

Appendix A. Reports of the Commissions for 2024

A1. Commission on Journals

Annual journal reports

Overview

| | 2019 | 2020 | 2021 | 2022 | 2023 | 2024 |
|-----------------------------------|-------|-------|-------|------|------|------|
| No. of submissions (all) | 2424 | 2121 | 1802 | 1523 | 1549 | 1703 |
| <i>without Acta E or IUCrData</i> | 1732 | 1528 | 1495 | 1148 | 1105 | 1260 |
| Rejection rate (%) | 32 | 28 | 24 | 24 | 31 | 24 |
| <i>without Acta E or IUCrData</i> | 35 | 31 | 30 | 28 | 38 | 40 |
| No. of published papers (all) | 1710 | 1583 | 1373 | 1220 | 1103 | 1220 |
| <i>without Acta E or IUCrData</i> | 1153 | 1079 | 1015 | 865 | 738 | 830 |
| No. of open-access papers (all) | 923 | 936 | 834 | 888 | 846 | 964 |
| <i>without Acta E or IUCrData</i> | 365 | 430 | 475 | 533 | 481 | 574 |
| No. of pages (all) | 12854 | 11819 | 11145 | 9644 | 8542 | 9753 |
| <i>without Acta E or IUCrData</i> | 10443 | 9539 | 9551 | 8065 | 6940 | 8013 |

IUCr Journals Editor-in-Chief's Annual report for 2024

The reports below summarize major developments for each journal during 2024. These reports reflect the hard work and dedication of all IUCr journal Editors, including the Managing Editors in Chester. Some of the general comments and highlights here preview items discussed in the individual reports that follow.

In March 2024, the Journals Management Board (JMB), comprising the Editor-in-Chief, Main (Section) Editors of each journal, the IUCr Journals Commissioning Editors, the Journal Managing Editors, other relevant Chester staff, and the IUCr President, held an in-person meeting in Chester, providing an impetus for several initiatives that have since been followed up. Significant issues affecting each journal were discussed among the editorial leadership teams.

Regular virtual meetings for the Main Editors of individual journals have increased and continue to be important for communication and journal development. Full Editorial Board virtual meetings have also become a more regular occurrence for many of the journals, allowing problems to be addressed, initiatives such as new special issue ideas for increasing journal submissions to be discussed, and improvements proposed to enable smoother review processes, hence faster reviews. Multiple opportunities for in-person meetings of editors and authors continue to be afforded at IUCr affiliate meetings in various parts of the world.

While the combined effects of the pandemic, major X-ray and neutron facility upgrade shutdowns, and continuing war situations involving major contributing countries to IUCr journals, have significantly reduced submissions and published articles for IUCr journals in recent years, 2024 saw some recovery with an increase of 10% in submissions, 11% in published articles and 14% in pages published, compared with 2023. There was also an increase of 14% in open-access articles published.

Throughout 2024 and into 2025, all members of the journal Editorial Boards have been encouraged to work collegiately bringing in new high-quality submissions, consistent with the respective journal scopes, with these undergoing significant updating where needed to address the changing needs of the structural science research community. New sections continue to be initiated to capture emerging areas of relevant structural science, supported by the appointment of new Main Editors and Co-editors with appropriate expertise while also increasing gender diversity and increased representation from developing parts of the world in structural science.

Finally, late 2024 saw the retirement of Peter Strickland as Executive Managing Editor of the IUCr journals in the Chester Office after many years of dedicated service, the subsequent appointment of Louise Jones as Head of Publishing Operations and, from the beginning of 2025, Krana Vukmirovic as Head of Publishing Strategy.

A. Allen, Editor-in-Chief, IUCr Journals

| | 2019 | 2020 | 2021 | 2022 | 2023 | 2024 |
|-----------------------------------|-------|----------------|----------------|----------------|-------|------|
| No. of submissions | 115 | 94 | 90 | 81 | 98 | 72 |
| Rejection rate (%) | 38 | 35 | 34 | 38 | 42 | 42 |
| No. of published papers | 88 | 79 | 65 | 57 | 55 | 51 |
| research papers – foundations | 59 | 50 | 42 | 36 | 40 | 36 |
| advances | 15 | 5 | 8 | 6 | 6 | 3 |
| short communications | 0 | 4 | 2 (1 advances) | 5 (1 advances) | 3 | 3 |
| lead articles | 0 | 2 (1 advances) | 1 | 0 | 0 | 1 |
| feature articles | 0 | 0 | 1 | 0 | 0 | 0 |
| topical reviews | 0 | 1 (advances) | 0 | 0 | 0 | 0 |
| editorial | 1 | 0 | 1 | 0 | 0 | 1 |
| commentaries | 1 | 2 (1 advances) | 2 | 0 | 1 | 0 |
| abstracts | 1217 | 227 | 1566 | 1020 | 390 | 693 |
| other | 12 | 15 | 9 | 10 | 5 | 7 |
| No. of open-access papers | 28 | 20 | 20 | 16 | 24 | 21 |
| No. of pages | 918 | 783 | 638 | 519 | 601 | 465 |
| Average length (pages) | 11.3 | 11.4 | 11.8 | 10.4 | 11.3 | 10.7 |
| Average publication time (months) | 6.1 | 6.2 | 5.8 | 6.0 | 6.1 | 5.4 |
| Impact factor | 2.0 | 2.3 | 2.3 | 1.8 | 1.0 | |
| 5 year impact factor | 3.1 | 3.3 | 2.7 | 2.2 | 2.1 | |
| Cited half life (years) | >10.0 | >10.0 | 8.2 | >10.0 | >10.0 | |

The journal scope has been updated to highlight more of the science covered by the journal and to encourage more submissions from the different areas. *Acta A* covers a very wide range of science and has two sections: Advances and Foundations. Articles for the Advances section are selected based on their likely impact and broad interest.

Four Advances papers were published in 2024

Deep learning applications in protein crystallography

S. Matinyan, P. Filipcik, J. P. Abrahams

<https://doi.org/10.1107/S2053273323009300>

(which is also a Lead Article)

Parameterized absorptive electron scattering factors

M. Thomas, A. Cleverley, R. Beanland

<https://doi.org/10.1107/S2053273323010963>

Understanding extended homometry based on complementary crystallographic orbit sets

Z. Zhang, Y. Shen, J. Sun

<https://doi.org/10.1107/S205327332400007X>

Symmetries and symmetry-generated averages of elastic constants up to the sixth order of nonlinearity for all crystal classes, isotropy and transverse isotropy

R. S. Telyatnik

<https://doi.org/10.1107/S2053273324007666> (this article was highlighted in a commentary)

The top three most highly cited papers in *Acta A* in 2024 were

Hierarchical topological analysis of crystal structures: the skeletal net concept, Blatova & Blatov

<https://doi.org/10.1107/S2053273323008975>

Algorithm for spin symmetry operation search, Shinohara *et al.*

<https://doi.org/10.1107/S2053273323009257>

Deep learning applications in protein crystallography, Matinyan *et al.* (the Lead Article mentioned above)

<https://doi.org/10.1107/S2053273323009300>

Commissioning Editor Thomas Proffen worked with Simon Billinge on a cross-journal virtual collection of papers on machine learning which was published in February 2024 (see https://journals.iucr.org/special_issues/2024/ML/). An accompanying Editorial reviewed developments in the field, from the earliest papers on machine learning to be published in IUCr journals to the wealth of papers in more recent years. The issue was widely publicised on social media.

The number of submissions to the journal fell in 2024 – 72 submissions were received compared with 98 in 2023. However, the rejection rate has remained steady at 42%. A total of 51 papers were published, comprising advances and foundations research papers, short communications, one lead article and one editorial.

In 2024 we welcomed Branton Campbell to the Editorial Board and we would like thank him and all the Co-editors who have worked on the journal throughout the year.

In Autumn 2024 we also welcomed Andrea Hill as the new Managing Editor of *Acta A*. We thank Nicola Ashcroft for her hard work on the journal over the years and wish her well in her new role as Managing Editor of *IUCrJ*.

A. Altomare and S. J. L. Billinge, Editors

| | 2019 | 2020 | 2021 | 2022 | 2023 | 2024 |
|-----------------------------------|-------|-------|-------|-------|-------|------|
| No. of submissions | 201 | 168 | 162 | 115 | 100 | 139 |
| Rejection rate (%) | 32 | 31 | 28 | 30 | 42 | 30 |
| No. of published papers | 136 | 117 | 112 | 95 | 63 | 82 |
| research papers | 120 | 107 | 102 | 81 | 52 | 72 |
| short communications | 0 | 0 | 0 | 0 | 0 | 1 |
| lead articles | 2 | 0 | 0 | 0 | 0 | 0 |
| feature articles | 1 | 0 | 0 | 0 | 0 | 1 |
| topical reviews | 1 | 0 | 0 | 2 | 0 | 1 |
| editorial | 1 | 0 | 1 | 1 | 1 | 1 |
| commentaries | 2 | 5 | 2 | 2 | 7 | 3 |
| other | 9 | 5 | 5 | 9 | 3 | 3 |
| No. of open-access papers | 12 | 17 | 30 | 22 | 19 | 36 |
| No. of pages | 1227 | 1147 | 1054 | 892 | 546 | 820 |
| Average length (pages) | 9.7 | 10.5 | 10.0 | 10.3 | 10.0 | 10.7 |
| Average publication time (months) | 5.2 | 4.6 | 4.5 | 4.7 | 4.6 | 4.5 |
| Impact factor | 2.0 | 2.3 | 2.7 | 1.9 | 1.3 | |
| 5 year impact factor | 4.7 | 4.7 | 4.9 | 2.1 | 2.0 | |
| Cited half life (years) | >10.0 | >10.0 | >10.0 | >10.0 | >10.0 | |

Marc de Boissieu retired as a Section Editor and was replaced by Andrzej Katrusiak in August 2024. C. Malla Reddy resigned as a Co-editor in 2024. Replacements for A. Katrusiak (formerly a Co-editor) and C. M. Reddy have not yet been made; these appointments are anticipated once the journal scope is updated and aligned with identified priorities.

In 2024, *Acta Crystallographica Section B* continued to publish six issues per year. The number of articles (and pages) published in 2020, 2021, 2022, 2023, and 2024 was 117 (1147), 112 (1054), 95 (892), 63 (546), and 82 (820), respectively. These numbers vary depending on the number and size of special issues published in a given year.

Over the past year, authors from 36 different countries contributed to the journal, with the top five being Russia (18%), the USA (13%), and Poland (8%), followed by Japan and France. For comparison, articles in *Acta B* in 2023 involved authors from 28 countries, with the top contributors being Russia (19.5%), Poland (15.5%), Germany (11%), France (7.6%), India (7.1%), and China (5.7%).

Between 2018 and 2023, the rejection rate was typically around 28%, with slightly higher values of 33% in 2023 and 30% in 2024. Recently, the average length of full articles has been 10.0 pages (10.7 pages in 2024), with some significantly longer articles. In 2024, the average time from submission to publication was 4.5 months, consistent with previous years (e.g. 4.6 months in 2023). A total of 139 articles were submitted in 2024 (up from 100 in 2023) and 82 were published.

The journal's impact factors for 2022 and 2023 were 1.83 and 1.3, respectively, which is in line with historical values, aside from occasional higher outliers due to the publication of exceptionally high-impact articles. The five-year impact factor stands at 2.0.

A special collection of papers on *The Seventh Blind Test of Crystal Structure Prediction* was published in *Acta B* in December 2024 and is expected to be particularly well cited.

In 2024, a special issue on *Magnetic Structures* was undertaken, with guest editors J. Manuel Perez-Mato (Spain), Branton J. Campbell (USA) and V. Ovidiu Garlea (USA). A total of 13 articles were published in 2024 for this special issue, with another five in progress for publication in 2025.

We greatly appreciate the efforts of all our Guest Editors in bringing these special issues to fruition. We also acknowledge the invaluable contributions of our Co-editors. In 2024, 138 peer reviews were received, while 364 requests for peer review were made. We recognize the significant effort required of our Co-editors, given that approximately two-thirds of review requests are declined or ignored.

The journal has received extensive support from the Chester staff, especially our Managing Editor, Amanda Berry, whose dedication and responsiveness to both editors and authors are greatly appreciated. We also extend our gratitude to Peter Strickland for his long-standing guidance and support. We look forward to working with Louise Jones and other Chester publishing professionals in 2025 and beyond.

L. Dawe, A. Katrusiak and A. Nangia, Editors

| | 2019 | 2020 | 2021 | 2022 | 2023 | 2024 |
|-----------------------------------|------|------|------|------|------|------|
| No. of submissions | 406 | 227 | 180 | 171 | 132 | 169 |
| Rejection rate (%) | 49 | 41 | 40 | 43 | 51 | 26 |
| No. of published papers | 197 | 143 | 105 | 96 | 62 | 104 |
| research papers | 186 | 137 | 98 | 93 | 60 | 92 |
| feature articles | 3 | 0 | 0 | 0 | 0 | 1 |
| topical reviews | 0 | 0 | 0 | 0 | 2 | 4 |
| editorial | 0 | 0 | 0 | 0 | 1 | 1 |
| commentaries | 6 | 2 | 4 | 3 | 3 | 4 |
| other | 2 | 4 | 3 | 0 | 2 | 2 |
| No. of open-access papers | 9 | 22 | 18 | 24 | 25 | 36 |
| No. of pages | 1697 | 1107 | 815 | 759 | 529 | 820 |
| Average length (pages) | 8.2 | 8.0 | 8.1 | 8.1 | 8.4 | 8.3 |
| Average publication time (months) | 2.8 | 2.9 | 2.8 | 2.7 | 2.9 | 2.7 |
| Impact factor | 0.9 | 1.2 | 1.2 | 0.8 | 0.7 | |
| 5 year impact factor | 6.3 | 7.3 | 1.0 | 0.7 | 0.7 | |
| Cited half life (years) | 4.8 | 5.8 | 6.8 | 7.7 | 8.7 | |

In 2024 *Acta Cryst. C* continued to encourage papers which combine structural chemistry with synthetic, biological and computational content. A further expansion to include electron diffraction papers has been facilitated by a special issue on *Electron diffraction for structural characterisation* (see below for further details).

There has been a significant recovery from the general decline in the number of papers which saw a low of 132 papers in 2023, with 169 papers being published in 2024. This recovery has been due in part to special issues (see below) and some relaxing on the content to accept papers which reported high-quality crystallography without the extra analysis which had been required previously. This has seen a reduction in the rejection rate from 51% in 2023 to 26% in 2024, which will also be a result of the generally zero rejection rate for special issue papers. The average page length remains just above 8 pages per paper. The predicted impact factor for 2024 is *ca* 1.1, which represents a significant improvement from 2023 (0.7) and sees a return close to the 2021 level.

The Review Board of referees (set up in 2016) continues to work very well and provides rapid and high-quality reports that help to maintain an average publication time of under three months, a publication time that has remained steady for a number of years. The review panel has recently been revisited and updated. Members were asked if they would like to stay on and were also asked for their ideas for the journal (*e.g.* topics for special issues and best practice articles). With the current level of submissions, the number of requests per member is 2-6 per annum, and most members were happy to continue on the Board. The large number of members (50+) means that there is no real urgency to add to the board at present.

The three following special issues/series featured in 2024

(i) *Crystallography in Latin America: a vibrant community* (edited by Maria Rosales-Hoz and Renata Diniz, both *Section C* Co-editors). This issue was completed in early 2025 with the publication of an associated editorial. The final issue was composed of 18 articles, ranging from structural reports to a memoir-type article, all highlighting the diversity and quality of research conducted by Latin American scientists.

(ii) *Advances in electron diffraction for structural characterization* [edited by Glenn Yap (*Section C* Co-editor), Eric Reinheimer (*Section C* Co-editor), Joe Ferrara, Laura Samperisi and Gunther Steinfeld]. This issue continues and will consist of 11 articles, including structural reports and topical reviews. All articles were of high-quality and were very well read.

(iii) *Best practice in crystallography series* (ongoing). This series was introduced by an editorial from *Section C* Main Editor Alan Kennedy and initially published three articles on crystal growth, photocrystallography and organic thin film resistors, each accompanied by a commentary. All have been well read and are expected to be highly cited. It is envisioned that the series will continue into the future, ideally adding three articles per annum.

Section C continued to publish commentaries on articles that were of note and four appeared in 2024, which is the usual number per annum for the journal.

The team of Co-editors have continued to do an excellent job reviewing submitted manuscripts, selecting referees and carrying out careful editing of the chemistry and crystallography. The Editorial board welcomed a new Chinese Co-editor, Zeng Song (University of Science and Technology Beijing), with a background in ceramics. Michael Gardiner (Australian National University) retired from the board after 5 years. Ton Spek also stepped down after serving on the Editorial Board since 1996. He was there for the adoption of CIF by the journal and developed *checkCIF*, which continues to be at the core of small-molecule structure checking for IUCr Journals (and worldwide). We thank Michael and Ton for their invaluable contribution to the journal.

The Editorial Board held its annual informal virtual meeting in February. Items discussed included the identity of the journal, transfers between journals, early career crystallographers and Co-editor experiences. These annual meetings are very useful and will continue in the future.

The *Notes for authors* were updated so that their structure was in line with the other IUCr journals. The scope was also updated to better describe the type of article and content wanted by the journal.

The main editors would like to thank all the Co-editors and Review Board members, past and present, for their support of the journal. This year saw the implementation of automatic notification for reviewers *via* a thank-you message when a paper for which they had provided a review was published. This has been welcomed warmly by reviewers. Finally, we wish to express our thanks to the Chester Editorial Office staff for maintaining the high professional standard for which the journal is recognised.

J. White, A. Sarjeant and A. Kennedy, Editors

| | 2019 | 2020 | 2021 | 2022 | 2023 | 2024 |
|-----------------------------------|------|-------|-------|-------|-------|------|
| No. of submissions | 160 | 194 | 186 | 153 | 113 | 97 |
| Rejection rate (%) | 29 | 15 | 20 | 24 | 22 | 27 |
| No. of published papers | 112 | 129 | 146 | 129 | 105 | 74 |
| research papers | 98 | 115 | 133 | 122 | 89 | 65 |
| feature articles | 2 | 2 | 1 | 1 | 1 | 2 |
| topical reviews | 1 | 1 | 3 | 2 | 1 | 1 |
| editorial | 2 | 3 | 2 | 1 | 3 | 3 |
| commentaries | 1 | 1 | 2 | 0 | 3 | 0 |
| other | 8 | 7 | 5 | 3 | 8 | 3 |
| No. of open-access papers | 60 | 69 | 93 | 83 | 77 | 59 |
| No. of pages | 1147 | 1279 | 1623 | 1473 | 1119 | 864 |
| Average length (pages) | 10.9 | 10.5 | 11.7 | 11.6 | 11.7 | 12.5 |
| Average publication time (months) | 4.9 | 4.7 | 5.4 | 4.9 | | 3.6 |
| Impact factor | 5.3 | 7.7 | 5.7 | 2.2 | 2.6 | |
| 5 year impact factor | 3.2 | 5.0 | 6.0 | 5.7 | 5.2 | |
| Cited half life (years) | 9.6 | >10.0 | >10.0 | >10.0 | >10.0 | |

As for the other IUCr Journals we have seen a steady fall in the number of submitted papers since 2020 (194 in 2020 to 97 in 2024), while the rejection rate has risen from 15% to 27% over the same time period, resulting in the publication of 74 papers in 2024, 65 of which were research papers (including 14 associated with the CCP4 Study Weekends and 5 from the CCP-EM meetings). This compares with 133 research papers published in 2021, which is a halving of the publication output over the last 4 years. We find these statistics deeply concerning (see possible actions at the end of this report).

Of the 9 non-research papers published in 2024, there were two feature articles (*A snapshot love story: what serial crystallography has done and will do for us* and *From femtoseconds to minutes: time-resolved macromolecular crystallography at XFELs and synchrotrons*), one scientific commentary (*Everyone is using biological structures, but how does one find the structure(s) one wants?*), one topical review (*Post-translational modifications in the Protein Data Bank*), one obituary (Peter Main) and one book review. In addition, there were also two editorials reporting the appointment of 5 and then 2 new *Acta D* Co-Editors, respectively, and a third editorial to introduce the 2022 CCP4 Study Weekend Special Issue.

Special issues continue to play a positive role for the journal, particularly those from the recurring series of annual CCP4 Study Weekends (2023, 13 papers collected together with introduction published in January 2025 entitled *Making the most of an abundance of data*), and the CCP-EM symposia. As instituted in recent years, the timeliness of the papers is ensured by publication in regular issues as soon as they are accepted and typeset, rather than waiting until all the papers in preparation are ready. Once all the papers for a special issue are available, they are also collected into a ‘virtual special issue’.

The *Acta D* 2023 impact factor (released in 2024) increased to 2.6 (the 2022 impact factor was 2.2), while the five-year impact factor remains above 5 at 5.2. Note that the new reference for the CCP4 software suite [Agirre *et al.* (2023), *Acta Cryst. D* **79**, 449-461] has already been cited 419 times and is likely to boost the impact factor for 2024. The proportion of open access papers has decreased to 59% from 73% in 2023. The average length of papers has increased steadily over the last 5 years from 10.5 (2020) to 12.5 pages over the last three years.

There was a reduction in the length of time for publication from 5.4 months in 2021 to 4.9 months in 2022 and 3.6 months in 2024. We have achieved this significant reduction by shortening the standard time given to authors for submission of revised manuscripts from two months to one month.

Acta D continues to publish material that keeps it relevant in the rapidly changing structural biology landscape. Research papers in 2024 included single crystal structure determination, X-ray free electron laser serial crystallography, fragment screening, cryoEM, computational structure prediction, quantum mechanical studies, UV-vis spectroscopy, in many cases using an integrative approach. *Acta D* continues to be acknowledged as a trusted, respected, reliable source of all structural biology studies. The name *Acta Crystallographica* may be acting as an impediment to some potential authors, though it should help to continue to emphasise the *Structural Biology* subheading in presentations mentioning the journal. A scientific comment on the future of provision of structural biology data to biologists was published as a call to arms to the community.

The ongoing attention to changes in the field of structural biology is reflected in the continued dialogue amongst the editors of *Acta D* and *F*, to ensure that journal guidelines are encouraging and useful to the community of potential authors.

As ever, we sincerely thank the highly efficient and excellent work of Louise Jones and Simon Glynn in the Chester office, under the supervision of Executive Managing Editor Peter Strickland (now retired and replaced by Louise Jones as Head of Publishing Operations) and Editor-in-Chief Andrew Allen. We are very grateful for their hard work, attention to detail and dedication, especially for Simon's sustained efforts to finalise the Special Issues.

C. S. Bond, E. F. Garman and R. J. Read, Editors

| | 2019 | 2020 | 2021 | 2022 | 2023 | 2024 |
|-----------------------------------|------|------|------|-------|-------|------|
| No. of submissions | 497 | 438 | 307 | 269 | 302 | 290 |
| Rejection rate (%) | 20 | 16 | 7 | 11 | 13 | 12 |
| No. of published papers | 392 | 365 | 263 | 261 | 242 | 263 |
| research communications | 392 | 362 | 262 | 252 | 236 | 262 |
| teaching and education | 0 | 0 | 0 | 2 | 4 | 0 |
| editorial | 0 | 0 | 0 | 1 | 1 | 1 |
| other | 0 | 3 | 1 | 6 | 1 | 0 |
| No. of open-access papers | 392 | 365 | 263 | 261 | 242 | 263 |
| No. of pages | 1952 | 1875 | 1329 | 1288 | 1227 | 1358 |
| Average length (pages) | 5.0 | 5.1 | 5.1 | 5.0 | 5.1 | 5.2 |
| Average publication time (months) | 1.3 | 1.1 | 1.3 | 1.6 | 1.6 | 1.7 |
| Impact factor | | | | 0.9 | 0.5 | |
| 5 year impact factor | | | | 0.6 | 0.6 | |
| Cited half life (years) | | | | >10.0 | >10.0 | |

In 2024, the number of submissions decreased by approximately 4%, but the number of published papers nonetheless increased compared to 2023 due to a lower rejection rate.

The journal continues to attract submissions from around the world, with an increase in the proportion of papers submitted from the USA, Ukraine and Vietnam, while the proportion of submissions from India and Türkiye decreased. The top three contributing countries were the USA (20%), Germany (15%), and India (8%). *Acta E* had the highest number of downloads (11.2 million) among IUCr Journals. The average publication time and the average length of papers have only slightly increased compared to 2023.

Submitted papers typically describe two or more structures, often analysed using complementary techniques such as UV-Vis, NMR, DFT and Hirshfeld surface analysis. However, the Editors would like to underline that, unless relevant to the discussion, the sections describing these complementary analyses should be transferred to the supporting information. The Section Editors also identify articles that lack sufficient scientific discussion at the pre-screening stage; these are either transferred to *IUCrData* or returned to the authors for resubmission after content improvements.

Since summer 2023, *Acta E* has had a new impact factor of 0.9, which has now settled at 0.5. A new scope for the journal is being prepared to include its new Education and Outreach Section, which will have a dedicated Editor. As part of the Early Career Boards project, *Acta E* will be grouped with *Acta C* and *Acta B*.

In 2024, 23 new papers were published in the AfCA-IUCr Virtual Collection, including a foreword by the Editors of the collection - Susan Bourne, Delia Haynes and Michele Zema - an article by Andreas Roodt on the creation of the African

Crystallographic Association and an article by Simon Billinge on the collaborative initiatives of JUAMI, the Joint US–Africa Materials Institute. Moreover, the March issue of the journal featured a highlight on the history and activities of the German Young Crystallographers.

Finally, we would like to express our thanks to our Co-editors for their dedication and excellent work as well as our gratitude for the constant and excellent support we receive from the staff in Chester, particularly Gillian Holmes, Sean Conway and Mike Hoyland. A special thank you to Peter Strickland for his sound advice and expert guidance. We wish him a very happy and well-earned retirement.

G. Diaz de Delgado, C. Massera, S. Parkin and L. Van Meervelt, Editors

| | 2019 | 2020 | 2021 | 2022 | 2023 | 2024 |
|-----------------------------------|------|------|------|------|------|------|
| No. of submissions | 122 | 98 | 97 | 70 | 54 | 85 |
| Rejection rate (%) | 32 | 26 | 26 | 29 | 32 | 30 |
| No. of published papers | 105 | 85 | 64 | 55 | 42 | 49 |
| research communications | 95 | 76 | 48 | 48 | 36 | 37 |
| topical reviews | 1 | 0 | 1 | 1 | 0 | 3 |
| editorial | 5 | 3 | 1 | 0 | 4 | 6 |
| commentaries | 1 | 0 | 1 | 0 | 1 | 0 |
| other | 3 | 6 | 13 | 6 | 1 | 3 |
| No. of open-access papers | 16 | 27 | 23 | 31 | 18 | 27 |
| No. of pages | 757 | 623 | 483 | 422 | 307 | 362 |
| Average length (pages) | 7.4 | 7.5 | 7.8 | 7.9 | 7.7 | 8.2 |
| Average publication time (months) | 3.9 | 2.8 | 2.8 | 2.7 | 3.3 | 2.9 |
| Impact factor | 1.0 | 1.1 | 1.1 | 0.9 | 1.1 | |
| 5 year impact factor | 0.9 | 1.1 | 1.1 | 0.9 | 0.9 | |
| Cited half life (years) | 6.5 | 7.5 | 8.1 | 8.8 | 9.7 | |

A number of changes have been implemented in the last year in line with the roadmap presented in one of our six 2024 editorials.

Interviews with Authors (<https://www.youtube.com/playlist?list=PL6UK2yPUlpxokIIPY0tohiqV2Yv8RFSz4>) was launched in April 2024. Five interviews have been conducted at the time of writing; the videos have been watched hundreds of times, and in general authors have felt positive about the possibility of doing an interview. An extended interview format (1 hour) with a senior crystallographer – John Helliwell was our first pick – was also trialled, although it seemed to be slightly less popular judging exclusively by the number of views. Longer videos seem to accumulate fewer views.

A focused issue on the use of structural genomics depositions in the education of protein crystallography was launched after a successful first paper by Prof. Krystle McLaughlin and her undergraduate students was published and highlighted in a commentary paper by Section Editor Jon Agirre. The focused issue is still ongoing, with about fifteen papers either published or still under review. The papers include pictures of the undergraduate students on the front page, highlighting the incredible diversity the crystallographic community has at early career stages; we aim to interview the students in a special series of interviews as part of our aim to amplify under-represented voices in structural biology.

Following discussions with CCP4, it was decided that *Acta Cryst. F* could be offered as an alternative destination to *Acta D* for shorter methods papers coming out of the annual CCP4 Study Weekend.

We were fortunate to appoint three new co-editors: Alejandro Buschiazzi (Institut Pasteur Montevideo, Uruguay), Stephen Muench (University of Leeds, UK), and Dorothee Liebschner (Lawrence Berkeley National Laboratory, USA).

In the last year, the number of submissions has picked up; with the rejection rate remaining stable at around 30%. This should correspond to more published papers in coming years. Papers are also slightly longer on average, but time to publication has stayed constant at three months. The impact factor remains stable, currently at 1.1, with the cited half-life increasing year by year between 2019 and 2024.

J. Agirre, M. C. Nonato and M. J. van Raaij, Editors

| | 2019 | 2020 | 2021 | 2022 | 2023 | 2024 |
|-----------------------------------|------|------|------|------|------|------|
| No. of submissions | 195 | 155 | 108 | 106 | 141 | 153 |
| Rejection rate (%) | 18 | 13 | 6 | 9 | 9 | 16 |
| No. of published papers | 165 | 139 | 94 | 95 | 123 | 127 |
| data reports | 162 | 138 | 92 | 94 | 122 | 126 |
| raw data letters | 0 | 0 | 0 | 2 | 1 | 0 |
| editorial | 0 | 0 | 0 | 1 | 0 | 0 |
| other | 3 | 1 | 2 | 0 | 0 | 1 |
| No. of open-access papers | 165 | 139 | 94 | 94 | 123 | 126 |
| No. of pages | 459 | 405 | 265 | 291 | 375 | 382 |
| Average length (pages) | 2.8 | 2.9 | 2.8 | 3.1 | 3.0 | 3.0 |
| Average publication time (months) | 0.9 | 0.9 | 0.9 | 1.2 | 1.0 | 1.0 |

The number of published data report papers in *IUCrData* has nudged up slightly compared to last year and there may be a rising trend compared with the low point in 2022. The quality of data report submissions is distinctly variable with some excellent papers (which might equally find a home in *Acta E*) but also many poorly prepared papers, which need a great deal of work from the Section Editors. Some of these are from inexperienced new submitters but there are also some ‘repeat offenders’, where the supervisor is apparently not properly checking and proof-reading student submissions. We thank the editorial team in Chester, above all Gillian Holmes, for their indefatigable efforts to maintain the highest scientific and presentation standards for the journal.

Authors are still not finding their way to Raw Data Letters, although the importance of raw data availability is well appreciated and there is interest in raw data re-use. Large scale facilities are developing raw data archiving and re-use policies. A poster for Raw Data Letters was created and presented at the ACA in Denver 2024, and flyers are being distributed. A paper in *Acta F* [Kroon-Batenburg, L.M.J. (2023). *Acta Cryst. F* **79**, 267] *Making your raw data available to the macromolecular community* continues to attract a large numbers of views. It seems that a hurdle has to be overcome to get a flow of submissions to RDL. However, we foresee a few papers coming and papers from the electron diffraction and the XFEL community are scheduled.

From the Raw Data Letter working group, a consortium has been established that received a grant (MC-ReDD) from OSCARS, a Horizons Europe project. The objective of MC-ReDD is the creation of a publicly available, easy-to-use tool for semi or fully automatic construction of imgCIF files from raw data sets and can be serviced from IUCr journals. While these imgCIF files are part of the Raw Data Letter accompanying the link to the raw diffraction data archive, they also represent a FAIR Digital Object allowing them to become part of open data collections hosted at Metadata Catalogues, enabling cross searching with other European Open Science Services (EOSC).

W. T. A. Harrison, L. M. J. Kroon-Batenburg, E. R. T. Tiekink, L. Van Meervelt and M. Weil, Editors

| | 2019 | 2020 | 2021 | 2022 | 2023 | 2024 |
|-----------------------------------|------|------|------|------|------|------|
| No. of submissions | 147 | 151 | 117 | 105 | 110 | 102 |
| Rejection rate (%) | 38 | 41 | 41 | 32 | 31 | 25 |
| No. of published papers | 120 | 129 | 108 | 89 | 80 | 98 |
| research papers | 94 | 100 | 79 | 62 | 56 | 63 |
| feature articles | 1 | 1 | 3 | 0 | 1 | 5 |
| topical reviews | 3 | 1 | 1 | 3 | 4 | 7 |
| research letters | 6 | 8 | 6 | 5 | 2 | 9 |
| editorial | 6 | 5 | 3 | 4 | 5 | 3 |
| commentaries | 8 | 11 | 11 | 12 | 9 | 11 |
| other | 2 | 3 | 5 | 3 | 3 | 0 |
| No. of open-access papers | 120 | 129 | 108 | 89 | 80 | 98 |
| No. of pages | 1133 | 1215 | 1034 | 791 | 771 | 1006 |
| Average length (pages) | 10.7 | 10.8 | 11.2 | 11.0 | 11.2 | 12.0 |
| Average publication time (months) | 4.3 | 4.3 | 4.5 | 4.9 | 4.9 | 4.7 |
| Impact factor | 5.4 | 4.8 | 5.6 | 3.9 | 2.9 | |
| 5 year impact factor | 5.7 | 5.8 | 5.4 | 4.4 | 3.3 | |
| Cited half life (years) | 3.0 | 3.5 | 3.8 | 4.2 | 4.9 | |

The number of submissions to *IUCrJ* decreased slightly in 2024, but the journal continued to establish itself within the wider scientific communities that use results obtained from diffraction methods, and impressions from authors, readers, referees and commentators remain positive.

Although the impact factor of *IUCrJ* decreased to 2.9 in 2024, the journal remains in the top quartile for Crystallography. [The projected impact factor for 2024 (to be released in 2025) is higher, around 3.7.] All submissions are first reviewed by a panel made up of the Main Editors (Dimitri Argyriou, Ted Baker, Richard Catlow, Henry Chapman, Susan Bourne, Sriram Subramaniam and Xiaodong Zou) and the Editor-in-chief (Andrew Allen). Articles that do not meet the journal's requirement for broad scientific significance are often transferred, with the agreement of the authors, to another IUCr journal. These transfers are smooth and do not require any additional work from the authors.

The six issues of *IUCrJ* published in 2024 have featured papers from a wide variety of areas including biology, chemistry, crystal engineering, cryo-EM, electron crystallography, materials, physics and FELs. The number of articles submitted to the journal was 102; a total of 98 papers were published with an average turnaround time of 4.7 months, of which around a month is from acceptance to publication. Articles have been publicised in *IUCrJ*'s social media feeds and by other methods, with 11 articles highlighted via in-depth commentaries.

The numbers of articles published in each section (excluding editorials and commentaries) were: Biology/Medicine 27, Neutron/Synchrotron 13, Chemistry/Crystal Engineering 12, Physics/FELs 10, Electron Crystallography 9, Materials/Computation 8 and CryoEM 5.

As seen from these figures, the Biology and Medicine section continues to receive a healthy number of submissions. These are quite varied in focus. Some focus primarily on biological structure, others on methods, and others can be strongly chemical (*e.g.* on optimization of small-molecule drugs). This is, appropriately, an author's choice, but also points to the fact that there is inevitably overlap between different sections of *IUCrJ*, and the names of the sections are important mainly for emphasizing the spread of areas covered by the journal. Probably the single most common theme in the Biology and Medicine section has been the growing importance of serial protein crystallography, a very important approach for understanding biological mechanisms.

In contrast, submissions to the cryo-EM section of *IUCrJ* were fewer than in 2023, with 5 articles published in 2024. The decline is in part from the almost universal adoption of cryo-EM by crystallographers and the growing adoption of cryo-EM methods by biomedical scientists working on interesting problems. As a result, the manuscripts received were more methodological in nature. It has thus been decided to explore whether it may be more effective to absorb the cryo-EM section into a section that covers structural biology more broadly.

In 2024, 15 manuscripts were published in the Chemistry and Crystal Engineering section, reflecting the continuing robust interest in chemical studies. No single theme is evident but a number of these papers report on molecular structures studied at high pressures with intriguing effects seen in bonding and phase transition behaviour. Other topics reported include isostructurality and molecular studies of proton transfer. It is encouraging to see the application of modern instrumental and computational methods being applied to molecular systems, and the increasing interest in ensuring interoperability of data collected by different methods. Crystal engineering concepts have matured and are well embedded in a range of chemical crystallography studies and this is reflected in the range of materials and subjects reported on in *IUCrJ* over the past year.

There were 10 papers published in the Physics/FELs section in 2024, two more than in 2023. Many of these papers presented or evaluated approaches to obtain structural information from diffraction measurements both from crystals and single particles. This included two papers investigating the use of higher-order correlations to improve diffraction analyses using FEL facilities, and applying iterative phasing algorithms for *de novo* phasing of SAD crystal diffraction. There were two papers on methods and software for serial crystallography, which has been a staple of the section since the beginning of *IUCrJ*, but generally the papers seem to be more diverse than previous years while still keeping to methodological or fundamental topics. The most read Physics/FELs paper was on the importance of definitions in crystallography.

We saw an increase in submissions to the Electron Crystallography section, with the number of published articles increasing from 5 in 2023 to 9 in 2024. Most articles were methods-oriented, including refinements with multipolar electron scattering factors, Hirshfeld atom refinement, and refinement of short-range order parameters. New data collection methods, STEM-SerialED and tilt-ePDF, were also reported. Applications of 3D ED on pharmaceutical crystals and covalent organic frameworks (COFs) were also published.

Three Editorials were published in 2024, and in January 2025 Andrew Allen contributed an Editorial celebrating the history and progress of *IUCrJ* in its first decade [*IUCrJ on passing its tenth anniversary and entering its second decade: progress, current status and prospects for the future*, *IUCrJ* (2025), **12**, 1-3].

The main goal of *IUCrJ* remains to attract high-quality scientific papers of broad significance from across the diverse scientific communities that utilize the results obtained from diffraction methods. We encourage you to consider publishing your work in *IUCrJ*, thereby helping to solidify the journal's position as a leading comprehensive science journal.

D. Argyriou, E. N. Baker, S. A. Bourne, C. R. A. Catlow, H. Chapman, S. Subramaniam and X. Zou, Editors

| | 2019 | 2020 | 2021 | 2022 | 2023 | 2024 |
|-----------------------------------|-------|-------|-------|-------|-------|------|
| No. of submissions | 284 | 297 | 282 | 275 | 317 | 313 |
| Rejection rate (%) | 32 | 33 | 33 | 26 | 37 | 33 |
| No. of published papers | 146 | 188 | 202 | 175 | 198 | 197 |
| research papers | 121 | 132 | 145 | 131 | 151 | 141 |
| short communications | 4 | 4 | 7 | 6 | 2 | 6 |
| feature articles | 0 | 0 | 1 | 0 | 1 | 3 |
| computer programs | 21 | 26 | 23 | 23 | 23 | 28 |
| editorial | 1 | 0 | 1 | 0 | 2 | 1 |
| commentaries | 0 | 2 | 1 | 0 | 1 | 0 |
| other | 0 | 24 | 41 | 15 | 18 | 18 |
| No. of open-access papers | 33 | 55 | 83 | 99 | 109 | 121 |
| No. of pages | 1468 | 1631 | 1902 | 1706 | 1884 | 2050 |
| Average length (pages) | 9.7 | 9.8 | 10.5 | 10.2 | 10.2 | 10.9 |
| Average publication time (months) | 5.6 | 5.7 | 5.8 | 6.1 | 6.0 | 5.5 |
| Impact factor | 3.0 | 3.3 | 4.9 | 6.1 | 5.2 | |
| 5 year impact factor | 3.4 | 4.2 | 4.5 | 4.6 | 5.0 | |
| Cited half life (years) | >10.0 | >10.0 | >10.0 | >10.0 | >10.0 | |

To help cover the number of submissions and ever-broadening scope, the journal appointed eight new Co-editors at the end of 2024: René Guinebretière (University of Limoges, France), James Harper (University of Utah, USA), Venkatesha Hathwar (Goa University, India), Karolina Jurkiewicz (University of Silesia in Katowice, Poland), Thomas Lane (DESY, Germany), Adrian Mancuso (Diamond Light Source, UK), Florian Meneau (Brazilian Synchrotron Light Laboratory, Brazil) and Katharine Page (University of Tennessee, Knoxville, and ORNL, USA). This substantial expansion of the Editorial Board sought to improve the journal's geographical coverage and ensure that we have the range of expertise needed to address the interests of cutting-edge applied crystallographic and structural science research. As well as enhancing existing expertise in areas traditionally covered by the journal, these new appointments look to rapidly evolving areas such as artificial intelligence and the new (for the journal) field of NMR crystallography.

The number of articles submitted and the number published in the journal in 2024 were almost the same as in 2023, with the impact factor staying relatively high at 5.2. The publication time (~5.5 months) has reduced slightly to its lowest over the past five year, while the average paper length (~10.9 pages) has slightly increased. The rejection rate has returned to its usual level (33%) after a rise last year. The number of open-access articles continues to increase, reflecting the impact of the various transformational deals administered by Wiley.

As usual, the high impact factor for 2023 was largely driven by two highly cited Computer Program articles. This is slightly down on the high of 6.1 in 2022 because one additional paper has fallen out of the impact factor window. We

expect the impact factor to drop significantly for 2024–2025 as the remaining two articles do the same. That a small number of articles can have such a large effect on the impact factor is sometimes advantageous, sometimes not.

A virtual collection of recently published articles on neural networks (Guest Editor Tomas Ekeberg, Uppsala University, Sweden) was published in January 2024. Guest Editors Elliot Gilbert (ANSTO, Australia), Jan Ilavsky (Advanced Photon Source, USA) and U-Ser Jen (National Synchrotron Radiation Research Center, Taiwan) are currently working on a focused issue collecting together selected full-length research, software and teaching articles related to work presented at the 19th International Conference on Small-Angle Scattering (SAS2024, Taipei, Taiwan, November 2024). The issue has attracted a large number of submissions and will be published later in 2025. The journal is also contributing a number of articles to the cross-journal focused issue on Quantum Crystallography and the collection from the IUCr2023 Congress to commemorate the 75th anniversary of the IUCr.

J. Hajdu, G. J. McIntyre and F. Meilleur, Editors

| | 2019 | 2020 | 2021 | 2022 | 2023 | 2024 |
|-----------------------------------|------|------|------|------|------|------|
| No. of submissions | 297 | 299 | 273 | 178 | 182 | 283 |
| Rejection rate (%) | 25 | 24 | 24 | 17 | 31 | 21 |
| No. of published papers | 249 | 209 | 215 | 169 | 129 | 175 |
| research papers | 203 | 158 | 151 | 130 | 95 | 125 |
| short communications | 10 | 14 | 9 | 4 | 5 | 6 |
| feature articles | 0 | 0 | 0 | 0 | 0 | 2 |
| beamlines | 27 | 23 | 39 | 19 | 22 | 23 |
| editorial | 1 | 2 | 3 | 1 | 0 | 4 |
| commentaries | 0 | 0 | 2 | 0 | 1 | 1 |
| other | 6 | 12 | 11 | 15 | 6 | 14 |
| No. of open-access papers | 87 | 91 | 100 | 169 | 129 | 175 |
| No. of pages | 2096 | 1754 | 2002 | 1503 | 1183 | 1626 |
| Average length (pages) | 8.7 | 9.0 | 9.9 | 9.4 | 9.6 | 9.8 |
| Average publication time (months) | 5.7 | 5.3 | 5.3 | 5.3 | 5.3 | 4.8 |
| Impact factor | 2.3 | 2.6 | 2.6 | 2.5 | 2.4 | |
| 5 year impact factor | 2.8 | 2.9 | 2.8 | 2.4 | 2.5 | |
| Cited half life (years) | 7.8 | 8.1 | 8.0 | 8.5 | 8.8 | |

JSR completed its third full year of being fully open access at the end of 2024. Submissions increased by 100 compared with the 2023 value, which is back up to the pre-2022 levels when JSR was a hybrid journal.

Average publication times came down to 4.8 months from 5.3, and the average article length has again increased this year and is now 9.8 pages. The top three countries for submissions were Germany, China and USA.

There were a couple of changes to the JSR Editorial Board in 2024. We welcome Helio Tolentino from the Brazilian synchrotron, so South America is once again represented on the board.

In addition, Yoshiyuki Amemiya decided to retire as one of the Main Editors, and Makina Yabashi agreed to step up from Co-editor to Main Editor as his replacement. So the board now consists of 3 Main Editors and 15 Co-editors, with a 12:6 male:female ratio.

In line with the above-mentioned increase in submissions, we will be looking to add a few more members to the board as it seems to be an increasingly common that there are few Co-editors available when authors come to choose a Co-editor during the submission process. We have noticed that submission from X-ray FEL is increasing so we will look into adding a few Co-editors expert in this area.

Two special issues were published in 2024. The first collected a selection of contributions presented at the Photon-MEADOW2023 workshop hosted by Elettra Sincrotrone Trieste in September 2023.

The title of the second was *X-ray spectroscopy to understand functional materials: instrumentation, applications, data analysis* and was organised by Main Editor Kristina Kvashnina and dedicated to Carlo Lamberti.

We ran an online Editorial Board meeting in December 2024, and in future hope to meet twice a year. We at JSR are also very much looking forward to working with the Early Career Board and mentoring young colleagues.

Finally, we are grateful to the readers of JSR for their ongoing interest and support, to the authors for choosing to publish in our journal, and to the Co-editors for their invaluable service to both the journal and the wider community. Thank you all.

D. Bhattacharyya, K. Kvashnina and M. Yabashi, Editors

A2. Commission on International Tables

International Tables for Crystallography is a major reference work published by the IUCr in conjunction with Wiley. Ten volumes designated A (and A1) through I are currently available; the tenth (on X-ray absorption spectroscopy and related techniques) was published online in 2024. The book *Teaching Edition: Crystallographic Symmetry* (the TE) is also a part of the series. The *Symmetry Database* is a related online resource.

Descriptions of activities during 2024 for the individual volumes follow:

Vol. A (*Space-group symmetry*; most recent online edition is dated 2016; editor Mois Aroyo)

TE (*Teaching Edition: Crystallographic Symmetry*; current edition is dated 2021; editor Mois Aroyo)

Symmetry Database server of the Online Edition of International Tables (updated continuously; editor Mois Aroyo)

Resources in Chester have been limited to the point that none of the items listed for Vol. A, the TE, or the *Symmetry Database* in the reports for 2022 and 2023 have been addressed yet. It is hoped that more staff time can be devoted to *International Tables* in 2025.

The version of Ruby on Rails (a server-side web application framework) used in the *Symmetry Database* has been updated.

A manuscript by M. I Aroyo & C. P. Brock for the Teaching Section of *J. Appl. Cryst.* about the many inconsistencies in the ordering of the 230 space groups and a proposed alternative order is nearing completion. It is possible that this article will be added to Vol. A and/or the TE.

Vol. A1 (*Symmetry relations between space groups*; most recent online edition is dated 2011; editor was Ulrich Müller, who has retired) (no activities)

Vol. B (*Reciprocal space*; most recent online edition is dated 2010; editor Gervais Chapuis)

The plans outlined in the 2023 report to move a revised version of Section 9.8 (*Incommensurate and Commensurate Modulated Structures*) of the 2006 edition of Vol. C into Vol. B are on hold because of limited resources.

The anticipated new contribution on *The Three-Dimensional Pair Distribution Function* method for single crystal diffuse scattering analysis by Arkadiy Simonov and Thomas Weber has not materialized because the authors have not responded to the referees' comments. It is possible that delays in handling have resulted in the article's becoming too out-of-date.

Vol. C (*Mathematical, physical and chemical tables*; online edition is dated 2006; editor Richard Welberry)

Nine chapters for the new volume are now available online. Two of the early-view chapters, both on data mining, were published in issue 4 of the 2024 IUCr Newsletter, and both chapters were made freely accessible for a limited period. Several other chapters are ready for typesetting.

Vol. D (*Physical properties of crystals*; most recent online edition is dated 2013; editor was the late André Authier) (no activities)

Vol. E (*Subperiodic groups*; most recent online edition is dated 2010; editor Gotzon Madariaga)

The paper *Complete online database of maximal subgroups of subperiodic groups at the Bilbao Crystallographic Server* by G. de la Flor, H. Wondratschek, and M. I Aroyo was submitted to *J. Appl. Cryst.* in 2024 and published in early 2025.

A paper titled *Scanning tables for the layer groups* by B. Field and S. M. Griffin was submitted to *Acta Cryst. A* in 2024. Acceptance in 2025 is expected.

Incorporation into Vol. E of these two papers is anticipated.

Several errors and inconsistencies in Vol. E have been noted and await correction.

The presentation of the scanning tables is being reconsidered with the aim of increasing their use.

The possibility of visualization in the online edition of Vol. E of the subperiodic groups is being considered. Collaboration with R. Hanson, the developer of *Jmol*, would be required.

Vol. F (*Crystallography of biological macromolecules*; most recent online edition is dated 2012; editors Liang Tong, Eddy Arnold, and the late Michael Rossmann) (no activities)

Vol. G (*Definition and exchange of crystallographic data*; online edition is dated 2006; editors Brian McMahon and James Hester)

The details of the content of the revised version have been finalized. The volume will consist of 8 Parts, 50 chapters in all, of which 27 are new content, 15 are significantly updated from corresponding material in the First Edition and 8 represent material which has been updated with technical changes only. Among the new material are seven new CIF or DDL dictionaries and accompanying commentary chapters. There are also extensive chapters describing the use of CIF in workflows for publishing and databases, and its relevance to more general aspects of experimental data management. Material is in hand for all except eight chapters.

The editors of Vol. G have already put most of the material in a form nearly ready for publication, so that the work needed from the staff in Chester will be minimized.

Vol. H (*Powder diffraction*; new volume in 2019; editors the late Henk Schenk, Chris Gilmore, who has retired, & Jim Kaduk) (no activities)

Vol. I (*X-Ray Absorption Spectroscopy and Related Techniques*; new volume; editors Chris Chantler, Federico Boscherini & Bruce Bunker)

Volume I was fully published in 2024; there are 152 chapters (1088 pages), with additional supporting material and tables also available online. Already there are many citations to the Volume, which is very welcome and perhaps indicative of widespread interest and appreciation from the XAS, XAFS, XANES and EXAFS communities and beamlines around the world.

Vol. I has also been a primary subject of the last two years of the joint meetings of the IUCr Commission on XAFS and the International XAFS Society on the Quality and Quantity of XAFS. A *Nature Review* on XAFS was written that particularly highlights Vol. I. Extensive work is also proceeding on the consequences of Vol. I, especially as regards coordinated work on data formats.

The publication of Vol. I was announced by inclusion of the Preface and Forward as the first two articles of the 2nd 2024 issue of the IUCr Newsletter. The cover of that issue is a picture of Editor Chris Chantler looking very pleased as he holds a spiral-bound set of sample chapters during the 2023 IUCr Congress in Melbourne.

Possible Volume J on magnetic crystallography

The Commission on Magnetic Structures organized a Special Collection of papers in Section B of *Acta Cryst.* to describe the important developments of the last decade in the analysis of magnetic structures. It is possible that sometime in the future these papers will form the basis of a new volume of *International Tables*.

Further information about the volumes can be found at <http://it.iucr.org> and at the home page of the Commission, <http://www.iucr.org/resources/commissions/international-tables>. The “Guided Tour” available at <http://it.iucr.org/services/guidedtour/> is highly recommended because it shows what is available electronically. Access to the Tables of Contents of all the volumes is free, as are sample pages (including author lists and prefaces); see the homepages for the individual volumes (e.g., <http://it.iucr.org/A/>).

An important event in 2024 was the retirement of Peter Strickland, who headed up publishing operations in the Chester Office for decades. Peter’s steady hand and very wise counsel were greatly valued by all who interacted with him. We hoped that he might never retire, but since the time did come (his garden was calling), we send him off with our very best wishes for many happy years.

While the retirement has affected operations in Chester, *International Tables* is fortunate that the staff most involved with the series have also been with the IUCr for many years. Louise Jones has taken over as Head of Publishing Operations. Nicola Ashcroft continues as Technical Editor of *International Tables* in addition to being the Managing Editor for IUCrJ. Volume I was technically edited by both Nicola and Simon Glynn (who is now responsible for Sections D and F of *Acta Cryst.*). Nicola and Simon have been especially skilled at interacting with the editors of the IT volumes and their authors, and providing them with tactful guidance. It is a pleasure to thank them for their continuing and very important contributions to the IUCr.

C. P. Brock, Chair

A3. Commission on Aperiodic Crystals

In 2024, the Commission on Aperiodic Crystals (CAC) actively continued to advance aperiodic crystallography, through organizing, supporting, and promoting meetings, workshops, and educational activities worldwide. In doing so, CAC continued its ongoing coordination of interaction between the various sub-communities and disciplines involved in the different aspects of research in aperiodic crystals, as well as the dissemination of research results to the wider scientific community.

In conjunction with the Special Interest Group 3 (SIG-03) of the European Crystallographic Association a common website is maintained for distribution of news and events as well as providing access to resources.

<http://sig3.ecanews.org>

<http://aperiodic.iucr.org>

The main activity of the commission in 2024 was the organisation and running of Aperiodic XI, 2024, the latest in a series of conferences supported by the Commission on Aperiodic Crystals (CAC). These conferences are held approximately every three years, with previous meetings taking place in Sapporo, Japan (2022); Ames, Iowa, USA (2018); Prague, Czech Republic (2015); Cairns, Australia (2012); Liverpool, UK (2009); Zao, Japan (2006); Belo Horizonte, Brazil (2003); and Nijmegen, Netherlands (2000).

Aperiodic 2024 was held from June 24–28, 2024, at the University of Caen Normandy, in Caen, France. This 11th edition of the conference was particularly significant as the first in-person gathering since the COVID-19 pandemic. It welcomed nearly 80 participants from 13 countries, fostering a rich exchange of ideas and research in the field of aperiodic crystals.

The scientific program covered a wide range of topics, from incommensurate structures to various aspects of quasicrystals, mathematics, and tilings. It featured 14 sessions, including presentations by 12 invited speakers and 40 contributed oral talks showcasing the latest advancements in aperiodic materials research. A dedicated poster session further enriched the discussions.

A highlight of Aperiodic 2024 was the presentation of the inaugural Janssen-Tsai Prize. Established in memory of Professor Ted Janssen (1936–2017) and Professor An-Pang Tsai (1958–2019), this prize recognizes outstanding contributions to the field of aperiodic crystals, from theoretical research to practical applications. Nominees must be under 45 years of age at the time of submission.

Prizes were awarded at Aperiodic 2024 to two distinguished researchers:

- Dr. Stefan Förster, for his outstanding contributions to quasicrystal research, particularly his discovery and study of ultra-thin films of decagonal quasicrystalline BaTiO₃. His work has significantly influenced the aperiodic crystal community and advanced our understanding of quasicrystal growth phenomena. - Dr. Tsunetomo Yamada, for his pioneering work on superspace atomic structure determination of icosahedral quasicrystals and his studies on phason diffuse scattering. His research has greatly enhanced our understanding of quasicrystal structures.

Each recipient was awarded a prize of 1,000 euros and a commemorative medal.

The conference took place in a warm and collegial atmosphere, with scientists from diverse backgrounds sharing their insights and experiences.

Other conferences and workshops

ECM34 | 34th EUROPEAN CRYSTALLOGRAPHIC MEETING Padova, Italy 26-31 August 2024

One microsymposium on “Aperiodic order and Complex structures” with two invited talks (L. Bindi and M. Diaz-Lopez) and 3 contributed talks (Sander van Smaalen, Leila Noohinejad, Anna Gagor).

EcmetAC Euroschool (3-8 November 2024, Jülich, Germany)

The Euroschool’s focus is on intermetallic compounds, advanced synthesis and characterisation techniques (<https://erc.org/index.php/conferences/euroschool/>)

S. Schmid, Chair

A4. Commission on Biological Macromolecules

The Commission (CBM) aims to support structural biology and macromolecular crystallography worldwide through scientific exchange, training, and promoting policies encouraging the generation and dissemination of knowledge and technologies.

- 1) The committee representing the CBM for the next IUCr Congress in Calgary Congress—comprising Matthias Bochtler (our representative to the IUCr Congress IPC), Dorothee Liebschner, Beatriz Guimarães, Alejandro Buschiazzi, with Diana Tomchick and Wladek Minor serving as observers—worked extremely hard and achieved a phenomenal outcome. The CBM program includes 17 sessions, not counting special sessions dedicated to George Sheldrick and other prominent crystallographers who have passed away.

We owe special thanks to Stephen Burley, who generously consulted with us on several occasions.

- 2) As reported last year, efforts are ongoing to improve the impact factor (IF) of the IUCr Journals. The CBM Chair has been in contact with several authors who submitted high-impact papers to bioRxiv and then had to wait up to a year for formal publication. Unfortunately, it seems that the journal’s IF continues to carry more weight than the timeliness of publishing cutting-edge research. That said, IUCr Journals have made significant progress in reducing the time between submission and publication, as well as in refining keyword selection to improve discoverability. These improvements are particularly notable across several IUCr titles. Authors should be encouraged to share their findings through modern and engaging communication channels. They should also notify their institution’s press office about papers with potential public interest. Furthermore, the IUCr should continue to promote media engagement, including television/radio interviews and articles in the popular press—to highlight important structural biology achievements. Finally, more attention should be given to designing visually appealing journal covers. Studies show that papers featured on the cover are more likely to receive wider publicity and attention.
- 3) A growing concern is the increasing number of PDB depositions that list “to be published” as the primary citation. In addition, discrepancies between the titles of deposited structures and the titles of their corresponding publications can be confusing, particularly for biomedical researchers relying on the PDB for structural information. Commission members, along with other crystallographers involved in data deposition practices, have been actively discussing standards that would make PDB records more accessible and understandable to non-structural biologists. A useful classification of common issues in macromolecular structures were presented in several papers. It is important to recognize that interpretations of structural quality can vary depending on whether the viewer is a crystallographer or a biologist. Special attention should also be given to the occupancy values of water molecules and metal ions, as misinterpretation of these features can lead to confusion or incorrect conclusions in biomedical research.
- 4) Following recommendations from the Committee on Data (CommDat) and the CBM, the Protein Data Bank (PDB) has, since September 2021, implemented a policy requiring the inclusion of the structure PI/Contact Author (also known as

the Depositor-of-Record) name, email address, and ORCID ID in the metadata of deposited structures within the public PDBx/mmCIF files. While providing this information for the PI/Contact Author is now mandatory, CBM and the IUCr should further encourage all contributing authors of PDB deposits to include their respective ORCID IDs to enhance transparency, traceability, and recognition of individual contributions.

- 5) IUCr should promote resources like Proteopedia as valuable resources for undergraduate and graduate students, as well as biologists. This page can be a valuable resource for students and researchers studying the virus and its impact on human health. (https://proteopedia.org/wiki/index.php/Lifecycle_of_SARS-CoV-2).
- 6) CBM chair works with CommDat chair Simon Coles to promote the deposition of diffraction images. Resource proteindiffraction.org may be closed in 15 months. Hopefully, the data will be transferred to PDBj.
- 7) Some CBM members are in contact with PDB to improve the validation report for X-Ray and CryoEM deposits.
- 8) Dr. Dr Matthias Bochtler and Dorothee Liebschner were added as consultants to CBM.

Meetings, workshops, and other outreach activities

The CBM has recommended the IUCr's support for several meetings and workshops that can be crucial in providing resources for teaching and disseminating results obtained through macromolecular crystallography.

W. Minor, Chair

A5. Commission on Crystal Growth and Characterization of Materials

The Commission has been engaged in several activities during the calendar year 2024. The membership of the Commission remained constant over the year with all members being active in various activities. The main and large meeting point was the 8th European Conference on Crystal Growth (ECCG-8) in Warsaw, and the European School on Crystal Growth, held in the neighbouring Jachranka, which preceded the conference. The conference organiser/Chair was Prof Mike Leszczynski (from our Commission), Institute of High Pressure Physics UNIPRESS, Polish academy of Sciences, Warsaw, Poland. Several members of our Commission attended the conference and had the opportunity to deliver invited as well as contributed talks. The conference offered us the first opportunity to meet in person after the events of the summer of the previous year. Our Commission provided a letter of support for funds to help early career and young researchers participate in the European School on Crystal Growth in Jachranka.

The organisers of the next ECCG conference in Berlin were present in Warsaw and gave a presentation welcoming us to Berlin in 3 years time. The proceedings of the ICCGE-20 which took place in Naples in July-Aug 2023 finally went online (special issue of the Journal of Crystal Growth, <https://www.sciencedirect.com/special-issue/1088WW7XJGX>) after a long process reviewing the contributed papers from the participants. The Proceedings were jointly edited by some excellent colleagues: Rosalba Fittipaldi, Luca Seravalli, along with Geetha Balakrishnan (Chair of this Commission). Prof Elias Vlieg of our Commission began work (following on from Prof Koichi Kakimoto) as the President of the International Organisation for Crystal Growth (IOCG), a prestigious and important role in the Crystal Growth community.

Dr Antonio Vecchione of this Commission, based on his extensive experience organising the ICCGE-20, has been chosen to represent the Commission on the International Programme Committee for the IUCr Congress to be held in Calgary in Aug 2026. Dr Vecchione has been gathering suggestions for Microsymposia in which the interests of the Commission members would be represented, and in which they could participate. It is hoped that our Commission would sponsor at least 3 Microsymposia as in the past IUCr Conferences.

G. Balakrishnan, Chair

A6. Commission on Crystallographic Computing

Commission Membership

There were no changes to the membership or board of the Commission during 2024. The current members have continued their commitment to advancing computational methods in crystallography.

Activities in 2024

The Commission's primary focus in 2024 was on preparations for the **2025 IUCr Congress in Calgary**. Key initiatives included:

Organization of the Computing School: This satellite event will emphasize the construction and understanding of Artificial Intelligence (AI) models in crystallographic research. The program is being developed with the active involvement of several IUCr commissions, including those on Computing, Mathematical and Theoretical Crystallography (MaThCryst), Teaching, Materials Science, and the Committee on Data. As AI continues to reshape the scientific landscape, this event aims to provide a timely and essential platform for crystallographers to engage deeply with algorithm development at a foundational level.

Planning and coordination of the Software Fayre: This event serves as a central hub for showcasing crystallographic on future directions in software development.

Development of Microsymposia and Keynote Lectures: The Commission contributed to the creation of program content focused on computational crystallography. These sessions are designed to ensure broad scientific representation and highlight emerging trends and challenges in the field.

In addition to these global efforts, the Commission continued to support **regional crystallographic congresses** in North America, Europe and Asia.

This support included contributions to scientific programming, recommendation of expert speakers, and promotion of initiatives that enhance the visibility and impact of computational crystallography worldwide.

Outlook for 2025

The Commission will continue preparatory activities for the 2025 IUCr Congress in Calgary into early 2025. This will involve finalizing the Computing School program, coordinating invited speakers, and integrating new computational tools and methodologies into the Congress framework.

S. Panjikar, Chair

A7. Commission on Crystallographic Nomenclature

The members of this commission (the CCN) are the editors of the Union's journals, the editors of the volumes of *International Tables*, the Chairman of the IUCr/OUP Book series Committee, the Chairman of the Teaching Commission, the Chairman of the Committee for the Maintenance of the Crystallographic Information File Standard, and both the IUCr President and General Secretary. At the end of 2024 the number of members was 53. There were also two appointed consultants (see <https://www.iucr.org/iucr/commissions/nomenclature>).

I. Nomenclature Problems

The Commission's webpage invites crystallographers to bring nomenclature problems to the attention of any Commission member. In June 2024 Dr. George Whitehead, the crystallographer at the University of Manchester, brought a problem to the CCN. He had determined a structure [now published *Chemical Science* (<https://doi.org/10.1039/D4SC04337E>)] for which he thinks Z should be $\frac{2}{3}$, but in Chapter 4.1 of Vol. G of *International Tables* the entry for `_cell_formula_units_Z` in the Core Dictionary states that the Z is an integer.

Several very experienced crystallographers were consulted; two of them re-refined the structure from Whitehead's data and confirmed his results. The reconstructed reciprocal lattice slices were examined for evidence of weak spots or diffuse scattering, but none was found. An expert in diffuse scattering noted that given the chemical formula and experimental conditions, observation of diffuse scattering would be unlikely.

Some of the crystallographers consulted believe strongly Z should always be an integer; others believe equally strongly that in this specific case, and a very small number of others, a fractional Z value is more appropriate. A description of the problem and of the two opposing viewpoints was forwarded to the CCN in mid-November. The discussion is ongoing, with a decision expected in the first half of 2025.

II. *Online Dictionary of Crystallography* (or, the *ODC*); the editor is Gervais Chapuis

The CCN is responsible for maintaining the *ODC*, which was established in 2006 as a wiki and continues to be run as such, *i.e.*, as a website of definitions that qualified members of the crystallographic community can add to or modify. One definition (of Z) was added to the *ODC* in 2024.

III. Other

In the CCN reports of 2022 and 2023 the possibility of starting a section of the CCN webpage giving answers to *Frequently Asked Questions* was proposed. In 2023 Carolyn Brock and Mois Aroyo planned to start drafting sample FAQs, but the first one, about inconsistencies in the ordering of space groups in Vol. A of *International Tables*, became a major project. The work for that project was completed in 2024 and a manuscript was begun with the idea of submitting it to the Teaching Section of *J. Appl. Cryst.* Submission in the first half of 2025 is expected. The manuscript will give the history of the current ordering and will detail its inconsistencies and then will propose an alternative. While it is unreasonable to think of replacing the current ordering, it is possible that an alternative could be added to the online version of Vol. A of *International Tables*.

C. P. Brock, Chair

A8. Commission on Crystallographic Teaching

During the 2024 the Commission on Crystallographic Teaching carried on its dues with different activities. The principal business has been the one of the evaluations of the schools and courses to be supported by IUCr through the Meeting Support Commission. In particular, the following events have been evaluated by the members:

- Early career diffraction methods seminar 2024 – Berlin (DE) 21-22 July 2024;
- VI Latin American Crystallographic Association School: Quantum Crystallography – Montevideo (UY) 19-21 September 2024;
- International Workshop on Magnetic Crystallography – Dongguan (CH) 24-30 November 2024;
- LACA Rigaku OpenLab 2024 – San Paulo (BR) 2-8 December 2024;
- 20th BCA/CCG Intensive Teaching School in X-ray Structure Analysis – Durham (UK) 29 March-5 April 2025;
- The Fourth Pan African Conference on Crystallography (PCCr4) Algiers (DZa) 20-24 April 2025;
- Structural Biology 2.0: Computational Tools and X-Ray Diffraction - Integrated to Solve and Understand 3D Protein Structures – Montevideo (UY) 21-30 April 2025

All of them were considered to be worth being endorsed even though sometimes the application was not fully and carefully prepared. It looks like in the last few years a boost in schools and courses dealing with crystallography has occurred. This is really a positive development considering that many of them are organized in countries where crystallography is not so well widespread and taught.

Several requests for evaluations came from the OUP Book Series Committee. Different texts arrived for the commission: Prof. Marie-Paule Pileni's manuscript on the nanoworld, the volume of Prof. John Helliwell on "Precision and accuracy in biological crystallography, diffraction, microscopies, and spectroscopies" and the chapter of Prof. Akio Takénaka et al. on "X-ray structural analysis of bio-molecular crystals".

In addition to those, Prof. John Hughes sent to the Commission on Crystallographic Teaching a piece of writing to be considered as a pamphlet on "Abundance of Elements and the Pressure and Temperature Conditions in the Earth's Crust". The possibility for this piece to be published on one of the educational sections of Acta was evaluated.

Some of the members of the commission and the consultant met online on May 6th and the Chair also informed the participants to start thinking about topics for the MS to be proposed for the IUCr Meeting in Calgary.

Prof. Rajni Kant volunteered to take part as representative of the CCT on the IPC. The first deadline that we will face is the one of the MS submission in March/April.

A. Guerri, Chair

A9. Commission on Crystallography in Art and Cultural Heritage

Awaiting report

K. Janssens, Chair

A10. Commission on Crystallography of Materials

Since the CCM is an important commission to the IUCr, the Executive Committee (EC) of the IUCr decided in Melbourne that the CCM needs to be re-formed. We are therefore in an "ad interim" status hoping to achieve to have a working commission again by the time of the next congress in 2026 in Calgary. The most important task of our ad interim Commission on Crystallography of Materials was the elaboration of the Terms of Reference. Different zoom meetings helped us to develop the Terms of Reference and to build the working group. Very important was the meeting which was enabled by the ECM-34 committee on Wednesday August 28th in Padua. We had an in-person as well as a Zoom meeting with our members and could finalize the Terms of Reference as well as the nominations.

It is also expected that our CCM will actively participate in shaping the Congress program 2026. We started therefore discussions with different commissions and are currently preparing different joint micro-symposium.

A. Dommann, N. Zhang

A11. Commission on Diffraction Microstructure Imaging

The imaging (DMI) Commission held a tutorial workshop "Elucidating 3D microstructures through diffraction-based imaging and simulations" as part of the Advanced Photon Source (APS) user's meeting in May 2024. The workshop provided use-cases and tutorials for maturing DMI techniques, and how to utilize these techniques to calibrate and validate complementary modeling efforts. Focuses of the workshop included: i) highlighting various DMI techniques and their application including high-energy diffraction microscopy, scattering tomography, and Bragg coherent diffraction imaging; ii) describing how to effectively manipulate, combine, and visualize this multi-modal data to gain insight into hierarchical material behavior at different length scales; and iii) discussing advanced materials simulation approaches instantiated with, and updated by, DMI data. The workshop had 10 invited talks and approximately 50 participants.

The DMI commission technique ontology & taxonomy effort, led by Dr. Kelly Nygren, is close to completion. After soliciting extensive feedback from preliminary drafts and extensive (sometimes contentious) deliberation, the commission has finalized definitions and classification for current DMI techniques. A manuscript providing an overview of current DMI techniques and their ontology is expected to be submitted to an IUCr journal in 2025.

The effort to benchmark instrument resolution and accuracy of DMI measurements at synchrotron beamlines around the world, led by the physical standards sub-committee, is continuing. Both nickel superalloy and titanium alloy test specimens were generated as representatives of often-used cubic and hexagonal engineering alloy systems respectively. These samples are now taking part in a worldwide tour. The specimens were preliminarily characterized at the Air Force Research Laboratory by Dr. Gregory Sparks and Dr. Paul Shade to provide baseline electron microscopy-based 2D surface characterization. The specimens then traveled to Argonne National Laboratory where they were characterized using DMI techniques by Dr. Jun-Sang Park and Dr. Peter Kenesei. Dr. Park next brought the specimens to Europe where they were characterized at Petra-III P21 in Germany. The specimens were then handed off to Dr. James Ball, where they were characterized at European Synchrotron Radiation Facility ID11 in France and the UK Diamond Light Source JEEP beamlines. Further measurements are planned in 2025.

D. Pagan, Chair

A12. Commission on Electron Crystallography

The main activity of the CEC and its members is devoted to the organization of schools and workshops where electron crystallography is one of the main subjects. In the following is a list of the events for 2024 and beyond.

Workshops.

Tatiana Gorelik (member) coordinated an ECA lunchtime webinar in February 2024, Sergi Plana Ruiz, “Liquid phase electron crystallography: the path to electron diffraction from protein crystals at room temperature”

Tatiana Gorelik (member) as Chair of SIG04 of the ECA coordinated the SIG04 publication award. Details can be found at https://www.iucr.org/news/newsletter/etc/articles?issue=159082&result_138339_result_page=16

Stephanie Kodjikian (consultant) co-organized the workshop “Practical 3D electron diffraction in Materials sciences” (Grenoble, France, 4-6/06/2024). This training workshop for X-ray crystallographers focused on the practical aspects of 3D electron diffraction in materials sciences, with alternation of demonstrations and manipulations on TEM, and tutorial sessions on computer.

Tatiana Gorelik (member) contributed to the Workshop on Advanced Precession-Assisted 4D-STEM and 3D-ED, June 19th – 20th 2024, Forschungszentrum Jülich with a lecture on Electron diffraction for structure characterization of novel materials.

Several CEC members contributed to the organization of the final meeting of the NanED EU project which hosted two lectures, one from Paulina Dominiak on charge-density analysis with ED data and one from Tamir Gonen on the use of MicroED in macromolecular crystallography.

Laure Bourgeois (member) co-organized an advanced materials characterisation microsymposium as part of the 8th Conference of the Combined Australian Materials Societies, CAMS 2024 (Adelaide, 4-6 Dec. 2024).

Hongyi Xu (consultant) organized and co-organized the following workshops:

- NordTEMHub
- ARTEMI 3D ED Workshop, Stockholm, April 2024
- MicroED workshop by ThermoFisher Scientific, Wollongong Australia, June 2024

Maciej Zubko (member) and other polish scientists co-organized the following events:

- „The XVIIIth International Conference on Electron Microscopy” in Zakopane Poland, 9-12.06.2024;
- „66 Konwersatorium Krystalograficzne (Polish Crystallographic Meeting)” in Wrocław Poland, 26- 28.06.2024;
- „14th Polish-Japanese Joint Seminar on Micro and Nano Analysis” in Toyama Japan, 3-6.09.2024; (co-organized by the Polish group from IMIM Krakow)

Schools

Several members of CEC have been actively involved in the organization of the electron crystallography school that was a satellite event of the ECM meeting held in Padova, Italy, in August 2024 (<https://elcrys24.sciencesconf.org/>). The school spanned two and a half days, focusing on three-dimensional electron diffraction (3D ED) and it had a participation of 38 students from Europe and Asia.

Cif for 3D ED data

Mauro Gemmi (member) and Lukas Palatinus (consultant) organized a meeting during ECM34 in Padova to discuss the issues with cif nomenclature in case of structures solved and refined with 3D ED. Thanks to that and to the work done in collaboration with IUCr in the NanED EU project with the great help of Brian McMahon we arrived to an approved modification of the core CIF dictionary for ED data.

M. Gemmi, Chair

A13. Commission on High Pressure

Awaiting report

K. Dziubek, Chair

A14. Commission on Inorganic and Mineral Structures

The Commission on Inorganic and Mineral Structures (CIMS) did not meet in person in 2024 but discussed issues as they arose by email. CIMS lent its support after due consideration to the 8th Moroccan School of Crystallography, to be held from November 5–8, 2025 at Cadi Ayyad University in Marrakech, Morocco, and the 7th Latin American Crystallographic Association and 27th Brazilian Crystallographic Association meeting Joint Meeting and the LACA-ABCr School, to be held in Fortaleza, Ceará, Brazil, from October 13th to 18th, 2025 (<https://laca-abcr-2025.abcrystalografia.org.br>). The commission website was discussed: it continues to be maintained by Massimo Nespolo at <https://www.crystallography.fr/cims/index.htm>. Michael Lufaso manages the “official” bond valence parameter reference file `bvparm20.cif` hosted by the IUCr at <https://www.iucr.org/resources/data/datasets/bond-valence-parameters>.

Roberta Oberti and Giovanni Ferraris chaired the international meeting "Minerals as a treasure trove" at the Accademia Nazionale dei Lincei, Rome, on 15-16 February 2024.

Chris Ling is chairing the Diffraction Methods Working Group for "A Future Lightsource for Australia and the Region" (4th-generation replacement for the Australian Synchrotron).

John M. Hughes, in order to increase the examination of mineralogy in the IUCr Commission on Crystallographic Teaching educational pamphlets, contributed a pamphlet entitled Abundance of Elements and the Pressure and Temperature Conditions in the Earth's Crust (#24), and was invited to prepare an additional pamphlet (#25) entitled Minerals: Naturally Occurring Compounds That Crystallize on Earth, currently underway.

C. Ling, Chair

A15. Commission on Magnetic Structures

After the 2023 IUCr Congress in Melbourne, the commission focused on completing the report on guidelines for the publication of magnetic structures, which had been started in 2023. This document establishes clear rules for reporting magnetic structures in a standardized and unambiguous form. Following extensive discussions and revisions, the final version was approved in May 2024. The commission also coordinated with the IUCr management of Acta Cryst. B the publication of a virtual issue focused on magnetic structures, led by the guidelines report. Acting as guest editors of this special issue, former commission chair Branton Campbell, vice-chair Ovidiu Garlea, and the current chair J. Manuel Perez-Mato have handled a collection of invited papers, which have appeared in the mentioned journal throughout the year. Many commission members and consultants have contributed to this issue. At this stage, nearly all planned articles (over twenty) have either been published or are in the editorial process. It is expected that within a few months, all articles will be made available into a single virtual issue of the journal dedicated to magnetic structures.

In July 2024, J. Manuel Perez-Mato, Branton Campbell, and Ovidiu Garlea attended and lectured at the school on "Magnetic Structure Determination from Neutron Diffraction Data" held at Kennesaw State University in Atlanta, USA. The program provided hands-on training and lectures on determining magnetic structures from both powder and single-crystal neutron data. Participants were introduced to the application of magnetic space groups and representational analysis, which were demonstrated through a series of practical exercises.

At the 2023 Melbourne Congress, the commission contacted Prof. T. Kamiyama and other scientists from the China Spallation Neutron Source (CSNS) in Dongguan, to organize an international workshop on magnetic crystallography, under the auspices of the commission. Supported by the IUCr, the workshop successfully took place in November 2024, with over 70 participants and many commission members serving as lecturers. The workshop provided an excellent opportunity to foster collaboration and engage with researchers from diverse scientific backgrounds. Participants benefited from direct interactions with experts, gaining insights into the latest methodologies.

Given the limited presence of magnetic structural research at the 2024 meeting of the European Crystallographic Association (ECA), we found it necessary to engage in increasing the visibility of magnetic crystallography within this association. The secretary of the commission, Françoise Damay, initiated the formal process for the creation of a Special Interest Group (SIG) on Magnetic Crystallography within the ECA. This SIG aims to represent and promote this type of research and its community within the ECA and its meetings. Thanks to her motivation and her continuous efforts, the bureaucratic process is now in its final stage, with more than 20 renowned European crystallographers having joined the group. The SIG is expected to receive formal approval this summer at the upcoming European Crystallographic Meeting in Poznan.

The expansion and long-term maintenance of MAGNDATA, the only available database of magnetic structures, hosted at the Bilbao Crystallographic Server, is of special importance to this commission. During this year, an effort has been undertaken to motivate authors to deposit their published structures in the database using the magCIF standard format and the software tools available. But to ensure in the long term the database sustainability, the commission has started to discuss more drastic and comprehensive measures.

After the success of the Erice school on Magnetic Crystallography in 2019, the commission reached out to Annalisa Guerri to organize a second edition. A reservation was finally secured for the year 2030. In principle, the secretary and vice-chair of the commission, Françoise Damay and V. Ovidiu Garlea, are in charge for overseeing this future school.

During this year 2024, there has been an upsurge of research on spin-group symmetry and its applications. Spin space groups are increasingly being used in DFT electronic band calculations as spin-orbit-free symmetries, particularly in the frame of altermagnetism and unconventional magnetism in general. Three different research groups have independently enumerated tens of thousands of spin space groups, each using different notations. These developments imply a new challenge for the commission, as one of its main aims, according to its terms of reference, is to "establish standards for the description and dissemination of magnetic structures and their underlying symmetries...". It is then expected that the commission will contribute in the next years to the establishment of a standard nomenclature for these symmetry groups.

J. M. Perez-Mato, Chair

A16. Commission on Mathematical and Theoretical Crystallography

Events

Introduction to Geometric Data Science

Tutorial at the Foundational Aspects of Neuro-Symbolic Computing workshop
<https://sites.google.com/view/fanesy-2024>
Santiago, Chile 4 – 8 March
Presented by Vitaliy Kurlin

A mathematical analysis of GNoME and other materials databases
<https://www.imsi.institute/activities/data-driven-materials-informatics/materials-informatics-tutorials-and-hands-on/>
Tutorial at the Materials Informatics workshop in IMSI
Chicago, USA 11 – 15 March
Presented by Vitaliy Kurlin

Computational Geometry and Graph Theory for Crystalline Materials
Mini-symposium series at the SIAM Mathematical Aspects of Materials Science
<https://www.siam.org/conferences-events/past-event-archive/ms24/>
Pittsburg, USA 19 – 23 May
Organized by Vitaliy Kurlin

Crystallographic Symmetry: Undergraduate Summer School Program
Shanghai University, China, 3 – 14 June
Lecturer: Mois Aroyo

Shanghai International Crystallographic School and Workshop on chirality in solid state physics and quantum materials
<https://www.crystallography.fr/mathcryst/shanghai2024.php>
International Center for Quantum and Molecular Structures, Shanghai University, Shanghai, China, 14-21 June 2024
The aim of the school was to provide an introduction to group theoretical methods and computational tools necessary for appropriate applications of symmetry properties in solid state material science.
Lecturers include: Mois I. Aroyo and Massimo Nespolo

Introduction to Crystallographic Symmetry: Summer Semester School Program
University of Science and Technology, Beijing 7 – 21 July
Lecturer: Mois Aroyo

Geometric Data Science
Minisymposium at the European Congress of Mathematicians
<https://www.ecm2024sevilla.com/index.php/program/ecm2024-programme-mini-symposia>
Seville, Spain, 15 – 19 July
Organized by Vitaliy Kurlin

Practice of Powder X-ray Analysis 2024
Sponsored by the Crystallographic Society of Japan
<https://crsj.jp/news/2024/240409xrd.html>
Tokyo Institute of Technology, Japan 25 & 26 July
Caretakers include Koichi Momma

Training course on symmetry and group theory: Sokendai Interdisciplinary Lecture
<https://www.crystallography.fr/mathcryst/TrainingCourseJapan.php>
Tsukuba, Japan, 22 – 26 July & 29 July – 2 August
Sponsored by The Crystallographic Society of Japan and the Institute of Materials Structure Science of the High Energy Accelerator Organization; co-sponsored by Sokendai
The training course is normally held biannually (March and August) and aims at providing a solid background in symmetry and group theory to students and scientists working on crystalline materials.
Lecturer: Massimo Nespolo

International School on Fundamental Crystallography: Seventh MaThCryst school in Latin America
<https://www.crystallography.fr/mathcryst/lima2024.php>
Universidad Nacional Mayor de San Marcos, Lima, Peru, 12-16 August 2024
Lecturers include: Mois Ilia Aroyo, Gemma de la Flor Martín, and Massimo Nespolo

Mathematics and Computer Science for Materials Innovation
<https://kurlin.org/macsmin/2024.php>
Liverpool, UK (& hybrid), 9-13 September 2024
Organized by Vitaliy Kurlin and Olga Anosova, Dan Widdowson, Will Jeffcott, Yury Elkin, Jonathan (Teddy) McManus et al.

VI Latin American Crystallographic Association Meeting
<https://www.laca2024.pedeciba.edu.uy/>
Montevideo, Uruguay from September 23 to 26
On the organizing committee: Leopoldo Suescun

Introduction to Geometric Data Science
Tutorial at the SIAM Mathematics of Data Science

https://meetings.siam.org/sess/dsp_programsess.cfm?sessioncode=80792
Atlanta USA 21 – 25 October
Organized by Vitaliy Kurlin

São Carlos OpenLab 2024
<https://www2.ifsc.usp.br/portal-ifsc/cristalografia-ifsc-usp-acolhe-o-sao-carlos-openlab-2024/>
Universidade de São Paulo, Brazil 2 – 8 December
Supported by ABCr, CAPES, DAIRIX, IFSC, Rigaku, USFP, IUCr, LACA, UNESCO
On the organizing committee: Leopoldo Suescun

Leopoldo Suescun was elected to the Board of Directors of the International Centre for Diffraction Data for 2024 – 2028
<https://www.icdd.com/who-we-are/#board>

M. Louise Antonette De las Penas continues as a Co-editor of Acta Crystallographica A

Mois Aroyo, Online Crystallography by the Bilbao Crystallographic Server
Indian Institute of Technology, India 18 April

Gemma de la Flor Martin, with Ulrich Müller, 2nd ed. of Symmetry Relationships between Crystal Structures: Applications of Crystallographic Group Theory in Crystal Chemistry

Koichi Momma, 3D Visualization System VESTA Basics: Visualization Methods for Crystal Structure and Electron Density & Application of the VESTA 3D Visualization System: Collaboration with Various External Programs
33rd Nanostructure Research Institute Materials Calculation Seminar
https://www.jfcc.or.jp/event/nano_keisan.html
Nagoya, Japan 22 October

Davide Proserpio, Topological Analysis of Reticular Framework Materials with ToposPro
PNWS Seminar, 25 – 25 September, Graz University of Technology

And various journal articles and presentations *G. McColm, Chair*

A17. Commission on Neutron Scattering

The Commission (CNS) promotes the use of neutron scattering by encouraging the publication of information on the capabilities of neutron sources and instrumentation and by supporting symposia, schools and workshops that educate researchers on the unique information that can be provided by neutron scattering. Several members of the Commission are actively involved in developing neutron sources and new neutron scattering technologies and methods.

Operation for major neutron facilities (HFIR, ILL, PSI, ISIS, Dhruva, JRR-3, OPAL, CSNS etc.) continues.

The construction of the European Spallation Neutron Source (ESS) in Sweden is progressing. Five diffractometers are under construction, the first one DREAM, will start in 2026 as one of the first ready for users. The Spallation Neutron Source (SNS) in USA is operating at 1.7MW from July 2024. FRM II is not running yet but a lot of progress has been made especially to prepare for the transition to LEU. The operation of J-PARC MLF in Japan was suspended due to target problems in late 2024. Operations are set to resume in April 2025. In Canada, the Canadian Long-Term Neutron Plan for 2025-2035 was formulated in October 2024. It recommends that the federal government allocate \$95 million over six years starting in 2025 to be managed by Neutrons Canada. In November 2024, McMaster University celebrated the launch of the Canadian Neutron Beam Laboratory (CNBL). The neutron scattering facilities at the McMaster Nuclear Reactor are expanding, including the addition of new neutron beamlines and a neutron radiography facility.

Commission supported the organization of several conferences (for example, the 2024 Workshop on Magnetic Crystallography at Dongguan, China).

Our commission members were also involved in organizing several meetings not only for neutron but also for quantum beam (synchrotron, neutron and ion radiation etc.) joint use that took place in 2024 (for example, the MLZ conference "Neutrons for Energy Storage" took place on at the Fuerstenried Palace in Munich on June 4th – 7th 2024.). Many workshops on instrumentation and/or data evaluation were held.

Neutron schools and crystallographic seminars to train the next generation of neutron scattering researchers are also important and are held at various facilities, and the Commission also supports the holding of these schools, such as the 8th Neutron and Muon School, which was held in Japan from December 9 to 13, 2024. In February, the future of the new generation of compact sources was discussed at UCANS-11 hosted by TRIUMF, Canada's particle accelerator centre in Vancouver.

Commission members were involved in planning activities for several important neutron-related conferences and schools in 2025.

The major event will be the ICNS2025 (International Conference on Neutron Scattering) in July 2025, hosted by ESS, Lund, Sweden.

T. Ishigaki, Chair

A18. Commission on NMR Crystallography and Related Methods

In 2024 the commission curated the organization of SMARTER-8 meeting in Aveiro (September 2024). This biannual interdisciplinary meeting brought together researchers from different areas of structural science, including diffraction, modelling, NMR and electron microscopy. The meeting was an excellent opportunity to present cases of the structure determination and analysis of properties of complex systems where synergistic application of different tools is essential. The strategy for future SMARTER meetings was discussed and the commission will work together with the SMARTER executive committee to ensure the organization of future meetings. IUCr sponsored the attendance of several early-career researchers for this meeting. The commission was also involved in promotion of the Faraday Discussion on NMR crystallography supported by Royal Society of Chemistry (Birmingham, September 2025).

The commission had several opportunities to meet both online and in person (in Aveiro in September 2025) to discuss its activities, membership and future directions. Prof Len Mueller (University of California Riverside) has joined the commission as a consultant to promote advances of NMR crystallography in the field of structure determination of biological macromolecules. This appointment will also help the Commission to develop links with the Commission of Biological Macromolecules. Prof James Harper (Utah Valley University) has joined the Editorial board of the IUCr Journal of Applied Crystallography.

The commission has proposed four microsymposia for IUCr congress in Calgary in 2026. These were formulated in collaboration with other commissions from the outset. Following the IPC meeting, these symposia reflect different scientific themes of the Commission and are to run in collaboration with Commissions of Structural Chemistry, Materials, Biological Macromolecules, Crystal Growth and XAFS. Prof Yaroslav Khimyak acted as a representative for the Commission at the IPC meeting. Professor Marta Dudek was actively involved in discussion of all matters related to the IPC (finalizing microsymposia, proposing the co-chairs and outlining potential speakers, nominating keynote and plenary speakers). She is to be nominated as the member of IPC committee for IUCr congress in 2029.

Y. Khimyak, Chair

A19. Commission on Powder Diffraction

Members of the CPD have been involved in discussions around powderCIF/pdCIF regarding how to improve the utility and utilization of cif files for reporting results from powder crystallographic experiments. This has involved two IUCr working groups initiated by the Chester office. The first, which includes Jim Kaduk, Dave Billing, Matthew Rowles, Graciela Diaz de Delgado and Angus Wilkinson, has focused on improving the use of pdCIF and modifying checkCIF to work better with powder CIFs. The second, which includes Dave Billing from the CPD, is coordinated by Loes Kroon-Batenburg and focusses on developing minimum specifications for depositing data to IUCr's Raw Data Letters.

The CPD has reviewed applications for meeting support, and backed applications for support, of the 2025 European Crystallographic Meeting, the 2024 PCCr4 (The Fourth Pan African Conference on Crystallography) meeting, and the VI Latin American Crystallographic Association Meeting.

The CPD considered a request to “collaborate” with a team writing a funding proposal for submission to the US National Science Foundation, which sought to create an open database of powder diffraction data suitable for use in training AI/ML tools that might be of service to the powder diffraction community. This request set off a lively debate amongst commission members and consultants regarding the role of the Commission on Powder Diffraction. Some members were in favor of supporting the proposing team while others felt that the CPD should not provide support to a particular group of people or engage in activities that might be viewed as competing with other organizations such as ICDD and “Momentum Transfer”. CPD declined to “collaborate” as we were divided in opinion.

Individual members of the commission and its consultants have engaged in a wide variety of activities to promote structural science in general and powder diffraction in particular. For example, Antonia Neels is Co-chair for the upcoming (2026) EPDIC meeting in Switzerland and she has been working on its organization. Fabio Furlan Ferreira is an organizer for the upcoming 1st Latin American Powder Diffraction Conference (LAPDiC). Cora Lind taught the powder diffraction component of the US National School on Neutron and X-ray scattering in July 2024, and both Jim Kaduk and Cora Lind taught part of the powder diffraction component of the American Crystallographic Association (ACA) Summer School in June 2024.

David Billing co-organized, along with Matteo Leoni and Dubravka Sisak Jung, the Erice Powder Diffraction School, which was run under the IUCr Banner (International School of Crystallography:: Welcome). The 2024 powder school also represented the 50th anniversary of the International School of Crystallography at Erice.

Dave Billing has also been in discussions with James Hester regarding an updated pdCIF specification to accommodate more complex powder datasets (i.e. one that include multiple measurements and multiple crystal structures such as in situ studies) in an effort to have this ready for the next Congress.

A. P. Wilkinson, Chair

A20. Commission on Quantum Crystallography

In 2024, the Commission on Quantum Crystallography (QCrComm) was actively involved in co-organizing scientific conferences, promoting and educating in the field of quantum crystallography (QCr), and standardizing QCr data through a dedicated CIF dictionary.

In June 2024, the 9th European Crystallography School was organized by E. Espinosa and D. Schaniel in Nancy, France. Many lectures and workshops during the school focused on quantum crystallography approaches.

In July 2024, a QCr session was organized for the second time at the ACA Annual Meeting in Denver, USA. The session, led by B. Patrick and M. Bodensteiner, was well received by ACA 2024 attendees. It was accompanied by a workshop on HAR.

In August 2024, four QCr sessions were organized by SIG-02 (A. Krawczuk) at ECM-34 in Padova. Many members and consultants of QCrComm gave lectures, including keynote lectures by J.-M. Gillet and A. O. Madsen.

In September 2024, several lectures on QCr were delivered during the LACA meeting in Montevideo, and a dedicated QCr School was organized. The school, strongly supported by QCrComm, was enthusiastically received by attendees from the LACA region, with approximately 50 students participating.

In November 2024, the Sagamore XX Conference on Quantum Crystallography was organized by QCrComm, with P. Munshi, D. Jayatilaka, and T. N. Guru Row serving as lead organizers. This long-awaited flagship conference of QCrComm had been postponed for three years due to the COVID-19 pandemic. It brought together participants from 14 countries—including Australia, Canada, China, Denmark, France, Germany, India, Italy, Japan, Poland, Russia, Switzerland, the UK, and the USA—to share their expertise. The five-day event featured five keynote and four plenary lectures, 41 invited talks, 13 oral presentations by young researchers, and a poster session with 40 participants. A one-day QCr workshop, covering various quantum crystallography methods, followed the conference and was well attended by Indian students.

In December 2024, a couple of lectures on QCr were given at AsCA18 in Kuala Lumpur.

In March 2024, the organization of a Focused Issue across all IUCr journals on Quantum Crystallography began, in celebration of the 100th anniversary of the development of Quantum Mechanics. The guest editors are P. Dominiak, A. Pendas, and K. Wozniak. More than 100 authors were invited, and over 30 articles have been published to date (many co-authored by QCrComm members and consultants).

Up to summer 2025, regular online meetings focused on the development of the quantum crystallography CIF dictionary continued. These meetings were attended by several members of the QCr community, including selected QCrComm members and consultants. They culminated in the first draft of the extended CIFrho definitions.

Throughout 2024, the Distinguished Lectures on Quantum Crystallography and Complementary Fields continued online. The series is jointly organized by the QCr Commission and the European Crystallographic Association SIG-2 on Quantum Crystallography, with support from the University of Warsaw (Poland) and the Crystallography Committee of the Polish Academy of Sciences. Nine lectures were broadcast in 2024, with more than 880 registered participants and 43–76 attendees per lecture. The lectures are recorded and posted on the website (qcrwebinar.chem.uw.edu.pl), with each 2024 recording receiving between 62 and 218 views.

P. Dominiak, Chair

A21. Commission on Small-Angle Scattering

The main commission activity for 2024 was advising and supporting the organization of the SAS2024 conference in Taiwan (<https://www.sas2024.tw/site/page.aspx?pid=569&sid=1535&lang=en>). Most members served on SAS2024 organization in various roles, e.g., as members of International Advisory committee. SAS2024 was 5 days long (with a two-day satellite SAS school before) conference in Taipei, which brought together around 400 small-angle scatterers from around the world presenting the latest from the small-angle scattering field. U-S Jeng and Mikihiro Takenaka, together with Professor Kazuo Sakurai, The University of Kitakyushu, organized “Cutting-Edge in Soft Matter Science 2024” as a satellite meeting to the SAS2024 in Kitakyushu, Japan.

During the conference CSAS – represented by 3 current members and 2 consultants - held a nearly hour-long open meeting attended by more than 50 participants. The meeting included introduction of the CSAS purpose and discussion with participants on their needs from CSAS in the future.

The SAS2024 conference proceedings will be published as virtual issue of JAC with four co-editors who are CSAS members or consultants. Multiple commission members are serving the community as Co-editors of IUCr journals (F. Meneau, J. Ilavsky, E. Gilbert, U-S Jeng); Dr A. Allen, consultant, is the main editor of IUCr journals.

Educational activities by CSAS members include various schools : Elliot Gilbert taught “Fundamentals of Small-angle scattering” at the 8th Neutron and Muon School, J-PARC, Japan; Jan Ilavsky taught “Synchrotron characterization of materials” at HUSI school, Hokkaido University, Japan; Florian Meneau organized and lectured at the annual synchrotron school at LNLS, Campinas Brazil, which covers wide range of SAXS related topics, and lectured at São Paulo school of Advanced science on 4th generation synchrotron techniques; U-S Jeng offers synchrotron classes at National Hsing-Hua University, Taiwan as well as a sum-

mer school on SAS; Mikihiro Takenaka gave a series of lectures on Research on polymer physics using scattering at the Advanced Softmaterial BL Consortium, SPring-8.

Community building activities: CSAS members are active in their local SAS community by serving as representatives on commissions, committees, etc. For example, Mikihiro Takenaka serves as Representative of the Small-Angle Scattering Research Group in SPring-8 Users Community (SPRUC), and Elliot Gilbert leads ANSTO's activities in Food Materials Science within which small-angle scattering (both neutron and X-ray) play an essential role. In this context, he has promoted and sought to increase this community in the last 12 months through a range of activities. Most recently this included a KEK-sponsored fellowship to develop the food materials science program in Japan.

Most members of CSAS are staff at large facilities in roles such as beamline/instrument scientists, beamline leads, etc., where they develop and operate the most advanced SAS tools and therefore facilitate top science for the wide user community. Elliot Gilbert is beamline scientist for the QUOKKA SANS instrument at the OPAL facility in Australia and Judith Houston is instrument scientist at ESS neutron source. Jan Ilavsky, Gregory Hura, and Florian Meneau are all scientists at synchrotron sources in their respective local areas. This engagement with the user community enables CSAS to effectively advocate for and represent small-angle scattering.

J. Ilavsky, Chair

A22. Commission on Structural Chemistry

The Commission on Structural Chemistry (CSC) encompasses a wide range of topics in the field of crystallography. There are extensive overlaps with other commissions including the Commissions on Inorganic and Mineral Structures, Powder Diffraction, and Crystallographic Teaching, as well as with important external bodies such as the Cambridge Crystallographic Data Centre.

The membership of the commission was renewed in 2023. The commission is fortunate to have several consultants who provide guidance and continuity. The members of the commission can be found at <https://www.iucr.org/iucr/commissions/structural-chemistry>.

The IUCr Executive Committee liaison remains Angela Altomare. In 2024, the CSC lent support to the following conferences and schools, which draw on crystallographers in the Structural Chemistry sphere:

- "VI Latin American Crystallographic Association Meeting", September 23rd through 26th, 2024, Montevideo Uruguay, Contact: Prof. Natalia Alvarez, Universidad de La Republica, Uruguay.
- "6th International Symposium on Halogen Bonding (ISXB6)", Dubrovnik, Croatia, October 2024, Contact: Mario Cetina, University of Zagreb, Croatia.
- "LACA IUCr-UNESCO Rigaku OpenLab 2024" São Carlos, São Paulo, Brazil December 2nd-8th, 2024, Contact: Javier Ellena, São Paulo University, Brazil
- "20th BCA/CCG Intensive Teaching School in X-ray Structure Analysis" 29th of March to the 5th of April 2025, Durham, UK. Contact: Natalie Pridmore, Durham University, UK.
- "Building Capacity in AI-Driven Drug Discovery and Vaccine Design: AlphaFold Training by BioStruct-Africa". Nairobi, Kenya, August 11–15, 2025, Emmanuel Nji, CRID Cameroon.
- "7th LACA – 27th ABCr Joint Meeting and the LACA-ABCr School" Fortaleza, Ceará, Brazil. 13-17 October 2025. Contact: Alejandro Ayala, Federal University of Ceara, Brazil.
- "1st Latin American Powder Diffraction Conference (LAPDiC)", which will be held from October 11th to 14th, 2025, in Fortaleza, CE, Brazil. Contact: Fabio Furlan Ferreira, Universidade Federal do ABC – UFABC, Brazil
- "Young Crystallographers Meeting #2" organized by the French Crystallographic Association (AFC) and scheduled to take place in Rennes Institute of Chemical Sciences (ISCR), Rennes, France, 2-5, December, 2025, Contact: Elen Duverger-Nédellec, Chair of the French Association of Crystallography Young Crystallographers Section.

The conferences and schools supported by the commission for 2026 so far are:

- "2026 Zurich School of Crystallography", June 29 – July 11, 2026, Zurich, Switzerland. contact: Gervais Chapuis ZSC Finance Committee Lausanne, Switzerland.

In all the cases the CSC members interrogated the degree to which structural chemistry was represented as a science, rather than simply a tool, at each conference. Aspects such as support for students or early-career researchers were taken into account. The diversity (gender, geographical distribution) of speakers was also identified as an important criterion for consideration of future applications for support. These factors play a key role in the degree of support expressed to the IUCr calendar committee. The CSC representative on the International Programme Committee for Calgary IUCr 2026 meeting is Javier Ellena, who provided a

liaison between the IPC and the commission to ensure that there will be a strong structural chemistry programme at the next IUCr Meeting. The CSC is planning a strong structural chemistry programme representing very well the commission in terms of subject matter with an extensive list of micro-symposia and keynote speakers, including some in collaboration with several other commissions. So far more than 20 microsymposia have been suggested and the commission is actively working in providing titles, descriptions as well as Chair and Co-chairs names, always bearing in mind always gender and geographic representation.

J. Ellena, Chair

A23. Commission on Synchrotron and XFEL Radiation

SXR Commission Membership

The current members and consultants listed at: <https://www.iucr.org/iucr/commissions/synchrotron-radiation>

Supported Meetings, Schools and Workshops

During 2024, the commission supported the following events:

1. Building Capacity in AI-Driven Drug Discovery and Vaccine Design: AlphaFold Training by BioStruct-Africa, that will take place in August 2025 in Nairobi, Kenya.
2. LACA Rigaku OpenLab 2024, that took place in December 2024 in São Carlos, Brazil.
3. VI Latin American Crystallographic Association Meeting that took place in September 2024 in Montevideo, Uruguay.

CSXR Member and Consultants Activities

The members of the Commission are active in key synchrotron and crystallography communities and conferences. For example:

Cinzia Giannini – Member, SPB/SFX Proposal Review Panel, European XFEL (since 2023 till now). Member, IUCr2026 International Program Committee for Commission on Synchrotron and XFEL radiation (2024-2026). Invited speaker at LNLS Annual User Meeting (07 nov.2024).

Eduardo Granado - Co-chair, SYNCLIGHT - São Paulo School of Advanced Science on 4th Generation Synchrotron Techniques, Campinas, Brazil, 14-25 Oct 2024. Chair of the Users Committee of LNLS (Nov 2023-Nov 2024).

Jose M. Martin Garcia – Developer and scientist of the Spain XFEL Hub (Since June 2021). Keynote speaker at the Symposium "Towards filming macromolecular movies" during the ESRF users' meeting (Feb 7, 2024). Trainer at the Time-resolved macromolecular serial crystallography EMBL workshop (ESRF, July 8-12, 2024). Organizer of the XFEL session at the AUSE-ALBA users meeting (Sept 5, 2024). Keynote speaker at the AUSE-ALBA users meeting (Sept 2-6, 2024). Invited speaker at BIFI (Zaragoza, Spain) for giving a seminar on TR-SFX (Sept 27, 2024). Lead CSIC representative to the European XFEL, as part of the strategic plan for singular scientific infrastructures (Since 2024).

Martin Saleta - Member of the scientific committee of the XIX annual meeting of the Argentinean Crystallographic Association (Nov-2024). Vice-president of the Argentinean Crystallographic Association (Since Nov 2024). Secretary of the Argentinean Crystallographic Association (Nov 2021-Nov 2024). Adjoint secretary of the Latin-American Crystallographic Association (since 2023). Invited Lecture at Second Aldo Félix Craievich School on Conventional X-ray and Synchrotron Radiation Techniques for Materials Characterization (Aug 2024).

Miguel A. G. Aranda – Member of the SAC of ELETTRA (since 2023). Beamline review panel committee member for ID22 ESRF (powder diffraction) (May 2024). Organizer of CoDI workshop (one-day meeting satellite to the Spanish synchrotron user association meeting). CoDI will be the long coherent-based imaging BL at ALBA synchrotron (September 2024). Co-editor for Journal of Synchrotron Radiation (Since 2022). Invited webinar at the LNLS Users Group Seminar series (May 2024).

Nadia Zatsepin - Member of Crystallographic Methods Working Group for planning 4th gen synchrotron in Australia, Australian Synchrotron 2.0. (since 2024). Advisory Board member for Computational Structural Biology node (currently being established) with the Australian Biocommons (since 2024).

Robert Feidenhans'l - Chair of the Council at MAX IV (since 2023). Member of the SAC at ALS in Berkeley (since 2024).

Shin-ichi Adachi - Chair, Japanese Society for Synchrotron Radiation Research (October 2023- September 2025). Council member, Asia-Oceania Forum for Synchrotron Radiation Research (AOFSTR, January 2024-December 2026). Member, FXE Proposal Review Panel, European XFEL (since September 2019).

E. Granado, Chair

A24. Commission on XAFS

The Commission on X-ray Absorption Fine Structure (CXAFS) meets regularly, once a month. The meetings are very well attended, even when the timings are inconvenient for some members, as they often take place very early in the morning or very late at night due to the worldwide distribution of the membership.

The activities of the CXAFS in **2024** were primarily focused on implementing the actions agreed at the 2023 International Conference on Improving Data Quality and Quantity in XAFS Spectroscopy (Q2XAFS2023). This conference was organized jointly with the International XAFS Society and was held at the Australian Synchrotron (ANSTO) as a satellite meeting of the **26th Congress and General Assembly of the IUCr** in Melbourne. As agreed during the meeting, the proceedings of Q2XAFS2023 are being published in a special issue of Radiation Physics and Chemistry.

In **2025**, the Commission's activities have been largely devoted to the preparation of our participation on the **27th Congress and General Assembly of the IUCr**, to be held in **Calgary in August 2026**. We have been actively preparing a full-day workshop on **X-ray Absorption Fine Structure (XAFS)**, to be held on the 10th of August. The workshop will provide an introduction to XAFS principles and advanced techniques for crystallographers, as well as tutorials and hands-on training sessions focused on data analysis and statistical methods. Applications of XAFS in several cutting-edge research areas spanning the physical sciences, materials science, and chemical sciences will also be presented. To promote the participation of young and early-career researchers, the Commission is currently seeking **financial support from the IUCr to cover travel and subsistence costs**.

In parallel with the workshop preparation, the Commission has been highly active in ensuring strong representation at the forthcoming Congress through the nomination of keynote and invited speakers, as well as through the organization of numerous microsymposia (MS), either as the main organizer, co-organizer, or supporting commission. **Dr René Loredó Portales**, from the University of Mexico, has been selected as a keynote speaker. His nomination was proposed by the CXAFS and supported by both the Commission on Inorganic and Mineral Structures and the Commission on Structural Chemistry. The CXAFS is the **sole organizer** of two microsymposia:

- Catalysis for the Net-Zero Transition
- Structural Characterization of Amorphous Solids, Glasses, and Liquids (Disordered Materials)

Both microsymposia are supported by the Commission on Powder Diffraction.

In addition, the CXAFS is **sponsoring six further microsymposia** in collaboration with other IUCr Commissions:

- Compositionally Complex Materials: Challenges and Opportunities for X-ray Absorption, Pair Distribution Function, and Related Probes (co-sponsored with the Commission on Powder Diffraction)
- X-ray Spectroscopy: High Energy Resolution Methods (co-sponsored with the Commission on Synchrotron and XFEL Radiation)
- Spectroscopy Meets Imaging and X-ray Spectroscopy for Biological Systems (co-sponsored with the Commission on Biological Macromolecules)
- Magnetic Order in Complex Materials: Applications of Resonant and Non-resonant X-ray Spectroscopy (co-sponsored with the Commission on Magnetic Structures and supported by the Commission on Powder Diffraction)
- X-ray Spectroscopy, Neutron and Muon Methods in Art and Archaeology (co-sponsored with the Commission on Crystallography in Art and Cultural Heritage)

The CXAFS is also **co-sponsoring four additional microsymposia**:

- Sustainable Energy Materials for the Future: Local Structure (sponsored by the Commission on NMR Crystallography and Related Methods)
- Statistical and Computational Analysis in Crystallography and Spectroscopy (sponsored by the Commission on Crystallographic Computing)
- Crystallography and Spectroscopy in Sustainable Resource Management (sponsored by the Commission on Inorganic and Mineral Structures)
- Crystallography and X-ray Absorption Spectroscopy Machine Learning Methods for the Development of Materials (sponsored by the Commission on CommDat)

Collectively, these microsymposia reflect the wide range of scientific areas in which spectroscopy, and XAFS in particular, is making a significant impact on structural science.

The organization and co-sponsorship of these activities highlight not only the high level of engagement of the CXAFS, but also its strong integration within the IUCr and good working relationship with other Commissions. The extensive collaboration

with other Commissions demonstrates the versatility of spectroscopy as a structural probe, its complementarity to traditional crystallographic techniques, and its relevance to many of today's major scientific and societal challenges.

Finally, it is important to highlight that several papers in **IUCr journals** have been published by Commission members during the period under review, demonstrating their continued scientific engagement and active contribution to the activities of the IUCr.

S. Diaz-Moreno, Chair