IUCr

Newsletter Archive

IUCr
International Union
of Crystallography

www.iucr.org

President's Letter – Summer 2024

Santiago García-Granda

The International Union of Crystallography is running the first year after our successful Congress and General Assembly in Melbourne and we are looking forward to the 2026 event in Calgary. The year since our Melbourne meeting has been a year of reflection on 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. In the past triennium we brought Alexandra Stanley on board as IUCr CEO. At the end of May, our Outreach Officer since 2014, Michele Zema, concluded his contract after 10 years of excellent contributions to IUCr marking a new era in the collaboration and promotion of Structural Science mainly in Africa, Latin America and Asia, bringing a substantial amount of funds, creating new and successful initiatives as with the 'Open Labs', new labs with modern equipment for Structural Science in less developed countries or the Light Sources withing the LAAAMP project.

The retirements of Peter Strickland and Andrea Sharpe will have a great impact on our activity in Chester and an extraordinary emocinal burden. Peter will retire in September, after xx years of the highest responsibilities not only in our editorial team, but also of undisputed leadership at Chester and at 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 yy, now completing with her retirement a career of xx years of service.

We will always be indebted to Peter and Andrea, 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.

In this first year between congresses the scientific protagonism corresponds to our regional Associations. The American Crystallographic Association has gathered in Denver in July, the European will meet in Padova in August, the Latin American will meet in Montevideo in September and the Asian will meet at the beginning of December in Kuala Lumpur, Malaysia. The African Crystallographic Association will meet in Algeria in April 2025.

It is very satisfying to note that the EPDIC meeting, EPDIC18 is being held jointly with ECM34 in Padova, which is very satisfying for both organisations that have common interests and which was very satisfying when it was held in Darmstadt in 2010. The attendance will benefit from the joint organization.

Although the Executive Committee will be represented at all regional meetings at the highest level, on this occasion the EC and the Finance Committee met in Denver at the 74th ACA meeting.

Given the importance of the upcoming meeting and General Assembly to be held in Calgary, Canada, in August 2026, this visit and the meetings with the ACA Council and the IUCr2026 Organising Committees in Calgary were essential. In particular, the plans for the formation and the work plan of the International Program Committee and other organizational and finantial isues.

All the discussions took place in an excellent atmosphere as well as the scientific level and the participation of the young generation of Structural Scientists was excellent. Also learning about the many initiatives that the ACA is putting in place was 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 finance committee analysed the Union's financial situation and adopted cost containment measures for 2024 and 2025, pending the recovery of our publishing revenues. Decisions were also taken on the investment of our funds and the desirability of augmenting the Finance Committee with new advisors to complement the current profiles and contribute to the diversity and rejuvenation of the committee.

As the 55 National Committees, which make up the General Assembly, and until the goal of incorporating all countries where there are structural scientists is achieved, the Associate program is an excellent way to become an individual member of the IUCr and enjoy the advantages of publishing in the 10 IUCr journals and other advantages that will be progressively increased, especially for younger associates.

Once the statutes of the International Science Council have been approved, the election of the Elections Committee has taken place and the election process for the renewal of the ISC Governing Board has started. The IUCr, together with the rest of the ISC member unions, is promoting a candidacy that defends the philosophy of rigorous and global science that our Scientific Unions promote.

Once again, many thanks to all those who form and make our organisation work, the Regional Associates, 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 for contributing to sustain and reinvent the IUCr from anywhere in the world.

Enjoy your summer hollidays!

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 articles in the Crystallography in Africa category, for which Michele played a significant role. For instance:

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

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

The first meeting of the Sengalese Crystallographic Association

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

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 (ref) and the other on the Berlin Natural History

Museum, and the scientists and crystallographers celebrated there (ref). 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 (refs) and in places like Thailand (ref).

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 (ref) and Larry Finger (ref) 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.

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.

Foreword to the AfCA collection: Celebrating work published by African researchers in IUCr journals

Susan A. Bournea, Delia A. Haynesb and Michele Zemac,d*

a Department of Chemistry, University of Cape Town, Rondebosch, South Africa.

b Department of Chemistry & Polymer Science, Stellenbosch University, Matieland, South Africa

c International Union of Crystallography, Chester, United Kingdom

d Department of Earth and Geoenvironmental Sciences, University of Bari “Aldo Moro”, Bari, Italy

*Correspondence e-mail: dhaynes@sun.ac.za

This 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, C. E. P., Acta Cryst. (2017). A73, C1394), 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 (https://www.iucr.org/outreach/openlabs; Zema, M. & Lecomte, C. (2015). Acta Cryst. A71, s177; Zema, M., Desiraju, G. R., Lecomte, C., Nalecz, M. & Ngome Abiaga, J. J.-P. (2017). Acta Cryst. A73, C363) 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 (https://www.xtechlab.co/, Agbahoungbata, M. Y., Bonou, S. A. S., d’Almeida, T., Zema, M. and Borna, C., (2021). Acta Cryst. A77, C606), which is an outgrowth of the IUPAP-IUCr-ICTP Lightsources for Africa, the Americas, Asia, Middle East and Pacific (LAAAMP) initiative (https://laaamp.iucr.org, Scandolo, S., Mtingwa, S. and Zema, M. Acta Cryst. (2017). A73, C1069) 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, the African Crystallographic Association 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 the 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 (REF: IUCr code vz2001). He begins with the early days of crystallography in the North (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, J. B., Diouf, N., Gueye, R. S., Gaye, M., Thiam, I. E. and Coles, S. J. Acta Cryst. (2023). E79, 1109–1114). 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 (REF: IUCr code vz2002). 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 form 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 the article by Kenfack Tsobnang et al. (Kenfack Tsobnang paper, https://www.iucr.org/news/newsletter/etc/articles?issue=155831&result_138339_result_page=15). 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 structures obtained using the remote lab concept have been published as part of this collection (add reference).

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. in this collection (REF: IUCr code ok5102). 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.

Adding Open Science to the Modern Discovery and Applications Toolbox in Crystallography

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

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. 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 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'S WORKING GROUPS

UNESCO then convened five ad-hoc Working Groups focusing on key impact areas, bringing together experts and open science entities, organizations, and institutions according to their field of activity and expertise on:

Open Science Capacity Building

Open Science Policies and Policy Instruments

Open Science Funding and Incentives

Open Science Infrastructures

Open Science Monitoring Framework

These UNESCO Working Groups each had at least three virtual events, some now four, and the recordings are available [3]. A key output of the Working Groups assembled by UNESCO is a helpful toolkit [4]. Within this toolkit is 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's sustainable development goals 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 analyse 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, e.g., see [9]. This approach addresses the challenge perceived by UNESCO for the Global South of article processing charges (APCs) for authors. 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 International Science Council 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 managing editor, Peter Strickland. This emphasized the importance of pre-publication peer review of articles with data and checking report, such as the IUCr's checkcif and the PDB's Validation Reports, which are both exemplary for 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 Professor Dick Marsh in the pre-2000s decades.

INDUSTRY AND THE UN SDG9

UNESCO's work involving industry's needs is not explicitly covered so far. This is important, as recognized by the UN's Sustainable Development Goal 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 which are very well described by the USA National Academies report [14]. They even advocate doing away with journals in favour of preprints.

The International Science Council [1] does realize, though, that different areas of science may vary in their approach. For us crystallographers, the very basis of the crystallographic tradition of careful validation of data underpinning our journals' 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

To conclude I would stress the following positives that commend adding or expanding Open Science in our research toolbox beyond what we already have achieved with such as our IUCr Journals open access publications (Acta Cryst E, IUCrData and IUCrJ). Firstly, I 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 a fully open global collaborative approach could deliver hugely. UNESCO, as well as the World Health Organisation, is aware that global funding schemes could really help here. Secondly, measured raw data that has not led to eventual publication needs opening to wider sharing and exploitation, as led by the EU's PaNOSC [18] project. 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, 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 minutes ‘basics’ video [21]. An easy win in my view of an OSF would be harnessing this 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, Managing Editor of IUCr Journals, and Mike Glazer, IUCr Newsletter Editor for detailed discussions and comments.

References

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

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

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

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

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

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

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.

http://paleo.esrf.eu/

202203-diamond-oa-action-plan.pdf (scienceeurope.org)

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

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

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

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

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

I. Bruno, S. Gražulis, J. R. Helliwell, S. N. Kabekkodu, B. McMahon, and J. Westbrook. (2017). Crystallography and Databases. Data Science Journal, 16, 38, 1-17. DOI: http://doi.org/10.5334/dsj-2017-038

https://www.nature.com/nature/for-authors/registered-reports#:~:text=It%20is%20a%20format%20in%20which%20the%20methods%20are%20peer-reviewed%20before%20data%20collection%20and%2For%20analyses%20are%20done.

https://dndi.org/

https://www.panosc.eu/

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

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. https://doi.org/10.1098/rsos.240286

https://help.osf.io/article/583-getting-to-know-the-osf-the-basics#:~:text=The%20OSF%20is%20a%20free%20open-source%20software%20project,the%20entire%20project%20publicly%20accessible%20for%20broad%20dissemination.

“APERIODIC CRYSTAL”

Istvan Hargittai

“An aperiodic crystal is a structure with sharp diffraction peaks, but without lattice periodicity.” [1].This is a modern definition thanks to crystallography having become a science of structures, ie, more than what classical crystallography is. As far as I know, the theoretical physicist Erwin Schrödinger (1887−1961) was the first who used the term “aperiodic crystal” in his most influential book, What is Life? published in 1944, that is, 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, eg, [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].

To Schrödinger, a small molecule would be an initial seed for the gene. Its extension by mere repetition – the way a crystal is being formed – could not lead to the gene because periodicity would exclude carrying information. The other way for extending the initial seed molecule would be building 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 gene since it had been hypothesized to be uniformly repetitive (see, eg, [6]).

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

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 of science in establishing the truth. Klug referred to the philosopher Alfred N. Whitehead (1861−1947), coauthor with Bertrand Russel 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.

LITERATURE

1 International Union of Crystallography (1992). “Report for the Executive Committee for 1991.” Acta. Cryst. A48, 922−946.

2 Schrödinger, Erwin (1944). What is Life? Cambridge University Press.

3 Avery, O.T., MacLeod, C.M., McCarty, C. (1944). “Studies on the chemical nature of the substance inducing transformation of pneumococcal types: Induction of transformation by a desoxyribonucleic acid fraction from pneumococcus type III.” J. Exper. Med. 79, 137−158.

4 Hargittai, Istvan (2024). “What is Life? – 80 years: from Erwin Schrödinger to Paul Nurse.” Struct. Chem. 35, doi.org/10.1007/s11224-024-02314-4]

5 Perutz, M. (1987). “Physics and the riddle of life.” Nature April 9, 326, 555−558; the quote is on p. 558.

6 Hargittai, Istvan (2009). “The tetranucleotide hypothesis: a Centennial.” Struct. Chem. 20, 753−756.

7 Conversations with Aaron Klug, on October 9, 1998, and, in February and March 2000, at the MRC Laboratory of Molecular Biology, Cambridge, UK. Hargittai, Istvan (2002). Candid Science II: Conversations with Famous Biomedical Scientists. Magdolna Hargittai, Ed., Imperial College Press, London, Chapter 20, “Aaron Klug,” pp. 306−329.

Bringing Crystallography to the Classroom: Kenyan Teachers Learn to Engage Students in the Wonders of Crystals

Patricia W. Gitari1 and Martin N. Mbugua2

1Consultant Chemist, AESA, 2Department of Chemistry, University of Nairobi

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

Figure 1: Group Photo of Participants during opening of the teachers training on 29 November 2023 © UoN and CSIC

Front row (L to R) 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 Garcia-Ruiz (CSIC-University of Granada), Fermin Otálora (CSIC-University of Granada) and Solomon Derese (UoN).

The workshop, entitled "Learning How Science Works with Crystals," was led by renowned crystallography experts Prof. Juan Manuel Garcia-Ruiz (Donostia International Physics Center and the Instituto Andaluz de Ciencias de la Tierra-CSIC) and Dr. Fermin Otálora (Instituto Andaluz de Ciencias de la Tierra-CSIC, in 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 and biology, biomedicine, engineering, mathematics, and arts." said Garcia-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 firsthand.

Figure 2: Interactive training on crystallography © 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 crystal and polycrystalline materials with specific properties. A diversity of Kenyan schools will now have the opportunity to participate in the first Africa Education Program for Crystallisation Contest in the 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. Fermin Otálora, and Prof. Juan Manuel García-Ruiz under the auspices of the Consejo Superior de Investigaciones Científicas, The University of Nairobi 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 next September after the ECA conference. It is also planned to display an African version of the exhibition "CRISTALES". 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 © UoN and CSIC

(L-R): Nyongesa, Martin Mbugua, Fermin Otálora, HE Ambassador Cristina Díaz Fernández-Gil, Ambassador of Spain to Kenya Juan Manuel Garcia-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 underrepresentation 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 © UoN and CSIC

(L-R): Martin Mbugua, Juan Manuel Garcia-Ruiz, Patricia Gitari, Solomon Derese, Joy Kiano and Fermín Otálora

25th Heart of Europe Bio-Crystallography meeting

Przemysław Grudnik

The 25th Heart of Europe Bio-Crystallography meeting (HEC24) took place in September 2023 in Salem, located in the state of Mecklenburg-Vorpommern in Germany. The attendees could appreciate the beautiful scenery of the Lake Kummerower. The meeting has been organized by the group of prof. Michael Lammers from Greisfald University. As previously, organization of HEC has been supported by 11 sponsors including the IUCr Journals.

This 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 Johanna Hakanpää (PETRA III, DESY, Hamburg).

Over the three days course, 27 PhD students and postdocs presented current topics of their research. At HEC25, numerous prizes were awarded for outstanding short-talks and flash-talks, made possible by the generous support from the IUCr (International Union of Crystallography), GBM (Gesellschaft für Biochemie und Molekularbiologie e.V.), and Structure/Cell Press. As typically 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 Rezanova's group, and Pawel Kochanowski from Przemyslaw Grudnik's group—received awards from Structure/Cell Press, presented by Karin Kühnel, the editor-in-chief of Structure/Cell Press.

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 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.

[HEC25 prizes recipients]

[Group photo]

Comprehensive Training Course in Macromolecular Structure Determination in Thailand

Leela Ruckthong, Department of Chemistry, KMUTT, Bangkok, Thailand; Ronan Keegan, CCP4, STFC Rutherford Appleton Laboratory, Harwell, UK; Garib Murshudov, MRC LMB, Cambridge, UK; Ruslan Sanishvili, The President’s Office, KMUTT, Bangkok, Thailand.

General

From January 29 to February 7, 2024, King Mongkut’s University of Technology Thonburi (KMUTT) in Bangkok, Thailand, hosted the 3rd macromolecular structure determination training course entitled South East Asian Crystallographic Overview And Systematic Training (SEA COAST) https://seacoast.kmutt.ac.th/2024/.

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, both from 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, the 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 cryoelectron microscopy 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; Dean Myles, Oakridge 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; Martyn Winn, STFC, UK.

First day of the 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 have added crystallographic data collection from students' crystals, conducted remotely on the I04 beamline of the Diamond Light Source (DLS). We 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. Oakridge 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

at the I04 beamline of Diamond Light Source

Martyn Winn introducing all phases of structure determination

with cryo-electron microscopy

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.

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

Results

12 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 10 participants who tried data collection at DLS, 6 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 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 the SEA COAST 2024. Additional funding was provided by the Faculty of Science of the KMUTT, the Chemistry Department of KMUTT, 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.

First Senegalese Day of Crystallography

Authors: Magatte Camara1, Ibrahima Elhadji THIAM1, Rokhaya Sylla GUEYE1, Mbossé Ndiaye GUEYE1, Adama SY1, Farba Bouyagui TAMBOURA1, Emmanuel WENGER2, Claude LECOMTE2

1Executive committee members of Crystallography Senegalese Association (ASC-Senegal)

2CRM2 - Cristallographie, Résonance Magnétique et Modélisations, Nancy

Introduction

The aim of this article is to report on the first Senegalese Day of Crystallography organized by the Crystallography Senegalese Association (ASC) on February 19, 2024, at Cheikh Anta DIOP Dakar University.

2. Context

The First Senegalese Day of Crystallography (Cristal O!) organized by the Crystallography Senegalese Association (ASC) took place on February 19, 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 Crystallography Senegalese Association (ASC, Association Sénégalaise de Cristallographie) 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 /CRM2 AFRAMED project (Doctoral Training and Research in Africa through remote X-ray diffraction measurements) , a remote laboratory led by Professor Claude LECOMTE. Launched on August 31, 2022, this project enables scientists from African laboratories to remotely control the CRM2 single crystal X-ray diffractometer located at CRM2, Université de Lorraine , France. This conference day was attended by 81 participants from five Senegal 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

3. The 2024 edition

Course of activities:

The scientific day began with under the auspices of the university authorities. The opening ceremony was presided by Professor Bassirou LO, Dean of the Faculty of Science and Technology at Cheikh Anta DIOP University, 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 off with an official welcome address by Professor Ibrahima Elhadji THIAM, Chairman of the day's organizing committee, followed by Professor Magatte Camara, President of Crystallography Senegalese Association, Professor Emeritus Claude Lecomte, the head of the Chemistry Department, and the Dean of the Faculty of Science and Technology.

Immediately after the opening ceremony, we moved on to the inaugural lecture by Emeritus Prof. Claude 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, with its large 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 Claude Lecomte . AFRAMED is a 5-year CNRS project: during one month, 3 or 4 young African colleagues are trained intensively to ‘drive ‘ single-crystal diffractometers by CRM2 researchers (Drs E. Wenger, E. Bendeif and C. Lecomte); Then , back to their home country , these colleagues can collect diffraction data on the CRM2 diffractometers in remote mode for teaching and research. Since September 2022: Egypt, Togo, Cameroon and Gabon ,Senegal, Congo Brazzaville, Ivory Coast, Algeria were involved ;in 2024 Madagascar, Burkina Faso and Mauritania will be the hosts of CRM2. The trainees are fully funded by the CNRS IRN and IUCr within the Africa Initiative project. .In 2024 UNESCO will join .

During the conference day , a remote session on single-crystal X-ray diffraction was led by Dr Emmanuel Wenger .Emmanuel centered a paracetamol single crystal on the diffractometer and taught all steps of XRD data collection. We noted a large enthusiasm of the 81 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, a fetish instrument in crystallography, the contribution of crystallography to their field of research and their prospects.

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

The Materials Chemistry and Physics Laboratory (LCPM) was born in 2010 and recognized by a Rector decree in 2017. It is attached to 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 published over 300 publications, 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 chemistry recovery) and synthesis methods for innovative molecules and molecular materials.

Organic Coordination Chemistry Laboratory (Dakar, 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) doctoral school. Its current Director is Professor Ousmane DIOUF, and collaborates internally with the 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) - Southampton (England) etc. Over 200 articles were published in international journals. Its field of research is the synthesis of homonuclear or heteronuclear coordination complexes, or transition metal or lanthanide co-crystals from Schiff bases. The physico-chemical and biological properties of the molecules are studied.

Physical, Inorganic, Organic and Therapeutic Chemistry Laboratory, LCPMOT (Dakar, UCAD)

The organic, and therapeutic chemistry laboratory, more than 50 years old, recently named the laboratory of physical, mineral, organic and therapeutic chemistry (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 the Cheikh Anta Diop University of Dakar (UCAD). The main line of research focused 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, 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 analyses 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)

Quantum Energy Photonics and Nanofabrication Laboratory (LPQEN) is headed by Professor Balla Diop NGOM. LPQEN is a laboratory working on synthesis and characterization of nanomaterials such as activated carbon, two-dimensional materials (graphene, MXene), metal oxides, metal oxi-nitrides, composites, nanocelluloses…. The materials are characterized using various techniques to study their physico-chemical properties. Application of these nanomaterials are electrodes for super capacitor applications. The experimental facilities of the laboratory are: electric and chemical vapor deposition (CVD) furnaces, 16-channel VMP300 Static Potentiometer, 8-channel Battery Analyzer, Autoclave with heating jacket, pressure-controlled button cell crimping machine.

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

Research team in Inorganic and Organic Materials Chemistry “ECMIO” is attached to the Physics-Chemistry doctoral program of Applied Sciences and Computer and Communication Technology UFR, Department of chemistry of the Alioune Diop University of Bambey. Team was headed by Professor Farba Bouyagui Tamboura. To its credit 57 publications in indexed and abstracted journals, 17 oral presentations and 11 poster presentations at various conferences and seminars. Partner universities and institutes are Université Cheikh Anta Diop, Dakar / Assane Seck University, Universities of Ziguinchor / Nouakchott (Mauritania) / Strasbourg / El Manar Tunis / Materials Institute Jean-ROUXEL, Nantes. 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 3 multidisciplinary teams: Electronics-Electrotechnics-Automatics & Computing; Renewable Energies and Materials and Water, Environment and Climate. Pr Amadou Seidou H. Maiga is the Director, he is assisted by Pr Elhadji Babacar LY, who is a lecturer and researcher in materials chemistry at the Université Gaston Berger of Saint-Louis. 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 bio-fuel, among others. 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. The X-ray laboratory (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, Université Iba Der Thiam de Thiès, University of Trento and Synchrotron Elettra, Trieste, Italy, and Université Gustave Eiffel, Paris, France. The laboratory has organized three international X-ray workshops: December 2005, January 2009 and January 2012.

Hot Topics in Contemporary Crystallography 6 (HTCC6)

Dr. sc. Aleksandar Višnjevac

Dubrovnik, Croatia, April 7th to 12th, 2024

Physical Chemistry Division

Ruđer Bošković Institute

Bijenička cesta 54

10000 Zagreb

Croatia

Email: aleksandar.visnjevac@irb.hr

Phone: +385 91 5000112

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 Judy Dench as Gertrude, Dubrovnik was 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 7th to 12th 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, student restaurants and cafeterias with the top-notch sports, recreation and conference facilities, all in one place. The Akademis is located only 15 mins 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 were routinely starting at 8:30 AM sharp, and lasted until very late in the evening (frequently until 11 PM), 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 demo/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 a 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 LCP crystallization

Daniel Day-Lewis and Judy 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 alphabetic order) Areej Abuhammad, Terese Bergfors, Martin

Caffrey, Elspeth Garman and Patrick Shaw Stuart. The students practiced '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 an 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, 9th of 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 on 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 the 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 a full justification of 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 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 the HTCC6. The day was jam-packed with a series of alternating lectures and tutorials delivered by people who actually create and develop CCP4 - 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 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.

Databases Hot Topic jam-packed with tutorials requires full attention of everyone

The workshop, which was this year again generously co-funded by the Croatian Science Foundation through project calixDNA (PI: 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. 16 students received bursaries to cover, partially or entirely, their registration fees and accommodation expenses. The bursary scheme was generously funded by the International Union of Crystallography, Croatian Association of Crystallographers and European Crystallographic Association.

Students presented 15 posters and 8 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 K. 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 and Kinga Pokrywka, best poster presenters with Ilaria Gimondi from the CCDC

Selvita best DTP award went to Boris Gomaz

As a devoted organizer, I am equally keen to motivate students and lecturers to fill and submit the online questionnaire on their impressions on 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 on 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 11 PM, 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 an 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 at https://htcc6.org, on the Facebook page "Croatian Association of Crystallographers", Instagram profile "Croatian Crystallographers" and on the X profile @hrvukris. We are very much looking forward to the HTCC7 and we invite you to keep an eye on our social networks so you don’t miss it.

CCDC Science Day — the most inspiring day of the year for our scientific community

Author not stated in source

The Cambridge Crystallographic Data Centre sponsors numerous PhD and Master's students each year and co-supervises them alongside leading scientists from academic and commercial institutions. As a charitable institution, our mission is to support the development of the next generation of scientists. Every year, we invite them and their external supervisors 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 started with Nathan Hennessy, a 3rd-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 2nd-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.

Blogs 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. Read more

CSD Tools in Action: Cocrystal Design and Structural Features Analysis

Izabela Madura and co-workers from the Warsaw University of Technology 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

Check out all our blogs here.

CCDC Online Events: Free Virtual Workshops in October and November

First Steps in Protein-Ligand Docking With GOLD

8th October at 16:00–17:45 (BST)

This workshop on GOLD is designed for beginners, working in drug discovery. You will learn the basics of performing protein-ligand docking using the CCDC's docking software GOLD.

Register

ConQuest to Mercury – From Searching to Data Analysis

22nd October at 13:00–14:45 (BST)

We will explore a workflow using ConQuest and Mercury to have an in-depth look at trends and behaviours of defined 3D parameters, such as inter- and intra-molecular distances, angles and torsions, and crystallographic parameters for relevant groups of structures in the CSD.

Register

Introduction to Pharmacophore Searching Using CSD-CrossMiner

5th November at 10:30–12:15 (GMT)

This workshop on CSD-CrossMiner is designed for beginners, working in drug discovery. You will learn how to perform pharmacophore searches to uncover new ligands using the CCDC's software CSD-CrossMiner.

Register

All sessions are 90 minutes long and will include presentations and demonstrations by CCDC expert tutors and a hands-on part for you to try the software, with the tutors available to help you and answer your questions. The workshops will be recorded and all registered participants will have access to the recording.

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, we want to hear your ideas! You can explore the resources created by the winners of previous years' engagement grants here for inspiration. Applications close on 30th September 2024 (11:59 pm BST).

Follow us on Social Media

Want to learn more about CCDC events, blogs, case studies, and software updates? Follow us on LinkedIn, Facebook, and Twitter.

Sign up for the CCDC newsletter to receive inspiring content, the latest data updates and product releases, and event announcements.

MINERALOGISTS AND CRYSTALLOGRAPHERS AT THE BERLIN NATURAL HISTORY (NATURKUNDE) MUSEUM

Istvan Hargittai and Magdolna Hargittai

The Berlin Naturkunde Museum. Photograph by the authors

The Berlin Naturkunde Museum – Natural History Museum remembers some mineralogists and crystallographers from the time when the interest in understanding nature was much less compartmentalized than today. 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 facing 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. Photographs 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 honor 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 4,500 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. 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

å

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 – natural philosophy. He is best known for his taxonomy of plants. His contributions to crystallography were considerable given the state of sophistication of this field at his time, but 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 Wernigerod, the 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; we cropped the photograph). File:René Just Haüy at MNHN.jpg - Wikimedia Commons, licensed under the Creative Commons Attribution-Share Alike 3.0

René-Just Haüy (1743−1822) was born in 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 (File:Berlin, Mitte, Humboldt-Universitaet, Standbild Eilhard Mitscherlich 03.jpg - Wikimedia Commons; licensed under the 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 in 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 the corresponding phosphates and arsenates crystallize in 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 Isaacs'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 hemoglobin by Max F. Perutz et al. [8]. Kendrew and Perutz shared the chemistry Nobel Prize 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 had 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 "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 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, the 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.

LITERATURE REFERENCES

[1] J. Lima-de-Faria, Ed., Historical Atlas of Crystallography. Kluwer Academic Publ. for the International Union of Crystallography, Dordrecht/Boston/London, 1990

[2] R. J. Haüy, Traité de Cristallographie, 1822. Reprinted by Culture et Civilisation, Bruxelles, 1968.

[3] E. Mitscherlich. „Sur la relation qui existe entre la forme cristalline et les proportions chimiques." Ann. Chim. Phys. 14, 172–190 (1820).

[4] I. Hargittai, "On the origin of isomorphous replacement in protein crystallography." Struct. Chem. 33, 635–639 (2022).

[5] M. Vijayan, A. Ramaseshan, "2.4. Isomorphous replacement and anomalous scattering." In International Tables for Crystallography, Volume B: Reciprocal space, U. Shmueli, ed., Springer, Dordrecht, 2006, 264–275.

[6] N. Isaac, "A history of experimental phasing in macromolecular crystallography." Acta Cryst. D: Structural Biology 72, 293–295 (2016).

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

[8] A.F. Cullis, H. Muirhead, M.F. Perutz, M.G. Rossmann, A.C.T. North, "The structure of haemoglobin VIII. A three-dimensional Fourier synthesis at 5.5 Å resolution: determination of the phase angles." Proceedings of the Royal Society A 265, 15–38 (1961).

[9] E. Mitscherlich, "Ueber das Verhaltniss der Form der krystallisirten Körper zur Ausdehnung durch die Warme." Poggendorff Ann. Phys. 1, 125–127 (1822)

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

Memorial of Larry W Finger (1940--2024)

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

Larry Finger , 2nd from right with Bob von Dreele (left) and others at the American Crystallographic Association Annual Meeting 1991

Larry Finger, a pioneer in the development of computer-controlled diffractometers, crystallographic software and high-pressure diffraction methods, passed away on June 21, 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, 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 NBS (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 4-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 24kb) 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 microVaxes 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 C60, rare gases, hydrogen, methane and their unexpected compounds to be determined. His key contributions to solving the Tc > 90K superconductor structures and his calmness under pressure are described in Hazen (1988).

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.

Larry Finger and his wife Denise.

Citations

Angel, R. J. & Finger, L. W. (2011). Journal of Applied Crystallography 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). Journal of Applied Crystallography 27, 892-900.

Finger, L. W., Hadidiacos, C. G. & Ohashi, Y. (1973). Carnegie Institution of Washington Year Book 72, 694-699.

Hazen, R. M. (1988). The break-though: 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). Journal of Applied Crystallography 12, 374-378.

Ralph, R. & Finger, L. W. (1982). Journal of Applied Crystallography 15, 537-539.

Stephen Edward Tarling (1960-2023)

Jeremy Karl Cockcroft, Department of Chemistry, UCL (Article adapted from Crystallography News)

(Photograph taken for Sway Council and used with permission.)

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, 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 Prof. Kathleen Lonsdale at 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 Prof. Paul Barnes and with co-supervision from Prof. 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 be 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. 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 3 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 80s to the early 90s, 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 update 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 University College London (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 5-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.

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 Material 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.

IUCr

International Union
of Crystallography

www.iucr.org