCCOB) was set up in 1998 by Professor Abdou Salam Sall and Professor Mohamed Lamine Gaye. It belongs to the Faculty of Science and Technology and the PCSTUI (Physics, Chemistry, Earth, Universe and Engineering Sciences) Doctoral School. Its current Director is Professor Ousmane Diouf, and it collaborates with several national faculties and institutes and with various public universities in Senegal. Collaborations with international laboratories include the universities of Marseille, Toulouse, Nancy, Grenoble, Paris, Tunis, Nouakchott, Conakry, Algiers, Lyon, San Carlos (Brazil) and Southampton (UK). Over 200 articles have been published in international journals. Its field of research is the synthesis of homonuclear and heteronuclear coordination complexes, and transition metal and lanthanide co-crystals from Schiff bases. The physico-chemical and biological properties of the molecules are studied.

Physical, Mineral, Organic and Therapeutic Chemistry Laboratory, LCPMOT (UCAD)



The Organic and Therapeutic Chemistry Laboratory, more than 50 years old, recently renamed the Physical, Mineral, Organic and Therapeutic Chemistry Laboratory (LCPMOT) according to the subjects taught, is housed within the Department of Pharmaceutical, Physical and Chemical Sciences of the Faculty of Medicine, Pharmacy and Odontology (FMPO) of UCAD. The main line of research focuses on the synthesis of ligands and transition metal coordination complexes with biological activity. Most complexes have antioxidant activities (evaluated with the DPPH radical) greater than those of the ligands, and the diazenes obtained present antimicrobial and anticancer activities on several tumor lines.

Inorganic and Analytical Chemistry Laboratory, LACHIMIA (UCAD)



Founded in 1978 by Professor Libasse Diop and currently headed by Professor Mamadou Sidibé, the Inorganic and Analytical Chemistry Laboratory (LACHIMIA) uses crystallography as one of its main methods for characterizing molecular structure and materials in general. LACHIMIA is involved in three major areas of research, namely coordination chemistry, mining environment and water chemistry. In the field of coordination chemistry, LACHIMIA favors single-crystal X-ray diffraction analysis to elucidate the structure of their materials. For the study of mining environments, particularly mine tailings and clay materials, X-ray powder diffraction is used to characterize their mineralogy and analyse their crystalline phases. LACHIMIA has characterized over 200 crystal structures of coordination compounds, resulting in more than 100 publications in international journals. Recently, the laboratory has also undertaken X-ray diffraction characterization of mine tailings from SABODALA and clays from various regions of Senegal, in collaboration with the SANTARGILE Company.

Quantum Energy Photonics and Nanofabrication Laboratory, LPQEN (UCAD)



The Quantum Energy Photonics and Nanofabrication Laboratory (LPQEN) is headed by Professor Balla Diop Ngom. LPQEN is a laboratory working on the synthesis and characterization of nanomaterials such as activated carbon, two-dimensional materials (graphene, MXene), metal oxides, metal oxi-nitrides, composites and nanocelluloses. The materials are characterized using various techniques to study their physico-chemical properties. These nanomaterials are used in supercapacitor electrodes. The experimental facilities of the laboratory are electric and chemical vapor deposition (CVD) furnaces, a 16-channel VMP300 Static Potentiometer, an 8-channel battery analyzer, an autoclave with a heating jacket and a pressure-controlled button cell crimping machine.

Chemistry of Inorganic and Organic Materials team, ECMIO (UADB)



The ECMIO research team, headed by Professor Farba Bouyagui Tamboura, is attached to the Physics-Chemistry doctoral program of Applied Sciences and Computer and Communication Technology UFR, Department of Chemistry of UADB. It has to its credit 57 publications in indexed and abstracted journals, and 17 oral presentations and 11 poster presentations at various conferences and seminars. Partner universities and institutes are UCAD; UASZ; the universities of Nouakchott (Mauritania), Strasbourg (France) and El Manar Tunis (Tunisia); and the Jean Rouxel Materials Institute (Nantes, France). Work focuses on organic and inorganic synthesis; complexation, magnetic, conductimetric, antifungal and antibacterial studies; and X-ray diffraction.

Environment - Engineering - Telecommunications and Renewable Energies Laboratory, LEITER (UGB)



LEITER is a laboratory that tackles issues linked to the production of scientific knowledge on renewable energies, energy efficiency and water and environmental engineering, from materials and their transformation to technological and engineering innovations to achieve greater energy efficiency in their use. The Laboratory promotes multidisciplinary research activities with a potential impact on the sustainable development of Senegal and Africa. LEITER comprises three multidisciplinary teams: Electronics-Electrotechnics-Automatics and Computing; Renewable Energies and Materials; and Water, Environment and Climate. Professor Amadou Seidou H. Maiga is the Director and he is assisted by Professor Elhadji Babacar Ly, who is a lecturer and researcher in materials chemistry at UGB. He conducts research into materials and their transformation for various applications such as construction materials, biocomposites, conductive polymers, paper and plastic packaging, membranes for water treatment, biogas and biofuel. He uses crystallography and diffractometers to identify chemical species and phases in materials, to design the best combinations of materials for a given application, and to interpret the results of his research.

X-ray Utilization Laboratory, LUX (FST-UCAD)



The LUX laboratory research team is currently headed by Dr Abdou Ciss Wade. LUX was set up in the Physics Department in 2000 by Professor Djibril Diop, with the help of the X-ray physics group at the University of Trento in Italy. In 2005, the lab was equipped with a Philips PW 1840 diffractometer, with Bragg–Brentano geometry θ–2θ, and in recent years has turned its attention to the study of local materials such as binders made from sewage sludge ash and lime, clays, eggshell powder *etc*. The objectives revolve around the design of materials by promoting interactions between technologies on the one hand, and physics and chemistry on the other; the development of composite materials with specific properties; understanding the electronic, structural and thermal behavior of fullerenes and fullerites; and determining the mechanical, physical, thermal and chemical properties of local materials (soils, ashes, clays, eggshells *etc*.). The laboratory collaborates with the Ecole Supérieure, UIT, University of Trento and Synchrotron Elettra (Trieste, Italy) and Université Gustave Eiffel (Paris, France). The laboratory has organized three international X-ray workshops, which took place in December 2005, January 2009 and January 2012.

Magatte Camara, Ibrahima Elhadji Thiam, Rokhaya Sylla Gueye, Mbossé Ndiaye Gueye, Adama Sy and Farba Bouyagui Tamboura are members of the ASC Executive Committee. Emmanuel Wenger and Claude Lecomte are at CRM^2 - Cristallographie, Résonance Magnétique et Modélisations, Nancy, France.

MEETING REPORT (IUCR SUPPORTED)

15th Biennial Conference on High Resolution X-Ray Diffraction and Imaging (XTOP 2024)



Olivier Thomas, Nathalie Mangelinck-Noël

The 15th Biennial Conference on High Resolution X-Ray Diffraction and Imaging (XTOP 2024) was held in Carry-le-Rouet, France, from 17 to 22 March 2024.

The first XTOP conference took place in Marseille, France, in 1992 and the last in Bari, Italy, in 2018. The main scope of the conference was set in 1992 to X-ray topography and high-resolution diffraction. However, over time the conference has covered other related topics such as X-ray tomography, phase sensitive scattering, scanning techniques *etc*. Nearly a third of the 150 participants at XTOP 2024, who came from 18 different countries, were young scientists.



Tutorials

The first day (18 March) was devoted to a companion school with five tutorial lectures, aimed at (but not exclusively for) students:

Basic concepts of X-ray scattering and prospects - Ian Robinson, London Centre for Nanotechnology, UK

X-ray surface scattering and its applications - Frank Schreiber, Eberhard Karls Universität Tübingen, Germany

Laue Diffraction X-Ray Microscopy - Jean-Sebastien Micha, Université Grenoble Alpes, UMR SyMMES, CNRS-CEA/IRIG, European Synchrotron Radiation Facility (ESRF), Grenoble, France

Bragg coherent diffraction imaging and its applications - Marie-Ingrid Richard, CEA Grenoble, France

X-ray ptychography microscopy and its applications - Virginie Chamard, Institut Fresnel, Marseille, France.

XTOP conference

The second day (19 March) saw the opening of the XTOP conference and ended with a lecture in honour of Professor André Authier, a specialist in X-ray topography, given by Michèle Sauvage, Emeritus Senior Scientist at SOLEIL, France. The sessions continued for the next three days, interspersed with a half-day boat excursion; an evening lecture on the history of the XTOP conference by José Baruchel, Emeritus Scientist at ESRF, France; and the gala dinner.



Poster sessions.

IUCr Young and Early Career Scientist Awards

The selection committee received 14 excellent applications from young researchers and PhD students, and decided to award four bursaries as follows (in alphabetical order):

Fabian Gasser, PhD student, Graz University of Technology, Austria
Poster contribution: "Intensity Corrections for Grazing Incidence X-ray Diffraction"

Merve Pinar Kabukcuoglu, postdoctoral research fellow, Karlsruhe Institute of Technology, Germany
Oral contribution: "Correlated 2D and 3D X-ray Diffraction Imaging revealing the Evolution of Dislocations during Thermal Processing of GaAs wafers"

Maya Wehbe, PhD student, Université Grenoble Alpes and Commission of Alternative Energies and Atomic Energy (CEA), Grenoble, France
Oral contribution: "Combining dark-field X-ray microscopy with scanning X-ray diffraction microscopy to study GaN coalescence"

Jiangtao Zhao, postdoctoral research fellow, ESRF, Grenoble, France
Oral contribution: "Bragg coherent modulation imaging".


IUCr
Fabian Gasser
Merve Pinar Kabukcuoglu
Maya Wehbe
Jiangtao Zhao

MEETING REPORT (IUCR SUPPORTED)

Hot Topics in Contemporary Crystallography 6 (HTCC6)



Aleksandar Višnjevac

Ever since the spectacular production of Shakespeare's *Hamlet* at Dubrovnik's St Laurent fortress (Lovrijenac) back in 1989, with Daniel Day-Lewis as the handsome Danish prince himself and Dame Judi Dench as Gertrude, Dubrovnik has been just a stone’s throw away from becoming an international star city of the performing industries. And, inevitably, it became one, as King's Landing, a mythical capital of seven kingdoms in the global blockbuster of the 2010s, *Game of Thrones*. Nevertheless, famous Academy Award winners, film makers and celebrities of all kinds are not the only ones wandering the charming alleys of this medieval jewel. Since pre-pandemic 2019, Dubrovnik has also been the scene of a series of macromolecular crystallography workshops – Hot Topics in Contemporary Crystallography (HTCC), organized by the Croatian Association of Crystallographers (CAC). The sixth edition (HTCC6) of this series took place from 7 to 12 April 2024 in the Akademis Academia, the very first embodiment of what is apparently to become a widespread new and unique Croatian format of an academic centre, combining student and commercial accommodation and student restaurants and cafeterias with top-notch sports, recreation and conference facilities, all in one place. The Akademis is located only a 15 minute easy walk (or just five minutes by public transport) from the old city gates.

HTCC6 was entirely dedicated to macromolecular crystallography (as were its two predecessors, HTCC4 and HTCC5, also held in Dubrovnik, in 2019 and 2023, respectively). During the four working days, which routinely started at 08:30 sharp and lasted until very late in the evening (frequently until 23:00), four topics were thoroughly tackled: crystallization (HT1), data collection (HT2), data processing and structure solution (HT3) and databases (HT4). This was achieved through a balanced number of lectures (17), tutorials (12) and demos/hands-on sessions (2). An absolute delight for the students and HTCC6’s *fil rouge* of a kind was the “Bring your own sample” activity, with two formal sessions and many informal gatherings, permitting students to bring their ill-crystallizing samples and improve the crystallization conditions using micro-seeding techniques with the help of a Douglas Instruments crystallization robot installed on site. Sadly, only two of the students (Sergio Müller from Argentina and Bilge Tosun from Türkiye) took advantage of this excellent opportunity to both improve their knowledge on the secrets of crystallization and work on their own troublesome samples. I was happy to see them both anxiously checking on their growing crystals even on the very last day of the workshop, and begging the organizers to delay the dismantling of the small wet lab.



Martin Caffrey’s demonstration of lipidic cubic phase crystallization.

Daniel Day-Lewis and Judi Dench may have been the megastars of *Hamlet* at Lovrijenac, but the stars of the HTCC6 were its lecturers and tutors, the list of whom I could not be prouder. Crystallization was masterfully presented, through an entire (long) day, by (in alphabetical order) Areej Abuhammad, Terese Bergfors, Martin Caffrey, Elspeth Garman and Patrick Shaw Stuart. The students practised 'crystal fishing' with the aid of a video microscope that projected onto the main screen, allowing everyone else to see exactly what was happening and to applaud when the 'fisher' was successful. They also had the opportunity to learn how to operate the Douglas Instruments crystallization robot and use this equipment for the crystallization of their own samples. The key word of the day was “seeding” – a magic that turns bad crystals into beautiful ones.



Late night crystal fishing competition.

Tuesday 9 April was a new day for a new topic – data collection. I wanted to shape this day so as to provide a practical and as-deep-as-possible insight into how data collection works on different platforms. Krešimir Molčanov gave an excellent talk on data collection on the home instrument, combining it with, as we realized by talking to students in due course and reading their honest answers and comments in our post-*festum* online survey, a much-needed basic crystallography crash course. It was followed by Annie Heroux's synchrotron experiment presentation with Nicola Demitri, who joined us live from an Elettra Synchrotron beamline in Trieste, Italy, and performed a typical experiment just for the eyes of the HTCC6 participants. The afternoon of the second day provided full justification for the very name of the workshop (Hot Topics in Contemporary Crystallography), with Henry Chapman, Saša Bajt and Dominik Oberthür introducing the theoretical foundations and practical aspects of serial crystallography, including a tutorial in which a typical experiment was presented step by step, by D. Oberthür.

Combined data processing, structure solution and refinement made up the third hot topic of HTCC6. The day was jam-packed with a series of alternating lectures and tutorials delivered by people who actually create and develop *CCP*4 – one of the most popular software packages for macromolecular crystallography: Eugene Krissinel, Rob Nicholls and Lucrezia Catapano. Finally, for the fourth topic, databases, we had with us contributors from both the PDBe (Paulyna Magaña and Genevieve Evans) and the CCDC (Ilaria Gimondi, Kepa Burusco-Gondi and Fabio Montisci), who demonstrated the up-to-the-minute features of these two important crystallographic databases with a particular emphasis on the zones where small molecule and macromolecular structures intertwine (docking). An entire lecture was dedicated to *AlphaFold*. Intensive hands-on sessions introduced students to the practical use of *PDB-KB*, CCDC *Crossminer* and *Gold*.



The databases hot topic was jam-packed with tutorials that required the full attention of everyone.

The workshop, which was this year again generously co-funded by the Croatian Science Foundation through project calixDNA (Principal Investigator: Aleksandar Višnjevac), and sponsored by Douglas Instruments, Labena, Selvita, Bruker and Jena Bioscience, gathered 52 registered participants from 16 countries (Argentina, Austria, Croatia, Czechia, Denmark, Germany, India, Ireland, Jordan, Latvia, Poland, Slovakia, Sweden, Türkiye, UK and USA) with 23 students and 17 tutors and lecturers. Sixteen students received bursaries to cover, partially or entirely, their registration fees and accommodation expenses. The bursary scheme was generously funded by the IUCr, the Croatian Association of Crystallographers and the European Crystallographic Association.

Students presented 15 posters and eight five-minute-long oral pitches called officially “discussion triggering presentations” (DTPs). The best presentations were rewarded with monetary prizes generously provided by Selvita (€150 in cash for the best DTP) and the CCDC (€100 in cash for the best poster). The reviewers (B. Zieba, T. Bergfors and A. Višnjevac for the Selvita best DTP award, and I. Gimondi, E. Garman and A. Abuhammad for the CCDC’s best poster prize) had a tough job indeed. It took firstly careful inspection and then long and sometimes fervent discussions to finally unanimously select the winners. Colin P. Wren from Ireland (for his poster *Symmetry Matched Protein – Macrocycle Assembly*) and Kinga Pokrywka from Poland (for her poster *Exploring the role of active site residues of Rhizobium etli L-asparaginase in catalysis*) shared the CCDC award for the best poster presentation. Boris Gomaz from Croatia won the Selvita best DTP award for his oral contribution entitled *Computational analysis of purine nucleoside phosphorylase dynamics*.



Colin Wren (left) and Kinga Pokrywka (right), best poster presenters, with Ilaria Gimondi from the CCDC.



The Selvita best DTP award went to Boris Gomaz (right).

As a devoted organizer, I am equally keen to motivate students and lecturers to complete and submit the online questionnaire on their impressions of the workshop, as I am curious about their answers and

determined to shape the future editions according to the opinions thereby gathered. I am particularly proud that this year the organization of the workshop, and communication with the organizing committee, as well as the quality of the lectures and expertise of the lecturers passed this test with flying colours. The overall impression of the accommodation, registration fee, lecture hall, website and online registration process was almost equally good. Most of the students who took part in the survey do feel, however, that the long hours were counterproductive, and that the workshop should rather be extended for a day or two, allowing some more free time to socialize and relax. However, I was puzzled by this overwhelmingly expressed opinion, as I sometimes had a hard time to chase students out of the lecture room at 23:00, as they were still enthusiastically discussing around the posters, whereas I had an agreement with the management to leave the room by this hour. Anyway, the answer to the question “Would you recommend the HTCC workshop to a colleague?” was almost unanimously (20 out of 21) positive. This is the ultimate encouragement to myself and my team of organizers not to spare efforts to keep HTCC running in the future.

More on HTCC6 is available on the Facebook page "Croatian Association of Crystallographers", on the Instagram profile "Croatian Crystallographers" and on the X profile @hrvukris. We are very much looking forward to HTCC7 and we invite you to keep an eye on our social networks so you do not miss it.

MEETING REPORT

FEBS practical crystallization course "Advanced methods in macromolecular crystallization X"



Under the leadership of Dr Jeroen Mesters (University of Lübeck, Germany), the yellow group works on the crystallization of their own proteins.

Ivana Kuta Smatanova, Pavlina Rezacova, Jeroen R. Mesters, Jose A. Gavira

The 10th FEBS practical crystallization course "Advanced methods in macromolecular crystallization“ took place at the Faculty of Sciences of the University of South Bohemia in Ceske Budejovice, Czechia, from 9 to 15 June 2024.

The course was organized by Ivana Kuta Smatanova (University of South Bohemia, Czechia), Pavlina Rezacova (Czech Academy of Sciences, Czechia), Jeroen R. Mesters (University of Lübeck, Germany) and Jose A. Gavira (National Research Council and University of Granada, Spain). It was primarily supported by the Federation of European Biochemical Societies (FEBS). Eleven companies also contributed by providing equipment and materials for lab exercises, covering registration fees for eight students through four YTF FEBS grants, two grants from the Czech Society for Structural Biology and two grants from the Czech and Slovak Crystallographic Association, and sponsoring three poster prizes and a special prize from Professor Bernhard Rupp (Innsbruck Medical University, Austria, and k-k Hofkristallamt, San Diego, CA, USA).

The course featured two practical workshops conducted by supporting companies including Douglas Instruments Ltd and Altium International s.r.o. A distinguished group of 33 speakers and tutors (12 female and 21 male) from 12 different countries with exceptional expertise in protein crystallization and crystallography led the course. They presented 31 morning and 2 evening lectures to 24 students (12 female and 12 male).

The course started with welcome addresses from Associate Professor Ludek Berec, vice-rector for science and development at the University of South Bohemia; Associate Professor Dagmar Skodova Parmova, the Mayor of Ceske Budejovice; and Professor Mutay A. Aslan, the FEBS Advanced Courses Committee (ACC) representative and Member in Charge from Akdeniz University, Turkey. Additionally, Dr Sara Fuentes, Managing Editor of *FEBS Open Bio*, delivered an online lecture titled "Tackling the Reproducibility Crisis in Scientific Research."

Following the opening ceremony, participants, including PhD students and postdocs, were greeted online by two former practical crystallization course organizers: Professor Rolf Hilgenfeld from the University of

Lübeck and Professor Juan Manuel García-Ruiz from LEC Granada. The participants were then introduced to new topics of structural biology (synthetic macrocycles, *PROTACS*, AlphaFold *etc*.) and advanced methods in protein crystallization (InCellCryst *etc.*).

The first day concluded with a welcome party where students had the opportunity to introduce themselves to the speakers on a one-to-one basis. From Tuesday to Friday, the course followed a rigorous schedule from morning (08:30) to night, featuring lectures and lab exercises. These sessions covered a range of topics, from biophysical techniques for analyzing protein properties and sample quality before crystallization (such as dynamic light scattering and protein labeling) to protein crystallization screening, crystal improvement and *in vivo* crystallization.



Red group: Professor Martin Caffrey (Trinity College Dublin, Ireland) demonstrates lipidic cubic phase crystallization. Blue group: Dr Lata Govada (Imperial College London, UK) explains crystallization under oil. Light brown group: Professor Claude Sauter (University of Strasbourg, France) explains crystallization in microchips. Green group: Dr Jose A. Gavira (LEC Granada, Spain) demonstrates capillary experiments. Orange group: Dr Terese Bergfors (Uppsala University, Sweden) and students prepare for crystal seeding experiments.

The students had the chance to perform experiments on their own proteins (with nine students bringing their own samples) or to use model proteins. Time was also allocated for poster sessions and discussions with the speakers. Three students were awarded the following poster prizes:

FEBS Open Bio to Tomas Brom (MU Brno, Czechia) for his poster “Insight into inherited anemia CDAI: disease associated mutations disrupt Codanin1CDIN1 complex”

IUCr Journals to Alexandra Knopp (Institute of Cancer Research, London, UK) for her poster “Structural Biology of RNA Helicases”

FEBS ACC to Yurii Dubanych (CU Prague, Czechia) for his poster “Characterizing the interaction between Galectin3 and the human natural killer cell activation receptor NKp30.

All awarded students presented the results of their work in a short lecture before the closing ceremony on Friday.

Additionally, a special prize was given to the most active participant, Anil A. Sohail (University of Oulu, Finland). He received a copy of Bernhard Rupp's book *Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology*, personally dedicated by the author.



Alexandra Knopp (centre), flanked by the four organizers, receives the IUCr Journals Poster Prize. Congratulations!

Saturday morning was devoted to crystal observation and the final evaluation of the practical results.

We would like to conclude by expressing our gratitude to FEBS and the sponsors for their support in sustaining this course. We also extend our heartfelt thanks to all the speakers and tutors, whose contributions created a warm and friendly atmosphere throughout the week.

The course webpage can be found here. The photos were taken by Petr Pachl, Klara Nohavova and Radomir Kuzel.

MEETING REPORT (IUCR SUPPORTED)

11th Zürich School of Crystallography: Bring Your Own Crystals



Hans-Beat Bürgi, Tony Linden, Course Directors

The 11th Zürich School of Crystallography, 17–29 June 2024, was held as usual in the Department of Chemistry at the University of Zürich (UZH). The 10 male and 10 female participants comprised one MSc and 13 PhD students, three postdocs, two research staff and one person from a pharmaceutical company. They came from 17 countries: Brazil, China (Hong Kong), Croatia, Denmark, France, Germany, Italy, Japan, Norway, Saudia Arabia, Singapore, Slovenia, Sweden, Switzerland, Tunisia, USA and Zimbabwe. The cohort included 11 full-time tutors and two local guest lecturers.

All of the participants were highly dedicated and worked tirelessly for the entire School, despite its intensity. While most participants were young scientists, the group this time included two upcoming service crystallographers. The levels of experience of the participants ranged from minimal to moderate. During casual interactions, we gained the clear impression that everyone felt happy that they had learnt something new and were more confident about tackling their own structure determinations.

Participants receive very personalised mentoring with our popular 2:1 student–tutor ratio and are additionally motivated by the "bring-your-own-crystals" concept of the School. They become well-equipped to determine their own structures when they return home and to recognise when they need to seek advice for a challenging problem. One participant was thrilled that the information on growing crystals, sent out before the School, had yielded instant results for the materials she had hitherto been struggling to crystallise. Many new friendships formed and it was pleasing to see everyone interacting with each other.



The aim of the School is to introduce the participants to the theory and practice of X-ray diffraction and single-crystal small-molecule structure determination. We cover all stages from crystal growth through to interpretation of the results and preparing material for publication. We deliberately limit the focus to single-crystal small-molecule crystallography so as to be thorough. The daily schedule combines a balance of lectures, tutorial exercises and practical work, including hands-on experience mounting crystals and collecting data from samples the participants provide. We use five diffractometers, which include dual-source Rigaku Synergy and Supernova instruments, as well as a Bruker Venture D8 diffractometer.



The concepts of symmetry are consistently a challenging theme, which appears in part to be related to the visualisation of objects and symmetry transformations in 3D. Online tools are useful, but are not truly 3D. In small tutorial groups, we use wooden and plastic models of solid shapes and molecules representing all point groups. The ability to hold and tumble such models helps the participants acquire the concepts more easily. It was also great fun watching people cutting their apples in the "La coupe du roi" exercise to illustrate stereochemistry and chirality, a demonstration initially presented during our Schools by Howard Flack.

An innovation introduced this time by Lukáš Palatinus was the use of short quizzes via the Kahoot platform. A multiple-choice question is beamed on the front screen and participants have a limited time (*e.g.* 30 seconds) to answer the question using their phones. The results are then displayed on the front screen, which allows quick discussion of the answers and clarification of any misunderstandings. Points are awarded for correct answers in the fastest time. The quizzes generated excitement and enthusiasm, while providing instant feedback and reinforcement of key points from the preceding lecture material.



During the practical component, the participants work on at least four example structures presenting varying degrees of difficulty. This facilitates learning how to use the software effectively and to handle frequently encountered challenges, such as entities lying on or across symmetry elements, disorder, absolute structure and the analysis of weak interactions. Participants learn about the actual procedures going on when various buttons and settings are selected in the software and to interpret whether appropriate results are obtained. Each participant then works on the data set collected from their own crystalline sample. We used *Olex2* once again, alongside the *SHELX* programs, *PLATON* and other readily available software. The extensive range of tools and graphics incorporated into *Olex2*, from routine tasks like atom-naming to modelling disorder, plus a range of quality indicators and statistics, allows us to demonstrate structure solution, refinement and results evaluation in a didactically beneficial way.

Most days concluded with a short discussion where participants can express their feelings about their experience that day. On the final morning, the participants sat a two-hour written exam either to obtain ECTS credit points or to self-test their knowledge. After the exam, the final day included some advanced topics and presentations designed to give the participants a taste of other possibilities, such as Hirshfeld atom refinements and electron diffraction.

The farewell banquet is an emotional time for everyone after making so many new friends. Each participant received a certificate, Swiss chocolate and a copy of *The Non-Ambient Guide* donated by Anton Paar. The two participants with the best exam results received additional prizes: an insulated UZH-branded coffee mug (first prize) and the old but still useful book *Crystal Structure Refinement, A Crystallographer's Guide to SHELXL* by Peter Müller (first and second prizes).



The personal impressions of two participants are given below. We anticipate organising the next School in June 2026.

We gratefully acknowledge the generosity of our sponsors and supporters: Department of Chemistry of the University of Zürich, Swiss Society for Crystallography, European Crystallographic Association, IUCr, Cambridge Crystallographic Data Centre, Rigaku Oxford Diffraction, Dectris Ltd, Bruker AXS, Anton Paar and Quantum Detectors.

Impressions from participants

Voon Kunn Ng (National University of Singapore)



My experience during the Zürich School of Crystallography 2024 was a truly rewarding one. Not only did I gain theoretical and practical knowledge on crystallography but also the interaction with tutors and participants introduced me to various cultures, forged friendships and created many fond memories.

The School was very well-organised, and students were very well taken care of. Even before the School started, we received the lecture notes and many reading materials to prepare us for the School. Detailed instructions on downloading the software were also provided in advance, giving us ample time to resolve any software issues. Tutors even made time to solve any software issues on the first day, ensuring that all of us were well-equipped when classes started the next day.

While instrument operation and data processing are not new to me, I was curious to understand what the significance behind every step was. In this aspect, the School did not disappoint and provided answers to my questions. There was still so much that I could learn despite having solved many structures myself. Small group tutorials were especially helpful to visualize space groups and symmetry operations, and tutors were very approachable to answer any queries that we had. I could feel the passion and enthusiasm that the tutors had for crystallography as they were teaching and explaining, making it extremely pleasant to learn from them.

Classes were highly intensive, and coffee breaks to take a breather were very much looked forward to. The free day in the middle of the School also provided some rest time and an opportunity to explore the city. Even though ten days of crystallography were exhausting, knowing how much effort the tutors put in made me determined to absorb the knowledge that they were passing on.

On the last day of classes, all students sat for a 2-hour examination to test our knowledge gained during the School. As someone who last sat for an exam many years ago, it was nerve wracking, yet I was eager to know how much information I had acquired in the past ten days.

To sum it up, the School has taught me to greatly appreciate crystallography. It was an engaging and enriching experience, getting to know people in the field and learning so much from them. I would like to thank the organisers, Professor Tony Linden and Professor Hans-Beat Bürgi, for the opportunity to participate in the School, and making sure that we were always getting the best out of it.

Andrea Vitale (Bologna, Italy)



During the second half of June, from the 17th to the 29th, I had the opportunity to spend time with 19 other young researchers from all over the world in Zürich, Switzerland, for the Zürich School of Crystallography 2024.

It was a beautiful and formative experience, offering one of the most comprehensive understandings of crystallography and its related fields, both in practical applications and research.

Professors Anthony Linden and Hans-Beat Bürgi organized and directed the school in an exceptional manner. From the incredible selection of well-prepared tutors, who guided us through this intense and educational journey, to the carefully chosen hotel and restaurants that facilitated socializing and provided opportunities to meet and converse with professors and fellow researchers sharing the same passion. These interactions were inspiring, offering various perspectives and topics in this field.

For me, the school greatly enhanced my understanding of the foundational aspects of my research, particularly concerning the theory behind structure solution and refinement models.

Every lecture was filled with information, tips and tricks that crystallographers can use in their daily work. All this magnitude of knowledge was provided in both paper and .pdf formats, which will be very useful for continuing my studies and supporting my research projects. Additionally, we had the chance to collect diffraction intensities from our own crystals using the most advanced diffractometers and detectors for single-crystal structure determination. This hands-on experience allowed me to learn more about the instruments and their software, and it gave me the opportunity to solve and refine my own synthesized structure, manage its disorder and study its packing within the unit cell.

In conclusion, the Zürich School of Crystallography has been the highlight of my first year in my PhD program. It has already significantly contributed to my future career, research and experiments, and it provided the chance to meet incredible people whom I look forward to encountering again in the future.



MEETING REPORT

CCDC Science Day



The Cambridge Crystallographic Data Centre (CCDC) sponsors a number of PhD and Master's students each year and co-supervises them alongside leading scientists from academic and commercial institutions. As a charitable institution, its mission is to support the development of the next generation of scientists. Every year, these students and their external supervisors are invited to the CCDC office in Cambridge, UK, to spend a day presenting their research, listening to their peers and sharing knowledge and ideas.

This year wasn’t any different. CCDC Science Day 2024 on 27 June started with Nathan Hennessy, a third-year student from the University of Leeds, presenting on “Cooling Crystallisation from Binary Solvent Mixtures: Relationships between Solvent Composition and Activation Barriers for Nucleation”. Nathan presented crystallization at the molecular level, focusing on the example of L-histidine and explained the process of solution and crystallization, emphasizing the importance of factors such as Gibbs free energy, enthalpy, entropy and solvent composition. His research goals involve determining activation barriers for dissolution and crystallization, correlating them to solvent composition and analyzing trends using computational data. The workflow created by Nathan involves assessing solubility profiles to determine the feasibility of crystallization using different solvent mixtures, and he is exploring how data from the Cambridge Structural Database (CSD) can be used to understand these processes.

Dori Gasparikova, a final-year student from Durham University, presented her research on glucokinase (GK) and its role in the body, particularly in the liver where it converts glucose into glycogen and in the pancreas where it is involved in glucose-stimulated insulin release. The importance of studying GK concerning diabetes management was emphasized, considering the adverse effects of current therapeutics. Dori also referred to potential binders of GK, including activators and inhibitors. Her project goals were divided into experimental and computational methods, involving protein expression and purification, as well as docking experiments to guide the design of molecules. The optimization of GK expression, purification and validation was described, along with the initial steps in protein purification using affinity chromatography with a HisTrap HP column.

Harry Nash is in his final year at Sheffield University, and he presented his work on exploring and predicting sigma-hole interactions in the CSD using machine-learning techniques to predict interaction energies. Harry explained the nature and characteristics of sigma-hole interactions, the expected trends and the reasons for the interest in these interactions. The workflow involves searching the CSD with *ConQuest*, using the CSD Python API for automation of searches, geometric trend analysis of the data, machine learning using a database of sigma-hole interactions and their calculated energies, and finally validation against a dataset of molecular cutouts from the CSD.

Emilia Prandini, a second-year student from Politecnico di Torino in Italy, was up next to present her project “Predicting particle quality attributes of organic crystalline materials using particle informatics”.

Her main topic was predicting the particle quality of crystalline materials using informatics methods, focusing on a case study of a quercetin dimethyl formamide solvate. Her presentation covered crystal engineering, particle informatics methods and the impact of crystal properties on particle quality attributes. The methodology combines computational and experimental approaches, including XRD, molecular modelling, surface analysis, thermal stability studies, crystal phase determination and crystal growth analysis. Emilia's research aims to correlate crystal structure with surface properties, particularly focusing on the desolvation behaviour of this complex quercetin/dimethyl formamide system.

As usual, we wrapped up the day with engaging lightning talks from our first- and second-year students. We started with Aaron Horner, from the University of Southampton, who is evaluating new methods to quantify complex molecular models. Henry Holleb, from Durham University, is researching the hydration of pharmaceutical salts. James Broster, from the University of Oxford, is studying physics-based and machine-learning docking methods. Alex Lee, from Durham University, is researching high-throughput conglomerate synthesis and analysis. William Midgley, also from Durham University, aims to use *GOLD* to aid PROTAC linker design. Finally, Omar El-Habbak, from the University of Strathclyde, is focused on correlating digital and experimental chemical space to pharmaceutical manufacturing processes.

The presentations covered a wide range of topics, from molecular level crystallization to predicting particle quality attributes of organic crystalline materials, showcasing the depth and breadth of scientific inquiry being pursued. The engagement and enthusiasm of both the students and their supervisors were evident throughout the day, highlighting the collaborative and supportive environment fostered by the CCDC. It was truly a day of knowledge sharing, inspiration and celebration of scientific inquiry.

Blog highlights

CCDC scientist awarded prestigious BACG Young Scientists Award



Dr Pietro Sacchi, Research and Application Scientist at the CCDC, has been awarded the British Association for Crystal Growth (BACG) Young Scientists Award for his exceptional research on the HIV drug Ritonavir. The award is granted annually to a candidate who has made the most significant advance in the understanding of crystal growth processes. Pietro won based on his ground-breaking paper "Crystal Size, Shape, and Conformational Changes Drive Both the Disappearance and Reappearance of Ritonavir Polymorphs in the Mill".

CSD Tools in Action: Cocrystal Design and Structural Features Analysis

Izabela Madura and co-workers from the Warsaw University of Technology, Poland, used crystal structure analysis from the CCDC to design and study two cocrystals of caffeine and phenylboronic acid. This study investigates two cocrystal polymorphs composed of caffeine and 4-chlorophenylboronic acid using solid-state informatics tools.

Read more here.

CCDC Online Events: Free Virtual Workshops in October and November 2024

8 October: First Steps in Protein-Ligand Docking With *GOLD*

22 October: *ConQuest* to *Mercury* – From Searching to Data Analysis

5 November: Introduction to Pharmacophore Searching Using *CSD-CrossMiner*

All sessions are 90 minutes long and will include presentations and demonstrations by CCDC expert tutors and a hands-on part for participants to try the software, with the tutors available to help and answer questions. See here for more information.

CCDC Engagement Grant

Applications for the 2024/2025 round of CCDC Engagement Grants are now open! Awards are available to fund the creation of new STEM outreach activities and resources about crystallography or structural science to inspire non-specialist audiences, such as children and the general public.

Whether it's a video, social media content, game, poster or any other related activity, the CCDC wants to hear your ideas! You can explore the resources created by the winners of previous years' engagement grants here for inspiration. **Applications close on 30 September 2024 (11:59 pm BST).**

HISTORY OF CRYSTALLOGRAPHY

Mineralogists and crystallographers at the Berlin Natural History (Naturkunde) Museum



The Berlin Naturkunde Museum. Photograph by the authors.

Istvan Hargittai, Magdolna Hargittai

The Berlin Naturkunde Museum – Natural History Museum remembers some mineralogists and crystallographers from a time when the interest in understanding nature was much less compartmentalized than it is today. Here, we present memorials of Carl von Linné, Martin Heinrich Klaproth, René-Just Haüy, Christian Samuel Weiss and Eilhard Mitscherlich.

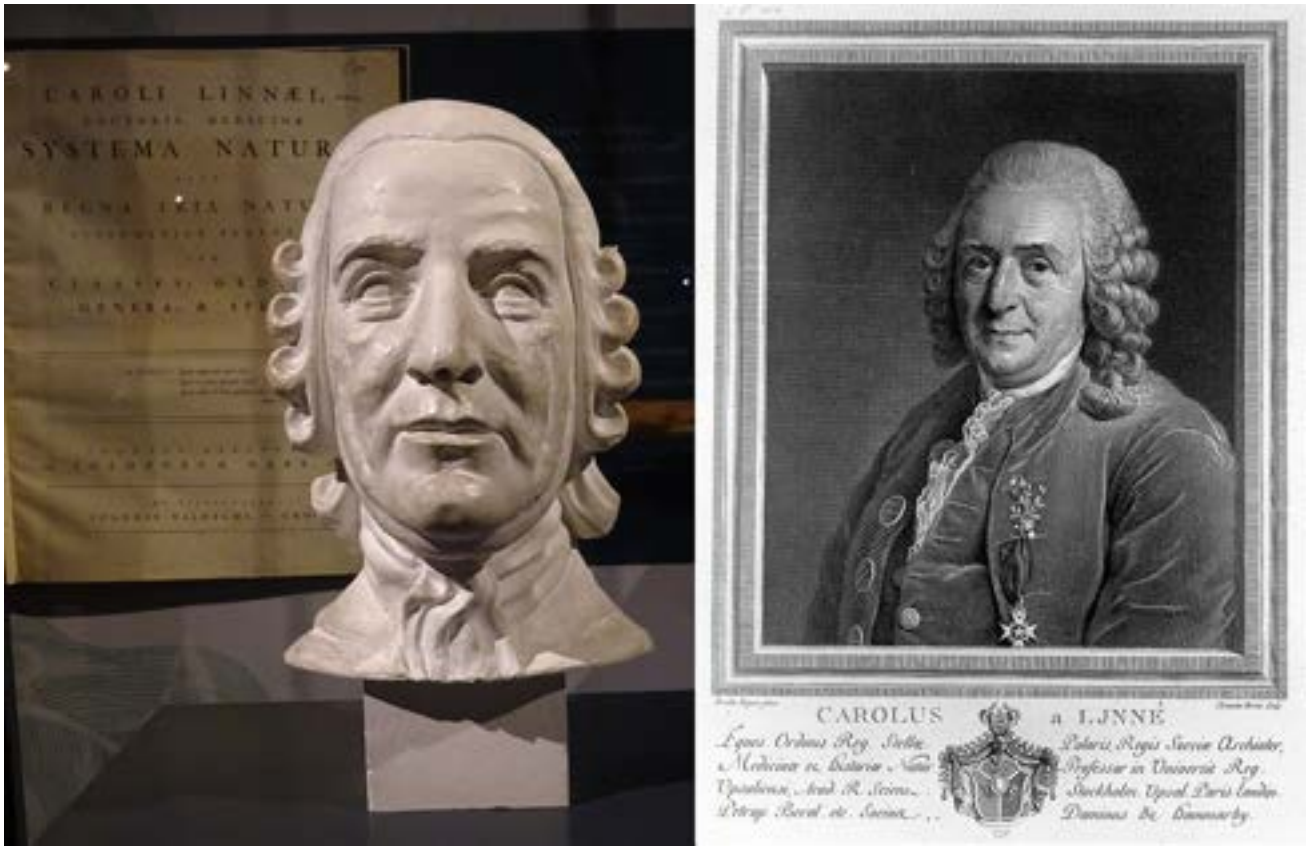


The two statues at the entrance of the building: Leopold von Buch to the left and Johannes Müller to the right. Photographs by the authors.



The central exhibition hall of the Museum. Photograph by the authors.

The Berlin Naturkunde Museum was founded in 1810 and has been at its present location, at Invalidenstraβe 43, since 1889. The two full-figure statues flanking the entrance honour the geologist and paleontologist Leopold von Buch (1774−1853) and the physiologist and anatomist Johannes Müller (1801−1858). The mineral collections of the Museum date back to 1700 and were initiated by the Prussian Academy of Sciences. They represent 75% of the minerals in the world. The Hall of Minerals exhibits 4500 specimens of a total of 250,000. The four scientists remembered below contributed to the development of classical crystallography to a smaller or greater extent. Eilhard Mitscherlich's discovery of crystallographic isomorphism has had relevance even for protein crystallography. Here, we present the images of their memorials in the Naturkunde Museum and augment them with selected other memorials elsewhere.



Carl von Linné (Linnaeus): bust at the Naturkunde Museum (photograph by the authors) and engraved portrait by C. C. Bervic (1779) after A. Roslin (1775). Wellcome Collection.



Statue of Linnaeus and one of its side figures, representing mineralogy, by J. Fr. Kjellberg (1885) in the Humlegården park, Stockholm. Photographs by the authors.

Carl von Linné (Carolus Linnaeus, 1707−1778) was one of the giants of science in the field of natural philosophy. He is best known for his taxonomy of plants. His contributions to crystallography were considerable given the state of sophistication of the field at this time, but were dwarfed in comparison with his other activities. Some early crystallographers, such as R.-J. Haüy, considered Linné a pioneer of the science of crystallography (see [1], p. 44). Linné was interested in the shapes of crystals; he drew them and prepared their wooden models. Incidentally, the authors of this contribution first learned about crystal shapes using wooden models in their studies at Eötvös University Budapest. Linné attempted to classify crystals according to their forms.



M. H. Klaproth: bust at the Naturkunde Museum (photograph by the authors) and drawing by E. J. B. Bouillon-Lagrande and H. A. Vogel (1810−1811), Wellcome Collection.

Martin Heinrich Klaproth (1743−1817) was a German pharmacist and chemist. He is best known for his discoveries of uranium and zirconium; co-discoveries of titanium, strontium, cerium and chromium; and for the validation of tellurium and beryllium having first been described by others. He originated from modest circumstances; he was a tailor's son and grew up in Wernigerode, Kingdom of Prussia. He studied pharmacy in Berlin and in several other cities, and he ran a pharmacy in Berlin for many years. He developed a true research laboratory adjacent to his pharmacy, conducted investigations, and published 84 papers. He became a member of the Berlin Academy of Sciences and, eventually, a paid officer of the Academy. He lectured in chemistry at the Prussian Royal Artillery, and his last appointment was a professorship in chemistry at Berlin University.

We feel motivated to say a little more about the discovery of tellurium. The Hungarian polymath Pál Kitaibel (1757−1817) worked at the medical school in Pest (Buda and Pest were separate cities at the time) and did research in chemistry, mineralogy, hydrology and botany. He discovered a new element in 1789 but did not name it. Eventually, he learned that it had already been discovered in 1782 by the Austrian mineralogist Franz-Joseph Müller von Reichenstein (1740−1825) in Transylvania (currently in Romania) while Müller was analyzing gold ores. It was not an easy discovery as it was difficult to distinguish it from antimony, an element already known. Müller called the new element *aurum*

paradoxium and *metallum problematicum* and sent a sample to Klaproth, who identified it and named it tellurium (the Latin *tellus* means earth). In contrast to frequent disputes in connection with the discovery of new elements, both Klaproth and Kitaibel readily acknowledged Müller's priority.



René-Just Haüy: drawing at the Naturkunde Museum (photograph by the authors) and statue by Isidore Hippolyte Brion at the Muséum National d'Histoire Naturelle à Paris (the National Museum of Natural History; photograph cropped by the authors) (René Just Haüy at MNHN.jpg - Wikimedia Commons, licensed under Creative Commons Attribution-Share Alike 3.0).

René-Just Haüy (1743−1822) was born into a poor family in the north of France. He studied thanks to scholarships and was ordained as a Roman Catholic priest in 1770. He had broad interests turning him to botany and then to crystallography. According to a story, his attention to crystal structures was first caught by the smooth planes of the crystal faces he observed when he accidentally dropped a crystal and it broke. His many contributions to the development of crystallography are documented throughout the chapters of the *Historical Atlas of Crystallography* [1]. The second, updated edition of Haüy's principal work, *Traité de Cristallographie*, appeared in 1822 and was reprinted in 1968 [2].



Christian Samuel Weiss: bust at the Naturkunde Museum, inside, and *bas-relief* on its facade. Photographs by the authors.

Christian Samuel Weiss (1780−1856) was a German mineralogist. He taught physics in Leipzig and was appointed Professor of Mineralogy at the University of Berlin in 1810. He was among the pioneers of modern pre-X-ray-diffraction crystallography. He introduced or expanded classification, instrumentation and mathematical techniques into his science.



Eilhard Mitscherlich. From left to right: bust at the Naturkunde Museum (photograph by the authors), statue by Carl Ferdinand Hartzer (1894) in front of the east wing of the main building of Humboldt University in Berlin (Berlin, Mitte, Humboldt-Universitaet, Standbild Eilhard Mitscherlich 03.jpg - Wikimedia Commons licensed under Creative Commons Attribution-Share Alike 3.0) and *bas-relief* portrait at Eötvös University Budapest (photograph by the authors).

Eilhard Mitscherlich (1794−1863) was a German chemist who, in 1819−1821, first described crystallographic isomorphism. He was born around today's Wilhelmshaven into an intellectual family. He studied philology at the University of Heidelberg. Then he switched to chemistry at the University of Göttingen. From 1818, he worked in a chemical laboratory in Berlin and established that corresponding phosphates and arsenates crystallize into the same form. This observation was the seed for his theory of crystallographic isomorphism (*isos* – equal and *morphe* – form). Mitscherlich first presented his observation in December 1819 at the Berlin Academy of Sciences and published it in French in 1820 [3].

The true significance for crystallography began appearing one hundred years later. Consider the following definition for isomorphous compounds: they have nearly identical structures except that one or more atoms are replaced by chemically similar ones. This is what was most successfully utilized in the structure determination of systems of ever-increasing size, the technique being called isomorphous replacement.

Recently, one of us followed the intricacies of how this utilization began in protein crystallography, including how some of the principal participants remembered it [4]. This paper was appended with a summary of selected references of the beginning of isomorphous replacement in crystallography ([4], pp. 638−639) based on the *International Tables of Crystallography* [5] and Neil Isaac's historical review [6]. The applications culminated in the first great successes of the isomorphous replacement method in the analysis of protein structures, *viz.* myoglobin by John C. Kendrew *et al.* [7] and haemoglobin by Max F. Perutz *et al.* [8]. Kendrew and Perutz shared the Nobel Prize in Chemistry in 1962 "for their studies of the structures of globular proteins." Application of Mitscherlich's observations remains fruitful even over two hundred years after he made them.

In his subsequent years, following the discovery of the law of isomorphism, Mitscherlich made substantial contributions in the area we would call today 'physical chemistry and catalysis', with results of lasting value in organic chemistry, inorganic chemistry, mineralogy and geology. He was among the pioneers of recognizing the phenomenon of crystallographic polymorphism, when the composition of the crystal is the same but its form is different [9]. This phenomenon has far-reaching consequences; suffice it to mention its pharmaceutical significance and the numerous lawsuits related to it.

Mitscherlich made a prescient observation in 1844 that a "solution of commercial tartaric acid rotated the plane of polarized light to the right while solutions of 'racemic' acid had no rotatory power" (see Jenny P. Glusker referring to Jean Baptiste Biot [1], p. 91). Mitscherlich carried on his research almost to the end of his life. He received national and international recognition for his work; among them was a gold medal from the Royal Society of London for his discovery of the law of isomorphism.

Acknowledgment

We thank Professor Johannes Vogel, Museum für Naturkunde Berlin, for kind assistance.

References

[1] Lima-de-Faria, J. (1990). Editor. *Historical Atlas of Crystallography*. Dordrecht: Kluwer Academic Publishers.

[2] Haüy, R. J. (1822). *Traité de Cristallographie*. Paris: Bachelier and Huzard. [Reprinted in 1968 in Brussels by Culture et Civilisation.]

[3] Mitscherlich, E. (1820). *Ann. Chim. Phys.* **14**, 172–190.

[4] Hargittai, I. (2022). *Struct. Chem.* **33**, 635–639.

[5] Vijayan, M. & Ramaseshan, A. (2006). *International Tables for Crystallography*, *Volume B: Reciprocal Space*, ch. 2.4, edited by U. Shmueli, pp. 264–275. Dordrecht: Springer.

[6] Isaac, N. (2016). *Acta Cryst.* D**72**, 293–295.

[7] Kendrew, J. C., Dickerson, R. E., Strandberg, B. E., Hart, R. G., Davies, D. R., Phillips, D. C. & Shore, R. G. (1960). *Nature*, **185**, 422–427.

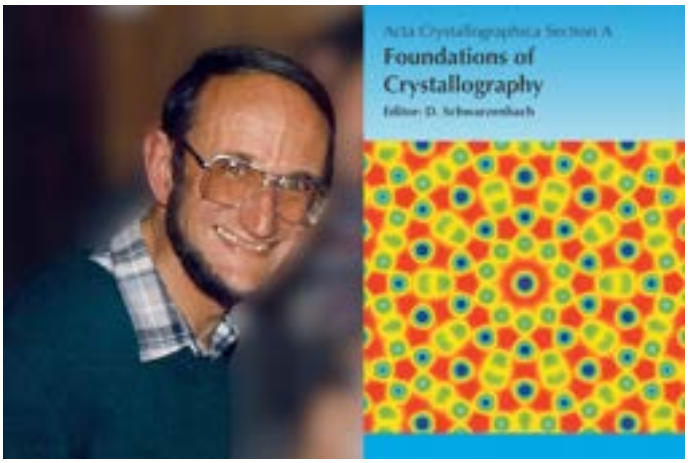
[8] Cullis, A. F., Muirhead, H., Perutz, M. F., Rossmann, M. G. & North, A. C. T. (1961). *Proc. R. Soc. Lond. A*, **265**, 15–38.

[9] Mitscherlich, E. (1822). *Ann. Phys.* **1**, 125–127.

Istvan Hargittai and Magdolna Hargittai are at the Budapest University of Technology and Economics.

OBITUARY

Dieter Schwarzenbach (1936–2024)



Dieter Schwarzenbach during the International Symposium on Accuracy in Structure Factor Measurement, Warburton, VIC, Australia, in August 1987. Photo credit: Sydney R. Hall.

Gervais Chapuis

Dieter passed away at the hospital in Lausanne, Switzerland, after a long neurodegenerative decline. He leaves behind his wife, Vera, and his two children, Charlotte and Thomas.

I met Dieter in 1966 when I started my doctoral studies at the Institute of Crystallography at the ETH in Zurich. That was shortly before his departure for a postdoctoral internship in the USA. In 1969 he returned to Zurich, bringing with him the newly developed *X-ray System* of programs for the solution of crystal structures. I was very fortunate to take advantage of it: it allowed me to crack a difficult structure by direct methods and finalize my PhD thesis. Later, it was also Dieter who helped me to find the most suitable place for a postdoctoral position, in David Templeton's group in the Lawrence Berkeley laboratory.

The experience gained by Dieter in America, first in Pittsburgh in Professor George Allen Jeffrey's Department of Crystallography and then at UCLA in Professor Ken Trueblood's Laboratory, in addition to his PhD with Professor Fritz Laves' group at the ETH in Zurich, formed an excellent basis for a successful career in crystallography. Indeed, shortly after his return from the USA, in 1970 he was offered a position as a lecturer in the Science Faculty at the University of Lausanne for a basic course in crystallography. Three years later, he was offered the opportunity to create and lead the Institute of Crystallography at the same institution with the position of Extraordinary Professor, which was later upgraded to full Professor in 1978.

My stay in Berkeley was coming to an end when Dieter visited me in 1973 and invited me to complete his team in Lausanne. Thus, in 1974, I returned to Lausanne to pursue my career in crystallography as a lecturer in Dieter's lab.

Since its creation, the Institute of Crystallography has delivered lectures and practical courses in various fields of crystallography to students of the University of Lausanne (UNIL) and of the Federal School of Technology (EPFL). In particular, students of physics, chemistry, materials and earth sciences have followed the basic and advanced courses. Our common book (Schwarzenbach & Chapuis, 2006) resulted from our experiences in teaching crystallography.

In parallel, the research work of Dieter and his team developed in numerous directions of crystallography. Measuring electron density in crystalline structures using diffraction methods was an important part of Dieter's interests. Would precise electron densities measured by diffraction be able to

reproduce certain physical quantities, such as electric field gradients (EFGs)? One of his most cited articles (Lewis *et al.*, 1982) concerned the charge densities and EFGs in corundum, α-Al_2O_3, where the capabilities and limits of diffraction methods were clearly demonstrated. Other important studies followed, including of the charge densities in cuprite, Cu_2O (Restori & Schwarzenbach, 1986), a paper published with his PhD student Renzo Restori in which the influences of the data-reduction processes, anisotropic displacements and the deformation models were explored. Other compounds like Li_3N, TiO_2, CoS_2 and NiS_2 were all part of an important programme of studies on charge densities.

During his career, Dieter developed some very fruitful collaborations with colleagues from nearby institutions. Hans-Beat Bürgi, head of the Laboratory of Crystallography in Bern, and Howard Flack from the University of Geneva were among them. The discovery of C_{60} resulted in many interesting studies, both in Bern and Lausanne. The development of the *Xtal* system of programs by Dieter's PhD student Eric Blanc contributed greatly to obtaining successful results. His *LSLS* ('Lausanne least-squares') program had some new capabilities regarding absorption, extinction corrections and twinning which led to the C_{60} paper by Bürgi *et al*. (1992). This fruitful collaboration on fullerenes resulted in four additional papers on various modifications and phases, improving models and obtaining more precise data on the orientational disorder and C—C bond distances.

Dieter and Howard Flack published an important series of well cited publications relating to some new theoretical developments in the methodologies of crystal diffraction. Both laboratories were involved in the software developments of the *XRAY* system and its successor, *Xtal*. About a dozen papers covering various topics from the use of least-squares restraints for origin fixing in polar space groups (Flack & Schwarzenbach, 1988) to the evaluation of transmission factors and their first derivatives with respect to crystal-shape parameters (Blanc *et al*., 1991) were published. Perhaps the most tangible result of their collaboration was the establishment of the Subcommittee on Statistical Descriptors by the International Union of Crystallography (IUCr). A panel of international specialists in statistical methods in physics and crystallography joined efforts to establish a series of recommendations for the proper treatment of statistical errors in crystallographic research. Dieter was the Chair of the panel, which also included Howard as a member. Two reports, *Statistical descriptors in crystallography* parts I and II, resulted (Schwarzenbach *et al*., 1989, 1995). They listed a series of 13 recommendations, the validities of which form the basis of the current statistical treatment of crystallographic data. It is owing to the second report that the commonly used term 'estimated standard deviations' (e.s.d.'s) was replaced by the more accurate term 'standard uncertainties' (s.u.'s).

While studying the impressive list of Dieter's scientific publications, close to 150, I was struck by the diversity of his interests, which covered a very large number of fields in crystallography. They extended from historical notices to mathematical crystallography, symmetry, diffraction theories and structure modeling, to cite only the most important topics. Dieter had an excellent memory and he always impressed his audience with his vast knowledge of crystallography.

The IUCr also benefited greatly from Dieter's expertise, as he served as a Co-editor for both *Acta Crystallographica* Section A (from 1992 to 2002) and Section B (from 1992 to 1999). He was then appointed as Section Editor for *Acta Crystallographica* Section A in 2002, a position he held to 2011, and as part of this role he was also an *ex officio* member of the Commission on Crystallographic Nomenclature.



Under Dieter's leadership, the Lausanne Institute of Crystallography attracted a large number of international visitors. This was facilitated by two other institutions in Lausanne: the Herbette Foundation from UNIL and the '3^{e} cycle' of physics (which would now be called a doctoral school) of the French-speaking part of Switzerland. Both institutions were able to support the visit of international lecturers for a few months. During that period, we could greatly benefit from the lectures of a very impressive panel of specialists, including Aloysio Janner, Ted Janssen, David Templeton, Pierre Toledano, Richard Welberry, Terry Willis, Hans Wondratschek and Akiji Yamamoto. The first version of Richard Welberry's book on X-ray diffuse scattering appeared in Lausanne as lecture notes on the same subject! It was also in Lausanne that Howard Flack developed the concept of his famous parameter during the visit of David Templeton and fruitful discussions on Rodger's η parameter.

Under Dieter's direction the Institute of Crystallography led to the creation of the very successful Swiss–Norwegian beamline (SNBL) at the ESRF in Grenoble. In the beginning, the essential problem for Dieter and Hans-Beat Bürgi (who was also interested in this facility) was not the financing of the beamline but rather finding first common objectives between the two participating countries and creating common visions to lead the project. It took a few years to solve all the administrative problems leading to the creation of the SNBL Foundation. Today the SNBL is a flourishing institution for the benefit of Swiss and Norwegian scientists.

Dieter was also admired by members of the Institute for his deep knowledge of the history of Switzerland. He could also cite entire poems from German and English literature, in particular extracts from Goethe's *Faust* and quotes from Shakespeare.

Dieter was a fine musician and very athletic. His career as a musician started as a student in 1957 as a violinist in the Zurich Academic Orchestra. He pursued his musical activities in Lausanne long after his retirement and participated actively in a few amateur orchestras, very often along with Vera, who is a respected violist. Dieter also rode his bicycle to the Institute of Crystallography and back home every day, a distance of about 12 km with a significant hill climb. He liked being accompanied by his son on

bike rides and sometimes cycled for more than 170 km to tour around Lake Geneva. He was also a real mountaineer and cross-country skier. I had many opportunities to climb several Swiss summits with him, both in summer and winter. I remember very clearly our party of four starting a ski tour from Rothenboden over Zermatt for the ascent of the Pointe Dufour, the highest point in Switzerland (4634 m). By the end of the ascent, only the two crystallographers had managed to reach the summit.

Dieter also joined from the outset a basketball team called OURRS that brought together professors from UNIL and EPFL. Every Tuesday during term time we would meet for an hour of physical exercise and a basketball game. Dieter participated actively in the team activities until his physical abilities started to diminish. Unfortunately, Dieter passed away just a few days before the celebration of the 50th anniversary of the team.

Dieter was not only my mentor but also a dear friend, whom I will miss.

Acknowledgements

The help of Vera Schwarzenbach, Alla Arakcheeva, Eric Blanc and the staff of the IUCr Editorial Office in Chester is acknowledged for providing useful information for writing this article.

References

Blanc, E., Schwarzenbach, D. & Flack, H. D. (1991). *J. Appl. Cryst*. **24**, 1035–1041.

Bürgi, H.-B., Blanc, E., Schwarzenbach, D., Liu, S., Lu, Y., Kappes, M. M. & Ibers, J. A. (1992). *Angew. Chem. Int. Ed. Engl.* **31**, 640–643.

Flack, H. D. & Schwarzenbach, D. (1988). *Acta Cryst*. A**44**, 499–506.

Lewis, J., Schwarzenbach, D. & Flack, H. D. (1982). *Acta Cryst.* A**38**, 733–739.

Restori, R. & Schwarzenbach, D. (1986). *Acta Cryst.* B**42**, 201–208.

Schwarzenbach, D., Abrahams, S. C., Flack, H. D., Gonschorek, W., Hahn, Th., Huml, K., Marsh, R. E., Prince, E., Robertson, B. E., Rollett, J. S. & Wilson, A. J. C. (1989). *Acta Cryst*. A**45**, 63–75.

Schwarzenbach, D., Abrahams, S. C., Flack, H. D., Prince, E. & Wilson, A. J. C. (1995). *Acta Cryst.* A**51**, 565–569.

Schwarzenbach, D. & Chapuis, G. (2006). *Cristallographie*. Lausanne: EPFL Press.

This article has been published in *Acta Cryst.* (2024). A**80**.

OBITUARY

Larry W. Finger (1940–2024)



Larry Finger and his wife, Denise.

Ross J. Angel, David Cox, Robert M. Hazen, Nancy L. Ross, Brian H. Toby

Larry Finger, a pioneer in the development of computer-controlled diffractometers, crystallographic software and high-pressure diffraction methods, passed away on 21 June 2024 at the age of 84. Larry was one of the most talented experimental scientists we have ever had the pleasure of working with – a unique combination of geologist, mineralogist, crystallographer and computer expert.

Larry grew up on a family farm, first in Iowa and then Minnesota, USA, where he developed the mechanical and problem-solving skills that would serve him so well throughout his professional life. After high school, he enrolled in the University of Minnesota, where he studied physics for his undergraduate degree and then joined Tibor Zoltai in the Department of Geology. His thesis in 1967 reported one of the very first determinations by crystal structure refinement of the cation site occupancies in a complex mineral. This required him to write his own program for crystal structure refinement for single-crystal data, which later evolved into the well-known *RFINE* package through a collaboration with Ted Prince at the National Bureau of Standards (Finger & Prince, 1974), in which form it is still used today. The same code was also the basis for the NIST Reactor's local Rietveld fitting code, remaining in use until the early 2000s.

Following his PhD, Larry moved to the Geophysical Laboratory of the Carnegie Institution of Washington, where he became the staff crystallographer until his early retirement in 1999. At Carnegie, he automated the manually driven Picker four-circle diffractometer, which involved the installation of stepper motors on the diffractometer. He interfaced the motors and the counting chain with a DEC PDP-11/20 minicomputer and wrote an entire diffractometer control package in a mixture of Basic and machine language (Finger *et al.*, 1973). This masterpiece of software design, which allowed the entire program to fit into the tiny amount of memory (12,000 words or 24 kb) then available, was achieved by Larry in just 150 hours of programming time. The published description concludes with the prophetic statement (Finger *et al.*, 1973):

In the future, this system should evolve into an extremely powerful tool for the study of crystal structures, thermal states, and the X-ray behavior of materials at elevated temperatures.

That turned out to be correct; the demand for the program and automation was so great that a company was established to retrofit an older generation of manual diffractometers and electron microprobes for chemical analysis, with what was named "Krisel Control" automation. It continued to sell until the late 1980s when the program itself was converted and developed as a Fortran program via MicroVAX computers and now PCs into the program *SINGLE* (Angel & Finger, 2011) that is still used in several

single-crystal diffraction laboratories.

What Larry had not foreseen in 1973 was the arrival of Robert Hazen at the Geophysical Laboratory in 1976 when they began a quarter-century of collaboration that established the field of high-pressure and high-temperature crystallography. Larry's major contribution was to develop the methods to obtain accurate and precise X-ray diffraction data from single crystals held at high pressures in diamond anvil cells (*e.g.* King & Finger, 1979; Ralph & Finger, 1982). These methods were described in the book *Comparative Crystal Chemistry* (Hazen & Finger, 1982), which also established from their own data the principles governing the response of mineral and inorganic crystal structures to temperature and pressure.

By 1980, Larry had already recognized the value of synchrotrons for powder diffraction. He built PDP-11 and later MicroVAX computers from spare parts to run Dave Cox's beamline (X13A, then X7A) at the Brookhaven light source. This was an indispensable contribution to a financially challenged beamline at a time when the cost of a computer was much greater than that of a new car. He then interfaced the CAMAC-based motor drivers and counters and wrote the initial data collection software. Larry was a major user of the beamline, which became the prototype for multiple generations of instruments worldwide. Out of this work also came Larry's most cited paper (Finger *et al*., 1994), an asymmetric peak function based on physical principles used for fitting powder diffraction patterns.

In the 1980s and 1990s, Larry provided the essential expertise in data collection and diffraction physics, particularly the effects of correlated thermal motions on diffracted intensities, which he had coded into the *RFINE* program two decades previously. This enabled the high-pressure crystal structures of molecular materials, including C_{60}, rare gases, hydrogen, methane and their unexpected compounds to be determined. His key contributions to solving the T_c > 90 K superconductor structures and his calmness under pressure are described in Hazen (1988).



Larry Finger, second from right, with Bob von Dreele (left) and others at the American Crystallographic Association Annual Meeting 1991 in Toledo, OH. Photo credit: W. L. Duax.

By his pioneering automation of X-ray diffractometers and electron microprobes, by sharing his software with the community, and, most importantly, by passing on his knowledge and expertise, Larry enabled many others to do cutting-edge crystallography. His approach might best be summarised by the title of one of his meeting abstracts: "difficult but possible". It is rare in science for one individual to open

pathways to discovery for so many others, and this was recognized by the award of a Humboldt Preis to Larry in 1996. His legacy will endure in his algorithms, experimental methods and crystallographic software that are, judging by the 300 citations they still receive annually, 25 years after his retirement, in continual use by the crystallographic community.

Citations

Angel, R. J. & Finger, L. W. (2011). *J. Appl. Cryst.* **44**, 247–251.

Finger, L. & Prince, E. (1974). A system of Fortran-IV computer programs for crystal structure computations. *NBS Technical Note 854.* Gaithersburg, MD, USA: National Bureau of Standards.

Finger, L. W., Cox, D. E. & Jephcoat, A. P. (1994). *J. Appl. Cryst.* **27**, 892–900.

Finger, L. W., Hadidiacos, C. G. & Ohashi, Y. (1973). *Carnegie Inst. Washington Year Book*, **72**, 694–699.

Hazen, R. M. (1988). *The break-through: The race for the superconductor.* New York: Summit Books.

Hazen, R. M. & Finger, L. W. (1982). *Comparative Crystal Chemistry: Temperature, Pressure, Composition and the Variation of Crystal Structure*. London: John Wiley & Sons.

King, H. & Finger, L. W. (1979). *J. Appl. Cryst.* **12**, 374–378.

Ralph, R. & Finger, L. W. (1982). *J. Appl. Cryst.* **15**, 537–539.

OBITUARY

Richard Alexander Pauptit (1954–2024)



Caitriona Dennis, Dean Derbyshire, Joacim Jaeger, Alan Riboldi-Tunnicliffe

It is with heavy hearts that we write this memorial for Dr Richard Alexander Pauptit, who died on 30 June 2024. Richard was well known and highly respected in protein crystallography circles and contributed hugely to the field. His enthusiasm, passion, and creativity for this area of structural biology was infectious, and those who were fortunate to work, study and collaborate with him will feel a profound loss on his passing.

Richard was born in Amstelveen, in the province of North Holland, Netherlands in 1954. Due to his father's work, he spent his formative years travelling the globe including time in the Middle East, Europe, Australia and Africa, and the love of travel continued throughout Richard's adult life.

Richard completed his schooling at the American Community School in Beirut, Lebanon, before enrolling at the University of Cape Town, South Africa (1973–75) where he received a BSc and excelled in Chemistry and Computing. It was during his time as an undergraduate that Richard's interest in X-ray crystallography was sparked. Richard began working in the field of small molecule crystallography in the laboratory of Professor Luigi Nassimbeni at the University of Cape Town, helping to solve four small molecule structures.

Richard's academic journey continued at the University of British Columbia, Vancouver, Canada, where he undertook an MSc (1976–78) and PhD (1978–1982) in the laboratory of Professor James Trotter. Here, he honed his understanding of crystallography in the field of chemical crystallography, working on organic compounds.

Richard continued to build on his knowledge during a postdoctoral and lectureship position (1982–83) at the University of Auckland, New Zealand, which resulted in the publication of several small molecule structures.

In 1983, moving across the globe again, Richard took up a research position in the Biocenter at the University of Basel, Switzerland with Professor Johan Jansonius. At this stage Richard extended his research activities to the study of macromolecules. Using his broad crystallography background and programming skills, Richard wrote and improved a wide range of computational programs in the area of molecular replacement and protein structure refinement. At the Biocenter, he led and collaborated on many challenging projects including proteases, transaminases and other enzymes as well as the nascent field of membrane protein crystallography on a number of different porins.

In 1991, Richard moved to Heidelberg, Germany, to become a Fellow with the European Molecular Biology Laboratory (EMBL), working with many current leaders in structural biology. At EMBL his scientific collaborations focused on Src homology 3 domains and other related proteins.

Following this research position, in 1992, Richard took up a Team Leader position with AstraZeneca pharmaceuticals (formerly known as ICI Pharmaceuticals), in Macclesfield, United Kingdom. He established protein crystallography facilities and integrated this technique into an ongoing programme of drug design. Together with other scientists, under Richard's leadership, target-compound complex structures were determined which led to development of many drug therapies for disease.

As a Senior Principal Scientist and Associate Director in Discovery Sciences, Richard continued to inspire and innovate, ensuring that scientists could collaborate, within and outside of the company, encouraging rich partnerships with universities and research institutes. He played an important role in various outreach initiatives, including a postdoctoral programme whose aim is to promote a supportive and collaborative research culture for scientists to thrive. Richard brought the crystallography group in AstraZeneca to both national and international arenas. He participated in and led many collaborative and strategic activities including: leadership of the Biological Structures Group of the British Crystallographic Association; he was an active member of the CCP4 committee; a member of Scientific Advisory Board for BIOXHIT (an EU Framework 6 high-throughput crystallography project); was a Member of the Scientific Advisory Committee for the Membrane Protein Structure Initiative (MPSi), a BBSRC SPoRT initiative; and was a peer reviewer for *JMB*, *Structure* and many other journals, including IUCr Journals where he also acted as a Co-editor on *Acta Crystallographica F*.

Richard instigated communities of practice and founded opportunities to share expertise and research news, including the international Protein Structure Determination in Industry (PSDI) meetings and the CCP4 Glasgow Protein Structure Workshop, a Northern UK regional protein crystallography event involving around 10 academic laboratories and AstraZeneca.

Richard was a leading voice in the world of protein crystallography with a long list of invited lectures at meetings and conferences. With his expertise in drug discovery, he held honorary positions in academia in addition to supervising researchers and being a PhD external examiner. He had an amazing portfolio of collaborations and authored many publications, but the wealth of influence he had on so many projects is priceless.

To have encountered Richard, to have worked with him and interacted in some way along his globe-trotting scientific journey is an unforgettable experience. Many people will have listened to, and have been inspired by, his talks at various conferences and lectures at universities. Colleagues will have sat with him on various committees and organized meetings and conferences with him, and will be marked by these encounters. As his former students, we were fortunate to benefit from his unorthodox yet effective teaching methods. His approach was always centered around the individual, offering a unique perspective on research and teaching: the strong, black coffee he served kept us going through the long periods of data collection; the crystallography tutorials delivered in the safe learning environment of the local pub will be forever etched in our memories; and the nail-biting journeys of course, in a battered, left-hand drive Volvo were character building.

Richard may have introduced us to crystallography, but his influence remains with us over the course of our varied careers. He taught us with humility, he was the most supportive, warm, funny and unusual mentor. He formed a community who were bonded by a scientific goal but also united a team through kindness, generosity and karaoke.

Richard retired from AstraZeneca in 2014 and spent time developing many of his other skills and talents. A big fan of motorbikes and skiing, he once stated that he enjoyed the feeling of the wind fast flowing through his long hair. He had a passion for music, played the guitar and was always keen on introducing people to lesser-known Canadian guitar bands. In latter years, Richard explored his creative side, demonstrating a talent in painting and exhibiting his art several times. He was an active member of a crossword setting community, sharing his method of setting, and solving puzzles on a regular basis. Many readers of *The Independent* will have in fact struggled with cryptic crosswords set by 'Dutch', Richard's alias as a puzzle setter.

Richard is survived by a loving family who have been a constant source of strength and inspiration for him. His children made him proud and will carry his generosity of spirit with them. Richard will be remembered not only for his scientific achievements and creative endeavors but also for his kindness, generosity, and the indelible mark he left on the lives of those who had the privilege to know him. A unique man, who will be sorely missed.

This article was previously published in *Acta Cryst.* (2024). F**80**, 191–192.

OBITUARY

Stephen Edward Tarling (1960–2023)



Jeremy Karl Cockcroft

Dr Stephen Tarling, who died suddenly from pancreatic cancer at the end of October 2023, was a larger-than-life figure. As an undergraduate, he studied chemistry at the University of Surrey at Guildford, UK, where he became interested in crystallography, no doubt as a result of the influence of Robin Shirley with whom he did his third-year project. Robin had started his PhD with Professor Kathleen Lonsdale at University College London (UCL), so Stephen was following in fine footsteps. Stephen then moved to the Department of Crystallography at Birkbeck College London, where he studied for a PhD supervised by Professor Paul Barnes and with co-supervision from Professor Alan Mackay. For his thesis, he worked on the structure of pigments, particularly ultramarine, as he had a CASE (Cooperative Award in Science and Engineering) studentship sponsored by the Colours Division of Reckitt & Colman. I still recall a great talk he gave on the subject, probably at a British Crystallographic Meeting (BCA) meeting, in which he discussed the importance of ultramarine in Renaissance paintings. At that time, ultramarine from lapis lazuli was a very valuable mineral pigment and would have been used for the blue colour in the clothes worn by the Virgin Mary.

It was at around this point in time that I first encountered Stephen as a fellow PhD student. Paul Barnes had taken what appeared to be his whole research group, known as the Industrial Materials Group, to do an experiment at the Institut Laue Langevin, Grenoble, France. Working on D1A at that time, I regularly interacted with any British-based team visiting the ILL, and I was immediately struck by this “cheeky chap” working on D1B on the other side of the guide tube to myself who was clearly enjoying his first visit to the ILL. I recall discussing powder diffraction with Stephen, amongst other topics, during his stay. I also learnt that the whole group had taken a ferry across the Channel to the Netherlands (which was perfect for Stephen as he was half-Dutch) and had driven down to Grenoble, presumably as the Science Research Council in those days would only fund flights for three people.

Following that early meeting, I encountered Stephen on several occasions through BCA meetings. In particular, via Paul Barnes’ contact with Mike Glazer in Oxford, Stephen started using his PXRD expertise to work in patent litigation. In particular, Stephen worked on many of the famous pharmaceutical patent cases from the late 1980s to the early 1990s, and I can vividly recall him giving several enjoyable talks on this subject with Mike Glazer at BCA events. Stephen was clearly in his element in this field: he had a brain that was very quick on the uptake and he was well suited to answering the sort of questions that lawyers try to use to trip up unwary expert witnesses. In another career, he might well have become an excellent patent attorney.

Stephen was also a great teacher and, with Paul Barnes, taught crystallography in the Department of Archaeology at UCL in the late 1980s. Stephen’s work on pigments led him to work with Anna Bennett, who worked at Birkbeck College and researched objects for the British Museum, especially whether the

objects were genuine or fake. Stephen also examined historical material from Uppark House, a National Trust property in Hampshire, after it was ravaged by fire. Many years later, following the restoration of the house, Stephen very kindly invited Martin Vickers and me to view it at a special opening, even though I had nothing to do with the analysis work. As I had no car at that time, Stephen even detoured on his trip from London in order to pick me up in his sports car. This was a typical example of Stephen's generosity.

On finishing his PhD, Stephen had a five-year appointment with British Gas. Around that time, British Gas consolidated its research facilities with its X-ray equipment, which was moved from London to Loughborough. When British Gas decided subsequently that they wanted to dispose of their STOE transmission powder X-ray diffractometer, Stephen very generously tipped me off. The only condition: it was free for us to collect but it had to be collected by the end of the week! Needless to say, I leapt at the opportunity, and I still recall dashing up the M1 with Martin Vickers in a small hire van to collect it, but unwittingly leaving behind around £10k of electronics, which were hidden out of sight behind an aluminium panel.

When Stephen's position at British Gas came to an end, he returned to a technical position he had held at the end of his PhD in the Department of Crystallography, for which he was well overqualified. Given that Martin Vickers had been appointed to run the PXRD equipment, Stephen had no future within the Industrial Materials Group, and he was given the role of interacting with the Estates team. I am told that he ran rings around them: he was noted for his famous clipboard on which he noted everything down at meetings. At the following meeting, when work had not been done as promised, he quoted back to them all of their promises! In addition, Stephen became heavily involved in writing web pages to benefit the Department, a job he took on with gusto and especially to the benefit of those needing it most, for example, the facilities provided by the workshop technician Paul Stukas.

One of my final interactions with Stephen as a crystallographer was at a satellite meeting to the IUCr Beijing Congress in 1996. We both attended the Powder Diffraction meeting in Hangzhou, and we both met up with Robin Shirley. Stephen was an enthusiastic cyclist and so he persuaded us to rent bicycles so that we could get easily around the city, this being a time when bicycles were still the dominant form of transport within most Chinese cities. Stephen had always been keen on going to restaurants and so we ended up having some great meals out together as well.



Photograph taken for Sway Council and used with permission.

The late 1990s saw a period of change in universities with lots of support roles being created. Stephen became a Scientific Staff Development Officer at Birkbeck College before he moved down the road to UCL in the same role, oddly enough at about the same time the Industrial Materials Group at Birkbeck College moved to the Department of Chemistry at UCL, with the old Department of Crystallography working purely on biological research. Stephen subsequently moved to Southampton University in a similar role, an opportunity for him and his partner Anita to set up home in the village of Sway in the New Forest. At a celebration to mark Stephen's life last November, I heard from many local people about how Stephen had been the life and soul of the village. For a number of years, he had been an active local parish councillor as well as being a board member of the New Forest National Park Authority. As at Birkbeck College, he had brought his internet skills to the fore again in creating local web pages for the benefit of others. At local fetes, he would interact with all of the stall holders, encouraging them when he could by buying local produce and, if not buying, encouraging them to sell their wares. Stephen's death came very suddenly: he had attended local meetings fortnightly as regular as clockwork, so it was notable when he missed the first one; by the next meeting he was sadly dead. Stephen will be missed by all of us who knew him well.

Jeremy Karl Cockcroft is at the Department of Chemistry, UCL, London, UK.

Article adapted from *Crystallography News*, published by the British Crystallographic Association.

For a list of papers by Dr Tarling 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