

Appendix B. Reports on Outreach and Education, the Crystallography in Africa Initiative and the *IUCr Newsletter*, and reports of the IUCr's Advisory Committees

B1. Meeting Support Committee (MSC)

For 2024 the MSC has received funding requests for a total of 31 events. Compared to 2023 (21) and 2022 (24), this presents a significant increase.

Among the 31 events were four regional associate meetings (ACA, ECA, LACA and AsCA) and one national crystallographic meeting (Turkey). An application for the Bangladesh National Crystallography Meeting conflicted with the AsCA dates in December 2024. Failure to produce a support letter from the AsCA organizers prompted the Bangladeshi Crystallographic Association to move their meeting to January 2025.

One of the 31 applications (ICCBM-18) was received at a very late stage, only 2.5 months before the event took place.

Of the 31 applications, 30 received support. Since at the time the ICCBM-18 application was received the funding decisions for the 2024 events had been completed and the funds for 2024 had been exhausted, ICCBM-18 could unfortunately not be funded. An overview of all events during 2024, which applied for IUCr funding and received funding, is provided below:

High Resolution X-ray Diffraction and Imaging, XTOP-2024, Carry-le-Rouet, France
Hot Topics in Contemporary Crystallography 2024, HTCC6, Dubrovnik, Croatia
RapiData2024, Stanford, USA
5th Turkish Crystallography Meeting, Samsun, Turkey
18th International Symposium on Metal-Hydrogen Systems, Saint-Malo, France
Real Materials in the Information Era, ISCoC, Erice, Italy
Zürich School of Crystallography 2024, Zurich, Switzerland
ACA Summer School on Chemical Crystallography, Purdue, USA
European Crystallographic School 9, Nancy, France
American Crystallographic Association Meeting 2024, Denver, USA
4th European School on Crystal Growth, ESCG4, Jachranka, Poland
8th European Conference on Crystal Growth, ECCG8, Warsaw, Poland
Early career diffraction methods seminar, Berlin, Germany
High Pressure Single Crystal X-ray Diffraction Summer School, Edinburgh, UK
International School on Fundamental Crystallography, MathCryst7, Lima, Peru
34th European Crystallographic Meeting ECM-34, Padova, Italy
European Powder Diffraction Conference EPDIC18, Padova, Italy
Electron Crystallography School 2024, Padova, Italy
13th International Conference on Inelastic X-ray Scattering, IXS2024, Himeji, Japan
SMARTER8, Aviero, Portugal
Latin American Crystallographic Association Meeting, LACA-2024, Montevideo, Uruguay
VI LACA School: Quantum Crystallography, Montevideo, Uruguay
2024 IUCr Commission on High Pressure Workshop, Lund, Sweden
6th International Symposium on Halogen Bonding, ISXB6-2024, Dubrovnik, Croatia
19th International Small Angle Scattering Conference, SAS-2024, Taipei, Taiwan
Fragment-Screening Workshop Sirius, FS-WS-2024, Campinas, Brazil
Sagamore XX Conference on Quantum Crystallography, Delhi, India
International Workshop on Magnetic Crystallography 2024, Dongguan, China
Asian Crystallographic Association Meeting 2024, AsCA-2024, Kuala Lumpur, Malaysia
LACA Rigaku Open Lab 2024, São Carlos, Brazil

The MSC has also decided to refurbish the funding guidelines. Work on this has begun.

M. Weiss, Chair

B2. Outreach and Education

The Outreach Committee (OuC) was established in 2024 by IUCr President as a Subcommittee of Executive Committee. Its purpose is to supervise and guide various IUCr Outreach activities (see <https://www.iucr.org/iucr/governance/advisory-committees/outreach-committee>). In 2024 OuC meet several times on ZOOM.

IUCr Outreach Activities traditionally are proposed, run and managed by experienced crystallographers who deeply care about propagating Structural Sciences and IUCr values around the world. All these actions are modestly supported by IUCr funding, the funds being distributed by IUCr CEO, Alex Stanley.

The OuC budget – as suggested by FC and approved by EC – is 30 K US\$ for each year, 2024 and 2025.

In 2024 the IUCr outreach activities were as follows:

Worldwide

Crystal growth competition for School Children organized by Luc Van Meervelt. Given the high quality and a high number (55) of the submitted videos, Luc added to the usual gold, silver and bronze medals, a number of honorable mentions. This year I participated in the judging panel and I enjoyed watching the videos immensely. The list of laureates of the video competition is presented in IUCr Newsletter.
https://www.iucr.org/news/newsletter/etc/articles?issue=159799&result_138339_result_page=11

Africa

2024 year was a very fruitful one for African crystallography. Three courses and Open Labs with remote facilities (connected to diffractometers at the CNRS Université de Lorraine CRM2 laboratory, Nancy, France) were organized by Claude Lecomte and Emmanuel Wenger as well as an AFRAMED session (funded by UNESCO – IUCr – CNRS)

https://www.iucr.org/news/newsletter/etc/articles?issue=158542&result_138339_result_page=21

with 4 participants from Burkina, Mauritania and 2 from Madagascar. A 10-day crystallography and diffraction school with remote experiments was organized in Togo (Université de Lomé) by P. Baneto and Dr A. Hounsi with help of Claude.

AFRAMED project was a part of IUCr Africa Initiative <https://www.iucr.org/outreach/africa>.

The 2025 activities in Togo and Ivory Coast will end the Africa Project. Future decisions and activities in Africa will be lead by AfCA, as Professor Lecomte plans to retire in 2026.

<https://www.iucr.org/outreach/africa/#afamed>

In Kenya, a team of scientists from Spain (Juan Manuel Garcia-Ruiz) and Kenya (headed by Solomon Derese and Martin Mbugua) successfully organised the first crystallisation contest, which finished on 25 January 2025. This contest was a second part of the programme “Learning how science works with crystals”, that started with the workshop “Crystallography at the School” held in late November 2023. During the workshop, high school teachers were trained on the fundamentals of crystallography and practical ways of growing crystals. This event featured sixteen teams involving sixty-six students from five schools. This contest was organized by a Spanish team (CSIC/DIPC) headed by Juan Manuel Garcia-Ruiz and Fermin Otalora in collaboration with a Kenyan team (UoN/AESA) <https://kenyancrystallizat.wixsite.com/blog> IUCr President Santiago Garcia-Granda attended the award Ceremony via video conference, enthusiastically praising the whole activity. For 2025 prof Garcia Ruiz is planning two new events in Kenya. One is the COSPAR-IUCr Capacity Building Workshop on "Mineral and Materials Sciences for Space Exploration", the other being a field trip to the Rift Valley with the team of the Sinergy project.

In Benin in 2024 Michele Zema organized a succesful Open Lab, he is also planning to provide crystallography assistance to UWI-Mona in Jamaica, supported by UNIBO- Global South as well as organize crystallography training session in Uzbekistan.

The full reports as well as captivating pictures of all the mentioned above activities will be presented at the Outreach IUCr website thanks to help of Kezia Bowman IUCr Marketing and Communications Manager.

In Dec 2024 an Open Lab in collaboration with Rigaku was organized in Sao Carlos Brasil by Javier Ellena

<https://www.ifsc.usp.br/lamucres/assets/pages/openlab2024.html>

LAAAMP project <https://www.iucr.org/outreach/laamp> started in 2016 continues.

IUCr v-president, Graciela Diaz Delgado is a new member of the LAAAMP Executive Committee and a Member of the Liaison Committee of the ISC Regional Focal Point for the Latin American and Caribbean Region.

The Outreach Committee would like to express their gratitude to all the Scientist and Staff Members working hard to make the Outreach Initiative such a success.

We are also grateful to the IUCr Journal's editors who donate their gratifications to the Outreach Fund.

Hanna Dabkowska, Chair of IUCr Outreach Committee

B3. Crystallography in Africa Initiative

2024 was a very fruitful year for African crystallography. Three courses and openlabs with remote facilities (connected to diffractometers at the CNRS Université de Lorraine CRM2 laboratory, Nancy, France) were organized as well as an AFRAMED session with 4 participants from Burkina, Mauritania and Madagascar (2 participants). A 10-day crystallography and diffraction school with remote experiments was also organized in Togo.

• Lomé, Togo

A crystallography course for ‘master de physique’ students was organized by Professor P. Baneto and Dr A. Hounsi (Université de Lomé). Claude Lecomte taught a course of crystallography and X-ray diffraction from March 21st to March 29th; this was followed by remote experiments on one of the CRM2 single-crystal diffractometers taught by Dr Emmanuel Wenger. 45 students participated in this 28-hour course and were evaluated as part of their physics master and/or engineering studies. Most students passed the exam with success.

• Sénégal

The Senegalese crystallographic association was inaugurated.

A one-day lecture was organized by Professors Magatte Camara (Ziguinchor Univ.) and Ibrahim Thiam (Dakar Univ.), with remote experiments organized by Drs El Eulmi Bendeif and Emmanuel Wenger in Nancy, February 19th 2024. Claude Lecomte was invited and gave a lecture “Cristallographie en Afrique Sub-Saharienne : Apport du projet AFRAMED”. UNESCO funded 25 bursaries for Senegalese participants. For efficiency this money was sent to IUCr and thanks to the IUCr CEO the bursaries were distributed easily. A report was published in the IUCr Newsletter, 5 October 24).

• Madagascar

Patrick Roge and Veroarisinina Ratsimbazafy (Antananarivo) and Claude Lecomte organized an openlab in Antananarivo (13 October to 23rd). Remote experiments with Emmanuel Wenger were performed thanks to IUCr who gave to Antananarivo University a PC, a video projector and connectors to Antananarivo University (1825 euros). 15 IUCr bursaries were given to Madagascar young colleagues to attend this openlab.

• C. Lecomte's team organized the third AFRAMED course, mostly funded by the CNRS AFRAMED budget and CRM2. Drs Brahim Sorgho (Burkina), El Waseda Thiam (Mauritania), Patrick Roge and Veroarisinina Ratsimbazafy (Madagascar) were taught single-crystal diffraction methods during one month (September 2024) by Drs Wenger and Lecomte. This AFRAMED training allows the trainees to run a single-crystal diffraction experiment independently: they can run the diffractometer remotely for their research or teaching from their home university. The IUCr contributes by paying the diffractometer fees.

Acknowledgements:

Special thanks are due to CNRS, IUCr, UNESCO, Université de Lorraine and SOLEIL, to Dr Emmanuel Wenger for his teaching and experimental demonstrations, and to Mrs. Anne Clausse for her help in the administration of the AFRAMED project.

Claude Lecomte, Chair of the IUCr Africa Initiative

B4. IUCr Newsletter

The IUCr Newsletter (<https://www.iucr.org/news/newsletter>) continues to provide material of interest to a broad audience. Not only does it report on the interests and activities of the IUCr and its Regional Associates and Commissions, but it also aims to inform, educate and entertain the global community of crystallographers and structural scientists.

This annual report covers four issues: Volume 32 Numbers 1–4 (2024). A large range of different articles was published, including 23 dealing with the IUCr journals and commentaries, 22 on meetings, 8 feature articles and 6 obituaries. Each issue contained letters from the President, Santiago García-Granda, and editorials from the Editor, Mike Glazer.

During this year, Andrea Sharpe retired and was replaced by Kezia Bowman. I can report that Kezia has quickly come to grips with the Newsletter and has been able to continue the excellent work carried out by Andrea, as well as in adding her own ideas. In each issue Istvan and Magdolna Hargittai as usual provided entertaining and interesting feature articles related to the history of crystallography and the persons involved. These were on Vladimir Koptsik, aperiodic crystals, the Berlin Natural History Museum and crystallographers, chirality, and quasicrystals.

IUCr Regional Associates contributed meeting reports, and meetings in Australia, Austria, Croatia, Czech Republic, France, Germany, Japan, Poland, Scotland, Senegal, Switzerland, Thailand, USA, – many supported by the IUCr – were also documented.

The email editions of the Newsletter were circulated to 13,000 crystallographers and structural scientists worldwide, and social media channels provided additional exposure. The complete Newsletter archive is available at <https://www.iucr.org/news/newsletter/archive>. Owing to the success of the Newsletter, the IUCr has decided that in future, 6 issues per year will appear instead of the 4 per year so far published.

I am most grateful to the staff at Chester for their help in putting the Newsletter together, and especially to Andrea Sharpe and Kezia Bowman, whose active help made possible the publication of each issue, as well as Jennifer Skade and Mark Bates who have both helped in editing and uploading of articles throughout 2024.

A. M. Glazer, Newsletter Editor

B5. Committee for the Maintenance of the CIF Standard (COMCIFS)

COMCIFS is responsible for development and maintenance of the CIF standard.

Dictionary licensing

COMCIFS voted to make the Creative Commons Attribution licence (CC-BY-4.0) the default license for CIF dictionaries. This means that dictionaries may be freely shared, as long as their origin is acknowledged and any changes to the original are noted. This decision has been conveyed to the Executive for their approval.

International Tables Volume G

A new chapter covering the NeXus format was commissioned and largely completed this year. Other chapters continue to be added to and refined, with the editors aiming for completion of the Volume this year.

Dictionary development

A new draft version of the modulated and composite structure dictionary was developed by G. Madariaga, and a number of data names relating to radiation damage were added to the core dictionary. COMCIFS was also involved in advising and reviewing an initiative of the European Nano Electron Diffraction (<https://naned.eu>) project to supply extensions to the core dictionary arising from 3D electron crystallography at the nanometre scale.

Looking forward

In the run-up to publication of Volume G all dictionaries will see formal releases. Work is ongoing to finalise the non-core dictionaries, with particular focus on powder CIF.

J. Hester, Chair

B6. Committee on Data (CommDat)

The Committee on Data was established by the IUCr Executive Committee at its meeting in Denver in July 2016. The specific terms of reference are: “CommDat will advise the IUCr Executive Committee on all aspects of data with respect to policy and actions to be taken.” Details, including membership and consultants, can be found here: <https://www.iucr.org/iucr/governance/advisorycommittees/committee-on-data>

There are the following matters to report for the period 2024/5 and 2025/6:

a) Raw Data Letters

The concentration of CommDat activity, and the most substantive outputs in this reporting period, has been around the establishment and development of the Raw Data Letters article category of the IUCr Data journal. This is an unusual publishing goal, in that it wishes to address the publication and reuse of RAW diVraction data – while this is an identified need and leads new territory in terms of publishing in general, it has caused a significant amount of follow-on work, due to its mode of operation and dependence on supporting a new type of data. There have been editorials and articles covering it, a number of exemplar articles published, presentations at various crystallographic conferences, conference posters, and conference leafleting etc. However, further sustained work is required to promote this article type – as it requires a cultural shift which is specific to diVerent communities ie the approach in Chem Cryst is diVerent to MX. There has been consultation with the Commission on Chemical Crystallography, as well as surveying and articles in the IUCr Newsletter. However, before this can happen in earnest and at scale, there is a requirement for some supporting tools to validate raw data. 18 months funding has been won from the EU OSCARS programme for the MC-ReDD project (Metadata Capture and validation for Reuse of raw DiVraction Data, <https://oscars-project.eu/projects/mc-redd-metadatacapture-and-validation-re-use-raw-diVraction-data>) is supporting a developer to build services around raw data validation that drive processes for its publication – this work is nearing completion. More recently, in the latest EU OSCARS programme, the Fail2FAIR project (Recovering discarded macromolecular crystallographic data, <https://oscarsproject.eu/projects/fail2fair-recovering-discarded-macromolecular-crystallographicdata>), was funded for 2 years and will provide ways to support the surfacing and reuse (particularly for AI/ML driven work/processes) of MX raw data.

b) Planning and preparation for IUCr 2026 Congress

CommDat was a significant participant in the work of the Calgary IUCr 2026 Congress Programme Committee, resulting in far greater involvement in the organising, themes and delivery of the programme than ever before. Involvement summarised as:

- The inaugural AI in Crystallography Summer School (<https://event.fourwaves.com/cryst-comp-school/pages>). Organised sponsorship and digital infrastructure (Dectris Cloud) to support the practical aspects, plus sessions on data considerations/preparation for AI
- Organising a 1 day workshop on Open Data and Global Open Science (<https://indico.esrf.fr/event/251/>)
- 4 Microsymposia and a Keynote primarily sponsored by CommDat, while a further 8 MS across a range of Commissions are heavily supported by CommDat.
- Advanced planning for an open data forum with Dectris Cloud

c) Raw Data availability policies, standards

CommDat had input into the ESRF data policy, which is leading the way in long term availability of central facilities data. Other synchrotrons, notably Soleil and SLS, are taking notice and following suit. There is a strong relationship with COMCIFS, and the committee has fed into their work in several areas, particularly High Pressure and Electron DiVraction CIF dictionaries / Core CIF additions. There has been representation at, and input into, a number of national or global scale activities, most notably the NFDI (Germany), PSDI (UK) and CO-DATA (global), developing standards.

d) Committee operations and communications

Publicising Raw Data Letters (posters, talks, IUCr stand) has occurred at numerous conferences including ECM, ACA and BCA. Awareness raising across various Commissions has been particularly good – as reflected in the Congress programme organisation. The IUCr forum has had some activity, however there has been a little less traffic more recently.

e) Considerations for the Future

Committee composition. Key members have become inactive / retired, most notably Brian McMahon as the CommDat Chair. Around the Calgary congress there will need to be some rotation of membership and establishing new roles (particularly considering the next point).

CommDat scope. The focus in recent years has been somewhat on raw data, which is expected as CommDat was established as a result of the DiVraction Data Deposition Working Group. However, all types of data have now come to the fore with the advent of Machine Learning techniques, as evidenced by coverage in the upcoming Congress, and so the coverage needs a little adjusting to remain current.

Simon Coles, Chair

B7. Committee for Gender Equity and Diversity (GEDC)

GEDC continued to review recommendations from previous years, and prepared for 2025 survey project to be distributed to IUCr regional affiliates

Two virtual meetings held in 2024 with Standing Committee of the Gender Equity in Sciences (SCGES) Group

GEDC Co-Chair Representative Santarsiero met in February 2024 with SCGES Group

- Attended two day sessions and presentations to discuss initiatives
- Attended Global Women's Breakfast
- Presentation on popularizing science without gender bias
- Presentation and discussion with representatives of Young Scientists' Organizations
 - IUBMB Trainee Initiative (Croatia, South Africa)
 - Global Young Academy (India, Indonesia)

Advancing Gender Equality in Scientific Organizations Project launched with SCGES, International Science Council (ISC), and International Academic Partnership (IAP)

- Identify key barriers and drivers to the leadership of women scientists in scientific organizations
- Combine quantitative data with qualitative insights to establish baselines, assess progress, and provide actionable recommendations to improve gender equality

GEDC Co-Chairs Nonato and Santarsiero involved in the SCGES working groups

Internet/Web, Communications, and Social Media

Best Practices

ISC Liaison

History Interview Project

IUCr continues to lead in promoting gender equality throughout conference leadership, awards, membership, and publications. Significant help provided to new regional affiliate, African Crystallographic Association, as they host their first Pan-African Conference on Crystallography

B. Santarsiero, Chair

B8. IUCr/Oxford University Press Book Series Committee

The books published within the book series, which was launched in 1987 (<http://ww1.iucr.org/iucr-top/genasm/rep93/oup.htm>), are commissioned in two categories: Monographs on Crystallography and Texts on Crystallography.

Due to an oversight there was no published report for 2024. The membership of the Committee has remained unchanged since 2023, when K. Friese (Germany) replaced R. Herbst-Irmer (Germany) and E.H. Snell (USA) took over the membership interest re-sponsibilities of J.R. Helliwell (UK). J. R. Helliwell retired in 2023 after 27 years on the book committee, including 6 as Chairperson. The current Chair is J. Gulbis (Australia), a member of the Book Series Committee since 2017.

Current members are: G. Chapuis (Switzerland), K. Friese (Germany), H. Maynard-Casely (Australia), P. Mueller (USA), M. Nespolo (France), E.H. Snell (USA), N. Yagi (Japan), X. Zou (Sweden) and J. Gulbis (Australia). As Chair of the commission of crystallographic teaching, A. Guerri (Italy) is an ex officio member, while S. Adlung represents ex officio liaison at Oxford University Press.

The Book Series Committee members provide individual assessments of book proposals, which are combined into a Chairperson's report. The IUCr-OUP Committee reports are provided to the IUCr Executive Committee, which can either endorse them or make suggestions, prior to submission to OUP.

2025 was a quiet year for the Committee. We evaluated one book proposal.

A highlight of 2025 was publication of a teaching text (hardcover): Precision and Accuracy in Biological Crystallography, Diffraction, Scattering, Microscopies, and Spectroscopies by John R. Helliwell. This featured in the IUCr newsletter Volume 33(5) 2025.

To ensure consistency with IUCr nomenclature policies, and to reduce introduction of errors, we continue to affirm to OUP the need for us to assign volunteer(s) with requisite subject expertise, ideally from our Committee, so as to review a full draft of a new text in our Book Series before publication by OUP in our, IUCr, name. In this vein, over the 2024-2025 period, previous and current IUCr-OUP members J. Helliwell, M. Nespolo and G. Chapuis, and external experts M. Cianci and G. Zanotti, reviewed all chapters of a teaching text X-ray Structural analysis of Biomacromolecular crystals by Akio Takenaka. J. Helliwell followed up with several rounds of editorial feedback. The prospective textbook is now with OUP. I would like to express my sincere appreciation of the efforts of all members of the IUCr-OUP Book Committee in 2025.

J. Gulbis, Chair