

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. The Sub-committee on the Union Calendar

Sponsorship of meetings

The Sub-committee on the Union Calendar considers and advises the Executive Committee on requests for IUCr sponsorship and financial support of meetings. Details of how to apply for financial support, along with guidelines, are available on the IUCr website.

Visiting Professorship Scheme

The IUCr Visiting Professorship scheme aims to support some of the costs of having internationally recognized scientists as lecturers for short courses at workshops or schools organized in developing countries. Support from at least one IUCr Commission is required. Applications will be considered by the Sub-committee on the Union Calendar.

During the IUCr Executive Committee meeting in Versailles in August 2022, the Sub-committee of the Union Calendar was renamed as the Meeting Support Committee (MSC). This renaming still needs to be approved by the General Assembly. Nonetheless, the working name of the committee is now the MSC. The new Chair of the MSC is Manfred Weiss, having taken over from Graciela Díaz de Delgado after the Versailles Executive Committee meeting.

The MSC received funding requests for a total of 19 events to take place during the calendar year 2022. Among these there were four meetings of the regional associates (ACA, ECA, AsCA and LACA), with zero, two, one and three associated satellite meetings, respectively, for which support was sought. The two ECA satellite meetings and the LACA satellite meeting were approved. AsCA did not provide additional details for their three satellites, so no funding was allocated to them. Nine further events applied for IUCr funding, of which seven were approved. The remaining two cancelled their applications. One cancellation was received from a Gordon Research Conference meeting due to the inability to meet the IUCr sponsor requirements. The other cancellation came from the meeting of the International School on Synchrotron Radiation due to a too-late allocation of funds. The other seven events were approved and received funds. The total funds requested were USD 118,000, and the total funds allocated were USD 73,000 (62%).

During 2022 a workflow for streamlining the application process was developed between the MSC Chair and the IUCr CEO, Alex Stanley. The plan is to roll out the new scheme after the Melbourne Congress.

The following meetings received support during the two-year period from 2021 to 2022:

6th Conference of the Bangladesh Crystallographic Association, virtual, 15–16 January 2021.

CCP4 Crystallographic School in South Africa: Data Collection to Structure Refinement and Beyond, Cape Town, South Africa, 31 March – 8 April 2020. (Moved to 22 February – 5 March 2021.)

17th European Powder Diffraction Conference – EPDIC17, Šibenik, Croatia, 26–30 May 2020. (Moved to 30 May – 3 June 2022.)

55 Erice School: Molecular Crystal Engineering – Virtual Meeting, 31 May – 4 June 2021.

2nd International School on Advanced Porous Materials (MOFschool2021) – Virtual Meeting, 21–25 June 2021.

European Crystallographic School (ECS6), Budapest, Hungary, 5–11 July 2020. (Moved to virtual, 4–10 July 2021.)

To.Sca.Land: Total Scattering for Nanotechnology in Al Andalus, University of Granada, Granada, Spain, 20–24 September 2021.

10th International Conference of the Hellenic Crystallographic Association, Athens, Greece, 15–17 October 2021 (originally scheduled for 2020).

Tunisian Powder Diffraction School, 21–24 January 2022.

LACA IV School on Powder Diffraction; Phase-ID & Microstructure, 24–28 January 2022.

56th Erice School: Crystallography Under Extreme Conditions, 3–11 June 2022.

57th Erice School: Diffuse Scattering, 3–11 June 2022.

Gordon Research Conference – Crystal Engineering, 19–24 June 2022 (withdrawn).

International Conference on the Chemistry of the Organic Solid State, ICCOSS XXV, 3–9 July 2022.

7th European Crystallography School, ECS-7, 10–15 July 2022.

16th International Conference on the Physics of Non-Crystalline Solids, PNCS-2022, 10–16 July 2022.

3rd European School on Crystal Growth, ESCG-3, 20–23 July 2022.

7th European Conference on Crystal Growth, ECCG-7, 25–27 July 2022.

72nd Annual Meeting of the ACA, ACA-2022, 29 July – 3 August 2022.

33rd European Crystallographic Meeting, ECM-2022, 23–27 August 2022.

ECM-2022 School on Spin and Charge Densities Modelling, 20–22 August 2022.

ECM-2022 School on Functional Materials under Pressure and Chirality in Crystals, 28–30 August 2022.

International School on Synchrotron Radiation, SILS-2022, 5–16 September 2022 (withdrawn).

XVIII International Small-Angle Scattering Conference, SAS-2022, 11–16 September 2022.

Asian Crystallographic Association Conference 2022, AsCA-2022, 30 October – 2 November 2022.

50th Annual Meeting of the Argentinian Biophysical Society, SAB-2022, 16–18 November 2022.

V Meeting of the Latin American Crystallographic Association, V-LACA, 28–30 November 2022.

LACA School: Polymorphism: Applications in Industry, 1–3 December 2022.

2022 IUCr Commission on High Pressure Workshop, CHP-2022, 6–10 December 2022.

B2. Outreach and Education

The IUCr is actively engaged in a number of outreach and education initiatives, targeting emerging countries worldwide and students of all ages, from schoolchildren to early career researchers and established crystallographers. Such initiatives are held in the spirit of the Crystallography for the Next Generation resolution (Morocco, 2015): to build on the success of IYCr2014, the IUCr and partner institutions committed to enhance the stature of crystallography; build capacity in developing regions of the world; and extend further the public understanding of science in general and crystallography in particular.

To increase the scope of the outreach programme and boost its impact, the IUCr is partnering with several other societies and organizations. Thanks to the great achievements reached since IYCr2014, the IUCr has reinforced its high reputation in the contexts of the global science diplomacy and advocacy debate, and of science capacity-building assessment through the implementation of actions towards developing scientific research, education and infrastructure worldwide. The IUCr is therefore playing a crucial and strategic role, while targeting the scientific community at large.

The pandemic imposed a re-organisation of the IUCr outreach efforts. Many in-person events were cancelled or postponed, but new formats and modalities allowed the crystallographic community to gather together so that momentum was not lost. Since 2022, a gradual resumption of in-person activities has allowed outreach initiatives to be revitalised and new actions are being implemented.

The present report highlights outreach and education activities implemented since the last General Assembly meeting held in Prague in 2021. Some activities are presently held within the framework of the IUPAP-IUCr-ICTP LAAAMP initiative (<https://laaamp.iucr.org>), hereafter referred to as LAAAMP, which stands for Lightsources for Africa, the Americas, Asia, Middle East and Pacific. The initiative was originally funded with a EUR 300,000 grant from the International Science Council (ISC) in 2016. The IUCr Executive Outreach Officer has acted as Chair of the LAAAMP Executive Committee during the triennium 2020-2022.

Reaching out to schoolchildren and schoolteachers

After being suspended from 2020 to 2022, the IUCr crystal growing competition (<https://www.iucr.org/outreach/crystal-growing-competition>) was re-launched in 2023. The competition, coordinated by Luc Van Meervelt, is open to all schoolchildren (three categories: under 11s, high-school middle forms and high-school upper forms) and aims to introduce students to the exciting, challenging and sometimes frustrating world of growing crystals. It has generated great enthusiasm among schoolchildren from several parts of the world in the six editions run from 2014 to 2019, and efforts are being made to reach a wider audience.

A new series of online workshops dedicated to schoolteachers was initiated in 2021 within the framework of LAAAMP to facilitate connections between science curricula and inquiry-based learning, with synchrotron research stories as a focus. The goal of the LAAAMP High-school Teachers Workshops (<https://laaamp.iucr.org/events/high-school-teachers-workshops-list>) is to introduce high-school teachers to science research, STEM, inquiry, and indigenous connections, and how they could connect these concepts to their classroom. Three editions have already been held in 2021 (in collaboration with the Canadian Light Source, CLS), 2022 (in collaboration with SESAME) and 2023 (in collaboration with Synchrotron Light Research Institute, SLRI, Thailand).

Reaching out to early-career researchers and young professors

Several actions are in place targeting early-career researchers and young professors, particularly from emerging countries worldwide. Such actions are aimed at expanding the scope of crystallography worldwide by offering new research and education opportunities and developing research infrastructure.

A LAAAMP mobility programme allows teams composed of a faculty member and a Ph.D. student from any of the targeted regions of LAAAMP (Africa, Mexico, the Caribbean, South America, Central and Southeast Asia, Middle East and the Pacific Islands) to spend a period of two months at a LAAAMP-participating synchrotron facility to be trained about the use of SR-based techniques (LAAAMP FAST Teams; <https://laaamp.iucr.org/calls>). Over a hundred individuals have been trained by this programme since 2017. The programme was re-launched in 2022, some FAST Teams are presently at synchrotrons for their training, and a new call is now active for training visits to be completed within 2024.

The LAAAMP SPARC (Synchronizing Partners to Advance Research Characterization) initiative, a mail-in access programme to advanced lightsources for researchers from targeted areas of the project, was launched while the mobility programme was suspended in 2020 to 2022 because of COVID-19. This initiative is still active, although priority is given to in-presence visits to synchrotron facilities.

The IUCr-UNESCO OpenLab initiative (<https://www.iucr.org/outreach/openlabs>), launched during IYCr2014, is still in full swing. Over 30 editions have been implemented in more than 25 countries, with different modalities and in partnership with several companies and organisations. Several hundred students have been reached by the programme. The essential need for reliable and up-to-date in-house equipment has become very clear. This has brought to design a new concept idea, developed by the IUCr Executive Outreach Officer within the framework of LAAAMP and in collaboration with the government of Benin, UNESCO and instrumentation manufacturers. The X-TechLab (<https://www.xtechlab.co/>) was founded in 2019. It is the first X-ray techniques facility established in Benin and acts as a hub for Central and Western Africa. The X-TechLab is funded by the government of Benin and is one of the flagship laboratories of Sèmè City (<https://semecity.bj/en/>), the International City of Innovation and Knowledge. It is equipped with new instrumentation including a Bruker AXS Quest Eco single-crystal diffractometer with an Oxford Cryosystems cryostat, a Malvern Panalytical Empyrean powder diffractometer and a Bruker X-ray micro-tomograph, the latter to be installed later during 2023. In addition, the facility has access to the CSD through the CCDC FAIRE programme, and to IUCr Journals and *International Tables for Crystallography*. Staff have been appointed on a permanent basis. The facility is devoted to education, research and service to local industry. Two OpenLabs of two weeks each are organised every year, and they have already reached over a hundred students from across Africa. A grand inauguration event of the powder diffraction lab is scheduled on 18 September 2023 and will be followed by an OpenLab. During the years of the pandemic, when travelling to Benin from abroad was not allowed, a training programme on crystal symmetry was offered by the X-TechLab staff, coordinated by the IUCr Executive Outreach Officer, to students from the Faculty of Science and Technology, U. of Abomey-Calavi, reaching over a thousand participants.

The X-TechLab model is now being implemented in another region of the world, namely the Caribbean. Work is in progress towards the establishment of crXstal (Caribbean Regional X-ray Science Toward Advancement Laboratory) at the University of West Indies, Jamaica. The project has been developed by the IUCr Executive Outreach Officer within the framework of LAAAMP, and in collaboration with UNESCO, ISC-LAC and Bruker AXS. More partners are expected to join soon. Negotiations and fundraising are ongoing for acquiring a new single-crystal diffractometer and the first OpenLab Jamaica is expected to be organised in early 2024.

In addition to the educational programme offered through the OpenLabs and the other initiatives reported above, several other schools and workshops are regularly organised as part of the outreach programme of the IUCr, and participation in congresses and conferences ensures visibility to the programme itself. Schools and workshops organised include: two editions of the LAAAMP-ICTP School on Synchrotron Light Sources and their Applications in December 2021 (107 participants) and February 2023 (180 participants), the SESAME-Africa Online Workshop (July 2022) and the LAAAMP-AfLS Africa Workshop (September 2022). Invited talks delivered by the IUCr Executive Outreach Officer include at the AfLS-AfPS-ePCCr conference (November 2021); the IMA conference (July 2022); "The Glory of International Cooperation" workshop (International Conference on Research Infrastructure; October 2022); the AfLS conference (November 2022); the inaugural meeting of the Synchrotron for the Greater Caribbean steering committee (January 2023); the PCCr3 conference (January 2023); the IUCr Journals Management Board meeting (March 2023); the IUCr Congress (August 2023); and the AIC Congress (September 2023).

Initiatives for new large-scale facilities

Around 50 synchrotron facilities are operational in the world and none of these is located in Africa, while Sirius in Brazil (which has recently become partner of LAAAMP) is the only facility operating in Latin America. Two major initiatives are presently active for an African Light Source (AfLS) and for a Synchrotron for the Greater Caribbean, LAMISTAD (the latter embedding the original initiative for a Mexican synchrotron). The IUCr is playing a fundamental political-diplomatic as well as scientific role in the whole process towards the establishment of these facilities. The IUCr Executive Outreach Officer is member of the Executive Committee of the AfLS Foundation and has participated in all the preliminary meetings for setting up a steering committee for LAMISTAD. Moreover, LAAAMP has signed an MOU with the AfLS Foundation and is leading in capacity building for the African Light Source project. In line with the generally agreed motto that "we need to build the users before building the facilities", the X-TechLab and crXstal facilities are considered by the international community as "feeders" of the two synchrotrons, and it is expected that future users of the synchrotrons will be trained in crystallography at these facilities, thus generating great enthusiasm and expectations around these initiatives.

Reaching out to the wider community and the general public

The IUCr is partnering with several other institutions for the organisation and implementation of the activities for the UN International Year of Basic Sciences for Sustainable Development (chaired by IUPAP and partnered by over 50 associations; <https://www.iybssd2022.org/en/home/>) and the Year of Mineralogy (declared by the International Mineralogical Association, IMA), to be

celebrated across 2022 and 2023. The IUCr Executive Outreach Officer is a member of the Steering Committees of both events, and was honoured to deliver the official opening speech of the Year of Mineralogy at the IMA 2022 Conference in Lyon, France.

Reaching out to new countries and regions

Since the first appeal signed at the IYCr2014 Summit meeting in Bloemfontein in 2014, envisaging the formation of an African Crystallographic Association (AfCA), and the inception of the first Steering Committee (chaired by Andreas Roodt) at the Hyderabad Congress in 2017, through all the Panafrican Conferences on Crystallography (PCCr), and to the formal foundation of the African Crystallographic Association (AfCA) under the leadership of Delia Haynes, the IUCr Executive Outreach Officer has participated in all the activities that have brought AfCA to apply for becoming the fifth Regional Associate of the IUCr (as a member of the Steering Committee first and as Advisor to the Executive Committee after its foundation). Of course, the capacity-building effort for reaching such a milestone started several years ago (perhaps, formally, with the launch of the IUCr Initiative in Africa back in 1999) and has involved many people and several initiatives that cannot be all mentioned here. In a relatively short period, AfCA represents today a large and growing community of crystallographers, has already gained strong credibility in the context of science, science education and science policy within the African continent, and has established excellent relationships with several organizations, like AfLS, LAAAMP, AfPS and many others. Several of the actions described in the present report are contributing to the development of the community and of the association as such, and continuous support will certainly be ensured through the outreach and education programme of the IUCr.

Other activities

The IUCr Executive Outreach Officer has been working with other members of the Chester staff on several aspects of general IUCr business, including promotion of activities, transfer of the outcomes of the outreach programme into the development of IUCr Journals, maintenance of some sections of the IUCr website and the *IUCr Newsletter* (both redesigned by the IUCr Executive Outreach Officer in collaboration with Brian McMahon in 2020 and 2018, respectively). Contributions to the work of other bodies include:

- IUCr Commission on Crystallographic Teaching (consultant);
- IUCr Gender Equity and Diversity Committee (member);
- IUCr2023 Congress (member of the IPC);
- IUCr Journals Management Board (guest);
- IUCr Journals (proposer and Guest Editor of the virtual special collection celebrating the foundation of AfCA);
- LAAAMP (co-founder and member of the Executive Committee; Chair from 2020 to 2022);
- X-TechLab (co-founder and Chair of the International Scientific Committee);
- African Crystallographic Association (advisor to the Executive Committee and previously ex-officio member of the Steering Committee);
- International Mineralogical Association (member of the Executive Committee);
- African Light Source Foundation (member of the Executive Committee);

The IUCr Executive Outreach Officer also regularly maintains liaison with several institutions and associations.

M. Zema, IUCr Executive Outreach Officer

B3. Africa Initiative on Crystallography

2022 was very fruitful for the Africa initiative with two OpenLabs: one in Congo Brazzaville and the other in Mauritania both, using remote facilities to collect data; the development of the concept of remote laboratories together with CNRS (AFRAMED); the signing of an MoU between the IUCr, UNESCO and CNRS; and an OpenLab during PCCr3 (Main Tutor E. Bendeif).

(1) The first OpenLab on Crystallography using remote diffraction facilities was held in Brazzaville, Republic of Congo, from 11 to 22 May 2022 at the Marien Ngouabi University. This OpenLab was organized by the Congolese Association of Crystallography (ACCr) in partnership with Marien Ngouabi University, the Geological and Mining Research Center (CRGM) of Brazzaville and the CRM2 laboratory (CNRS/Université de Lorraine). This event was attended by 28 young academics and PhD students in chemistry. After the opening ceremony, theoretical courses and tutorial sessions were conducted by Claude Lecomte. These courses focused on crystal lattices, crystallographic calculations, point groups, space groups, the *International Tables for Crystallography*, Fourier series and transforms, X-ray scattering by atoms and molecules and diffraction by crystals, an introduction to single-crystal and powder diffraction, and resolution and refinements of crystal structures from single-crystal and powder diffraction data. After 3.5 days of lectures and tutorials, practical activities were carried out for 5 more days. These activities focused on the remote use in Brazzaville of the Bruker D8 Venture single-crystal and Panalytical X'pert PRO powder diffractometers (Drs Emmanuel Wenger, Florence Porcher, Pierrick Durand and El Eulmi Bendeif, CRM2, were the main tutors). WINGX was used for this purpose with a special emphasis on SHELXS, SHELXL, and Mercury and CIF software. The powder analysis was performed using Qualx software (Rietveld refinement) and the Crystallographic Open Database (COD).

(2) The first Mauritania OpenLab on Crystallography was held at the University of Nouakchott, from November 14th to 19th, 2022. This OpenLab was organized by the Mauritanian Chemical Society (Professor A. Barry) in partnership with the Faculty of Sciences and Technics of the University of Nouakchott and the CRM2 laboratory (CNRS/ Université de Lorraine). Forty-three young professor-researchers, post-doctoral researchers, PhD and master's students in chemistry, geology and physics attended this OpenLab, mainly from the Islamic Republic of Mauritania, Senegal and Guinea. The programme was close to that of the Congo one; one of the highlights of this event was the remote visit to the French Synchrotron SOLEIL. On this occasion, for more than 2 hours Dr Jean Daillant, director of SOLEIL, offered a guided tour of SOLEIL followed by a discussion with the OpenLab participants. Practical activities were carried out over 3 days (days 3 to 5). For participants of group A (single-crystal XRD) the activities were focused on the remote use of the Bruker D8 Venture single crystal diffractometer of the CRM2 laboratory.

(3) Remote diffraction experiments: the CNRS AFRAMED (Appui à la Formation Doctorale et à la Recherche en Afrique par des Mesures à Distance) network is based on the possibility of a diffractometer from the CRM2 laboratory being remotely driven by an African colleague previously trained in the use of a CRM2 diffractometer during one full month. The colleague is thus able to use the diffractometer remotely for their own research and for their master's and doctoral teaching. The sample to be measured is centered by a CRM2 researcher (Dr E. Wenger), who then authorizes the African colleague to take control of the instrument for the duration of the experiment (about ten hours) via a secure internet connection. The proof of concept was validated in December 2021 with a remote experiment between the Plateforme de Mesures de Diffraction et Diffusion des Rayons X of the CRM2 in Nancy and the University of Dschang in Cameroon, and then by the OpenLab at the University Marien Ngouabi in Brazzaville in May 2022. This project is supported by CNRS, the IUCr and soon by UNESCO. During September 2022, Drs Patrice Kenfack (Cameroon), Adam Bouraima (Gabon), Ayi Hounsi (Togo) and Seham Kamal (Egypt) were trained in Nancy and are now using the CRM2 diffractometer remotely.

(4) An MoU between the IUCr, CNRS and UNESCO has been signed; this is a result of the Chair's work to organize remote experiments in Africa. Each participant sponsors the AFRAMED remote project with EUR 10,000 a year for 5 years, starting in 2022.

(5) An OpenLab in Nairobi in January 2023 was organized by Dr E. Bendeif, who was supported by the Africa initiative.

(6) Two 2023 projects have already been realized at the time of writing: a Master course in Lomé in March and an OpenLab in Franceville in May. Other 2023 projects will include AFRAMED training of colleagues from Senegal, Congo and Algeria in Nancy in September, and an OpenLab in Guinea in November.

Claude Lecomte, Chair of the IUCr Africa Initiative

B4. IUCr Newsletter

The *IUCr Newsletter* (<https://www.iucr.org/news/newsletter>) has something for everyone. 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 30 Numbers 1–4 (2022). An average of 32 articles were published in each issue, leading with a Letter from the President, Hanna Dabkowska, and an Editorial from the Editor, Mike Glazer.

Still reeling from the effects of the COVID-19 pandemic, the world suffered another shock when Russia invaded Ukraine in February 2022. The IUCr was quick to condemn this action, and the *Newsletter* published statements denouncing the invasion and declaring the Union's solidarity with the international scientific community in calling for a peaceful end to the crisis. Later in the year, the *Newsletter* included a Letter highlighting the dire situation facing students and scientists in Iran.

In 2023, the IUCr celebrates its 75th anniversary and hosts its 26th Congress. In 2022, the *Newsletter* invited its readers to participate in a timely refresh of the IUCr's vision/purpose and values and kept them abreast of news from the Congress organisers.

In other IUCr business, the *Newsletter* advertised for Alex Ashcroft's successor and subsequently introduced the new CEO, Alex Stanley; called for nominations for the 2023 Ewald, W. H. and W. L. Bragg and Struchkov Prizes, and for members of the Executive Committee and Commissions; and introduced changes to the procedure for applying for meeting support.

Each issue republished scientific commentaries from IUCr Journals and included other journal news, such as information about Special Issues, the new electron crystallography section in *IUCrJ* and the launch of Raw Data Letters in *IUCrData*.

Reviving a feature of the old series, a report on Crystallography in France was included, just ahead of ECM33 in Versailles. In Regional Associate news, the ACA's new logo and the ECA's 25th anniversary were celebrated. The Crystallography in Africa section reported on the launch of the Senegalese Crystallographic Association, the African Crystallographic Association's outreach activities and the 2022 OpenLab in Brazzaville, Republic of Congo, which used remote diffraction facilities for the first time.

Topical issues such as the impact of machine learning and artificial intelligence on crystallography, protein structure prediction, and recent advances at the world's synchrotrons, including the use of augmented and virtual reality and solutions to the Big Data challenge, were covered in this volume. Another article described the use of synchrotron powder diffraction experiments to investigate the mineralogy of waste-to-energy ashes – an application of crystallography that is key to finding alternative feedstocks for energy-intensive industries and enhancing environmental sustainability.

But these developments would not be possible without the ingenuity of our forefathers, and articles describing their lives and work – a regular feature of the *Newsletter* – make for very interesting reading.

The e-mail editions of the *Newsletter* were circulated to 13,500 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>.

During 2022, I was pleased to welcome Professor Nan Zhang from Xi'an Jiao Tong University as a Regional Editor to represent China; I look forward to hearing more about crystallography in their part of the world.

I am especially grateful for the staff at Chester for their support and especially the help from Andrea Sharpe.

A. M. Glazer, Newsletter Editor

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

COMCIFS is responsible for maintaining and developing the suite of standards known as the Crystallographic Information Framework (CIF) on behalf of the IUCr. These standards include a data format (CIF), a multitude of discipline-specific dictionaries describing the contents of data files, and the language in which these dictionaries are written (DDLm). The Worldwide Protein Data Bank (wwPDB) is separately responsible for a large and rapidly expanding collection of CIF definitions that encompass concepts and techniques used in the macromolecular community.

COMCIFS currently has 4 voting members and a broad collection of advisers and observers. The voting members are James Hester (Chair), John Bollinger (Co-Secretary), Brian McMahon (Co-Secretary), and Herbert Bernstein. Ongoing COMCIFS business is conducted via the associated IUCr mailing lists.

Brian McMahon has now retired from the IUCr office in Chester, and has indicated that they will also be stepping down as Secretary.

Dictionary development

New categories and data names for more detailed descriptions of elemental composition analysis were added to the core dictionary. The powder dictionary also saw significant work related to detailed calibration specifications for intensities and angles, as well as ongoing work on preferred orientation data names.

International Tables Volume G

COMCIFS members are closely involved with the preparation of the second edition of *International Tables Volume G (Definition and exchange of crystallographic data)*. This year saw several more chapters become ready for technical editing, and the remainder of the applications chapters commissioned. Further information is available in the report of the Commission for *International Tables*.

Interactions with other groups

COMCIFS is represented on the NeXus International Advisory Committee (NIAC), which primarily develops the NeXus raw data standards for large facilities. J. Hester continues to participate in the crystallography domain of the European Materials and Modelling Ontology (EMMO) consortium, who are developing a semantic description of crystallographic knowledge and practice.

COMCIFS is also closely involved with the IUCr Committee on Data (CommDat).

S. Grazulis represented COMCIFS on the IUCr 2023 Programme Committee.

Looking forward

As flagged in previous years, a small group of people is drawn upon to support CIF maintenance and development. This situation is not sustainable, particularly as the first generation of CIF experts move into retirement.

The original set of six voting members of COMCIFS has now shrunk to three. A slate of replacement candidates from stakeholder communities will be prepared for the 2023 IUCr General Assembly.

J. Hester, Chair

B6. Committee on Data (CommDat)

For 2022 there are the following matters to report:

(i) The IUCr Forum for Public Input to CommDat at <https://forums.iucr.org/viewforum.php?f=39> has had various new published reports and announcements posted there. These have been extensively accessed.

(ii) CommDat has participated fully in the work of the Melbourne IUCr 2023 Congress Programme Committee including a one-day workshop on raw diffraction data reuse, with a wide range of invited speakers; details are at <https://www.iucr.org/resources/data/commdat/melbourne-workshop>. Two microsymposia from CommDat were accepted, one on interoperability of data and one on raw diffraction data reuse.

(iii) *IUCrData* launched a new article category in September 2022 entitled Raw Data Letters, led by CommDat Member, as Main Editor, Dr Loes Kroon-Batenburg, see <https://iucrdata.iucr.org/x/issues/2022/09/00/me6192/index.html>. A checkcif for raw data to automate the reusability was developed in collaboration with COMCIFS, IUCr Journals staff and the Photon and Neutron Open Science Cloud EU project staff from ESRF and EuroXFEL.

(iv) CommDat members spoke at sessions dedicated to crystallographic data at the US National Academies Course on Crystallographic and Structural Databases, at the Stanford Linear Accelerator Center 2022 Users Meeting and at the German national project DAPHNE4NFDI (<https://www.daphne4ndi.de/english/>), which focuses on data archiving and reuse for research with photons and neutrons at large-scale research facilities.

(v) Close ties remain strong with COMCIFS, the IUCr technical committee maintaining the CIF standard, which is chaired by James Hester. James has been a very active member of CommDat and is involved in the Raw Data Letters initiative [see point (iii) above].

J. R. Helliwell, Chair, and B. McMahon, Secretary

B7. Committee for Gender Equity and Diversity (GEDC)

The GEDC was very active in 2022, providing advice and recommendations to the IUCr Executive Committee (EC) on a number of issues.

During 2022, the GEDC members developed a toolkit for inclusive conference organisation and this is now on the IUCr GEDC web page.

The GEDC recommended to the EC that the IUCr vision be refreshed in line with the 75th anniversary of the Union in 2023. The recommendation was approved by the EC and subsequently an article was printed in the December 2022 issue of the *IUCr Newsletter* to advise crystallographers of a 2023 survey on this topic, and a workshop to be held at IUCr2023 in Melbourne.

The GEDC advised the IUCr that the following four (of ten) recommendations from the International Standing Committee for Gender Equality in Science be implemented as priorities for the IUCr in 2023:

- Actively promote the visibility of female scientists, in particular at conferences.
- Actively promote gender balance at every level of the organization, including its leadership, committees and institutional events.
- Welcome families in scientific activities.
- Encourage the diversification of scientific awards, actively encouraging the nomination of women.

Related to the last of the four priorities, the Executive Committee tasked the GEDC with developing guidelines for IUCr prizes.

J. L. Martin, 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.

The membership of the Committee has remained stable and very active. See <https://www.iucr.org/iucr/governance/advisory-committees/book-series>.

The Book Series Committee members individually provide assessments of book proposals, which I brought together as a Chair's report in each case. These reports were first provided to the IUCr Executive Committee, which endorsed them, and then they were submitted to OUP.

In 2022 Richard Welberry's book *Diffuse X-ray Scattering and Models of Disorder* (2nd edition) was published.

In order to ensure consistency to IUCr nomenclature policies, and to reduce the chance 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, the IUCr's, name.

J. R. Helliwell, Chair