

Appendix A. Reports of the Commissions for 2022

A1. Commission on Journals

Overview

	2017	2018	2019	2020	2021	2022
No. of submissions (all)	2685	2678	2424	2121	1802	1523
<i>without Acta E or IUCrData</i>	1694	1880	1732	1528	1495	1148
Rejection rate (%)	28	27	32	28	24	24
<i>without Acta E or IUCrData</i>	36	34	35	31	30	28
No. of published papers (all)	1880	1793	1710	1583	1373	1220
<i>without Acta E or IUCrData</i>	1047	1139	1153	1079	1015	865
No. of open-access papers (all)	1129	999	923	936	834	888
<i>without Acta E or IUCrData</i>	296	345	365	430	475	533
No. of pages (all)	11565	12473	12854	11819	11145	9644
<i>without Acta E or IUCrData</i>	8564	9856	10443	9539	9551	8065

The reports below summarize the major developments for each journal during 2022. Each report reflects the hard work and dedication of the respective Editorial Boards as well as the Managing Editors in Chester. Here, it is appropriate to make some general comments as well as preview a few highlights discussed further in the individual journal reports below.

The Journals Management Board (JMB) comprises the Main (Section) Editors of each journal, the IUCr Journals Commissioning Editors, as well as the Journal Managing Editors and other relevant Chester staff. Due to residual effects of the pandemic, the JMB continued to meet virtually up to July 2022 but a small group of experienced Editors met in person, together with the Editor-in-chief and Executive Managing Editor, immediately prior to the 2022 ECM in Versailles, France, after which it was agreed that full in-person annual JMB meetings should resume, starting with a March 2023 JMB meeting in Chester.

During 2022, virtual meetings of the individual journal Editorial Boards, involving the respective Main Editors and Co-editors, Commissioning Editors, Managing Editors, and sometimes the Editor-in-chief, became more established. The objectives of such meetings are to discuss individual journal development and scope, develop plans for commissioning Special Issues and Lead/Feature articles, discuss any problematic issues coming up in review, and to mentor new or less-experienced Co-editors, so that the entire Editorial Board can progressively develop a common understanding both of journal scope and how this should develop.

The international conditions for scientific journal publication, ongoing effects of the pandemic, as well as the new major conflict in Ukraine, have all presented major challenges for the IUCr journals during 2022, and the continuing fall in submissions is now a major concern. Despite these challenges, the IUCr journals have continued to hold their own in terms of quality research publications and impact factors, at the same time increasing the proportion of open access papers published across the journals. Several new initiatives started in 2021 and 2022 have continued to develop to engender new submissions and encourage the greater dissemination of open science and data. These are discussed in the individual journal reports, but we highlight here the first year of full open access for *Journal of Synchrotron Radiation (JSR)*. This has gone well with high-quality papers published and an initial decrease in submissions within projections.

In connection with the critical need to increase the number of high-quality submissions and published papers, a much greater focus is being placed on commissioning of papers and Special Issues. To this end, we are seeking new ways to empower all members of the journal Editorial Boards to work collegiately with the Commissioning Editors, Main Editors, and the Managing Editors, to bring in new papers, consistent with the respective journal scopes, and to consider new sections aimed at emerging new areas of the relevant structural sciences covered.

As such initiatives call for the appointment of new Main Editors and Co-editors, we will continue the IUCr's commitment to furthering diversity in new Editorial appointments, including diversity in geography, background and gender, subject to meeting the scientific scope, interest and range of expertise needs of each Editorial Board.

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

Reports by Commissioning Editors

Biology

Roberto Steiner finalised the virtual thematic issue on Room Temperature Biological Crystallography. The virtual issue consists of a total of 13 articles (12 research papers + 1 review): 4 papers from *IUCrJ*, 7 from *Acta D* and 2 from *Acta F*.

Roberto also wrote the foreword and assembled a cover picture for the issue.

R. Steiner, Commissioning Editor, Biology

Chemistry

Work continued on the commissioning of articles in the high-pressure, chemical crystallography, and crystal growth fields, and in crystallography of molecular materials and pharmaceuticals. Discussions were held with the Editors of *Acta B* on potential topics for new Special Issues and Lead and Feature Articles.

E. Boldyreva, Commissioning Editor, Chemistry

Materials, Methods and Instrumentation

Activities in 2022 included participation in Editorial Board meetings and discussions related to *IUCrData*. Two Special Issues are currently under consideration: one on machine learning in crystallography (*Acta A, JAC*) and an issue on 3D printing and additive manufacturing (*JAC*).

Th. Proffen, Commissioning Editor, Materials, Methods and Instrumentation

Acta Crystallographica Section A

	2017	2018	2019	2020	2021	2022
No. of submissions	93	150	115	94	90	81
Rejection rate (%)	40	29	38	35	34	38
No. of published papers	62	76	88	79	65	57
Research papers –						
Foundations	34	45	59	50	42	36
Advances	5	9	15	5	8	6
Short communications	5	2	0	4	2 (1 advances)	5 (1 advances)
Lead articles	0	0	0	2 (1 advances)	1	0
Feature articles	0	1 (advances)	0	0	1	0
Topical reviews	0	1	0	1 (advances)	0	0
Editorials	0	1 (advances)	1	0	1	0
Commentaries	3	0	1	2 (1 advances)	2	0
Abstracts	1864	1124	1217	227	1566	328
Other	15	0	12	15	9	10
No. of open-access papers	5	13	28	20	20	16
No. of pages	488	713	918	783	638	519
Average length (pages)	9.9	11.1	11.3	11.4	11.8	10.4

Average publication time (months)	5.6	5.7	6.1	6.2	5.8	6.0
Impact factor	7.9	1.9	2.0	2.3	2.3	
5 year impact factor	4.2	4.6	3.1	3.3	2.7	
Cited half-life (years)	>10.0	>10.0	>10.0	>10.0	8.2	

Acta Cryst. Section A publishes articles reporting advances in the practice and theory of all areas of structural science. As well as traditional crystallography, this includes nanocrystals, metacrystals, amorphous materials and quasicrystals. It also covers electron crystallography, diffuse scattering, pair distribution function studies, time-resolved XFEL studies, cryo-EM, tomography, small-angle scattering, coherent scattering, diffraction imaging, and the structure of strain and defects in materials. We also welcome contributions on advances in analysis tools that are foundational to crystallography, including descriptions and applications of methods, algorithms and software, and the use of emerging computational approaches such as artificial intelligence and machine learning as applied to structural science.

The journal has two sections: Advances and Foundations. Articles are selected for the Advances section based on their likely impact and broad interest. They benefit from rapid publication and may be highlighted by an accompanying scientific commentary, and tend to be our most read and most highly cited articles. A list of all the Advances papers we have published since the section was launched in 2014 can be found at <https://journals.iucr.org/a/services/advances.html>.

Some of the most popular articles we published during 2022 (based on number of downloads) were:

Towards a machine-readable literature: finding relevant papers based on an uploaded powder diffraction pattern. B. Özer, M. A. Karlsen, Z. Thatcher, L. Lan, B. McMahon, P. R. Strickland, S. P. Westrip, K. S. Sang, D. G. Billing, D. B. Ravnsbæk & S. J. L. Billinge (2022). *Acta Cryst. A* **78**, 386–394.

A finite difference scheme for integrating the Takagi–Taupin equations on an arbitrary orthogonal grid. M. Carlsen & H. Simons (2022). *Acta Cryst. A* **78**, 395–401.

Crystallographic phase retrieval method for liquid crystal bicontinuous phases: indicator-based method. T. Oka (2022). *Acta Cryst. A* **78**, 430–436.

Origin of irregular X-ray mirage fringes from a bent, thin crystal. T. Fukamachi & T. Kawamura (2022). *Acta Cryst. A* **78**, 422–429.

Identification of a coherent twin relationship from high-resolution reciprocal-space maps. S. Gorfman, D. Spirito, G. Zhang, C. Detlefs & N. Zhang (2022). *Acta Cryst. A* **78**, 158–171.

Objective crystallographic symmetry classifications of a noisy crystal pattern with strong Fedorov-type pseudosymmetries and its optimal image-quality enhancement. P. Moeck (2022). *Acta Cryst. A* **78**, 172–199.

A simplified relationship between the modified O-lattice and the rotation matrix for generating the coincidence site lattice of an arbitrary Bravais lattice system. H. Liu (2022). *Acta Cryst. A* **78**, 139–148.

The first of these papers, 'Towards a machine-readable literature', was the preliminary result of a project between Simon Billinge's research group and the IUCr, exploring the idea that the wealth of crystallographic data held by the IUCr could be used as the basis for literature searches.

Like many of the other IUCr journals, the number of open-access papers we publish has been increasing over the last few years. We have found that open-access articles are around 4 times as likely to be viewed, and almost twice as likely to be cited, as articles that are not open-access. Other things that can help to boost readership and citations are featuring the article in a scientific commentary (which can be particularly beneficial for the more theoretical or mathematical papers), highlighting it on the cover or the home page of the journal, tweeting about it from the journal's account @ActaCrystA, and featuring it in the *IUCr Newsletter* (<https://www.iucr.org/news/newsletter>).

An Editorial published in January 2021 (*Acta Cryst. A* **77**, 1) outlined some simple steps that authors could take to help maintain the relevancy, vibrancy and broader impact of the journal. These include making sure that the crystallographic context of the work is emphasized early on in the article (e.g. in the title, synopsis, keywords or abstract), thus making it clear who in the materials or structural communities will use it and what they will use it for. Throughout 2022 all our Co-editors and the staff in the Editorial Office have been encouraging authors to emphasize the broader context of their work, if necessary by requesting that this is done before an article is sent out for review.

We were very pleased to welcome two new Co-editors to the Editorial Board in 2022: Louise De Las Peñas from Ateneo de Manila University, Philippines, and Tatiana Gorelik from the Helmholtz Centre for Infection Research in Braunschweig, Germany. In addition, Vitaliy Kur-

lin (University of Liverpool, UK) has been acting as a Guest Editor, alongside Mois Aroyo, for a Special Issue on crystal lattices, which is now well under way. A Special Issue on machine learning (joint with the *Journal of Applied Crystallography*) is also still planned.

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

Acta Crystallographica Section B

	2017	2018	2019	2020	2021	2022
No. of submissions	175	168	201	168	162	115
Rejection rate (%)	34	43	32	31	28	30
No. of published papers	134	75	136	117	112	95
Research papers	118	63	120	107	102	81
Short communications	0	1	0	0	0	0
Lead articles	1	0	2	0	0	0
Feature articles	0	1	1	0	0	0
Topical reviews	0	3	1	0	0	2
Editorials	3	1	1	0	1	1
Commentaries	3	1	2	5	2	2
Other	9	5	9	5	5	9
No. of open-access papers	8	8	12	17	30	22
No. of pages	1199	744	1227	1147	1054	892
Average length (pages)	9.8	10.7	9.7	10.5	10.0	10.3
Average publication time (months)	5.7	5.0	5.2	4.6	4.5	4.7
Impact factor	6.5	6.7	2.0	2.3	2.7	
5 year impact factor	4.2	4.7	4.7	4.7	4.9	
Cited half-life (years)	>10.0	>10.0	>10.0	>10.0	>10.0	

In 2022 *Acta Crystallographica Section B* continued to publish six issues per year, the number of articles (pages) published in 2019, 2020, 2021 and 2022 being 136 (1227), 117 (1147), 112 (1054) and 95 (892), respectively. These numbers are highly dependent on the number and size of any Special Issues published in a particular year.

In 2022, a major concern for the journal was the impact of the war in Ukraine on the number of submissions from Poland and Russia, then the two largest sources of articles submitted to the journal, together accounting for around one-third of the total. So far, the proportion of submissions from these two countries has reduced but they are still the second and third highest: the main sources of articles in 2022 by author affiliation were France (12.9%), Russia (10.7%), Poland (8.6%), USA (8.2%) and Germany (8.0%). Articles in *Acta B* involved authors from 35 countries.

Over the period 2017–2022 the rejection rate has usually been around 30%, with one outlier of 43% in 2018, so the value of 30% for 2022 is typical. Recently the average article length has varied between 9.7 and 10.7 pages, despite several articles of around twice that length. In 2022 the average time between submission and publication (4.7 months) was in line with recent years. Although slightly lower in absolute terms than in 2021, the number of open access papers (22) still represents a significant fraction (23%) of the total published.

Except when we can publish exceptionally high-impact articles, the journal's base impact factor is around 2.0 and we expect a broadly similar value for 2022. In 2021 the impact factor was 2.7.

In June 2022 we published a Special Issue entitled *Structure Correlation and Dynamics in Crystals – a Tribute to Professor Hans-Beat Bürgi* (Guest Editors: Simon Grabowsky and Mark Spackman). A virtual Special Issue on *Chemical Aspects of High Pressure Crystallography* across *Acta B/C/D*, *JAC* and *JSR* (Main Guest Editor: Elena Boldyreva) is ongoing. We are very appreciative of the work of all our Guest Editors for their efforts in bringing about these Special Issues. Invited articles and commentaries are regularly sought from prominent scientists, including Keynote Lecturers at IUCr Congresses and Regional Associate Meetings.

The journal has been extensively supported by the Chester staff, especially our Managing Editor Amanda Berry: we wish to express our appreciation for all their help and advice.

A.J. Blake, M. de Boissieu and A. Nangia, Editors

Acta Crystallographica Section C

	2017	2018	2019	2020	2021	2022
No. of submissions	367	441	406	227	180	171
Rejection rate (%)	47	43	49	41	40	43
No. of published papers	178	234	197	143	105	96
Research papers	169	227	186	137	98	93
Feature articles	1	3	3	0	0	0
Topical reviews	2	0	0	0	0	0
Editorials	3	1	0	0	0	0
Commentaries	0	0	6	2	4	3
Other	3	3	2	4	3	0
No. of open-access papers	3	6	9	22	18	24
No. of pages	1159	1782	1697	1107	815	759
Average length (pages)	6.7	7.7	8.2	8.0	8.1	8.1
Average publication time (months)	2.7	2.9	2.8	2.9	2.8	2.7
Impact factor	8.7	0.9	0.9	1.2	1.2	
5 year impact factor	3.0	4.4	6.3	7.3	1.0	
Cited half-life (years)	9.2	3.9	4.8	5.8	6.8	

In 2022 *Acta C* continued its push towards being a journal with appeal not only to the broad range of structural chemists but also synthetic, computational and biological chemists. The page length has been maintained at just over eight pages per article, a result of the increased non-crystallography content.

The number of submissions has continued to decline since the start of the pandemic; however, the rate of decline has tapered off significantly (35% in 2019–2020, and 27% in 2020–2021 to 7% in 2021–2022) and hopefully this will stabilise or indeed we might see an increase in submissions in 2023. The rejection rate remains fairly stable at ca 40%, an analysis of rejected articles up to May 2022 shows that 17% returned and were eventually published in *Acta Cryst. C*, 9% were resubmitted to *Acta Cryst. E*, 31% were published elsewhere while the remaining 42% do not appear to have been published as of February 2023. The impact factor is expected to drop down to 0.7 this year.

A Special Issue was commissioned in 2022 entitled ‘Halogen, Chalcogen, Pnictogen and Tetral bonds: Structural Chemistry and Beyond’ with Guest Editors Lee Brammer, Anssi Peuronen and Thomas Rosaveare (University of Sheffield). The submissions are essentially complete (10) and the issue is expected to be officially launched in early 2023 with a Lead Article to take the form of a short Topical Review by the Editors. The ten papers have a healthy number of downloads with two being promoted as front covers.

The team of Co-editors have done an excellent job reviewing submitted manuscripts, selecting referees, accepting or rejecting the submissions and carrying out careful editing of the chemistry and crystallography. Co-editor retirements were Tong-Bu Lu, Chris Frampton and Eugene Cheung. Two new Co-editors have been appointed: Carol Hua (recently appointed at University of Melbourne, Australia) and Xiaoping Wang (Oakridge National Laboratory, US) who bring a combined expertise in synchrotron radiation and neutron diffraction. Amy Sarjeant and Alan Kennedy have been appointed as *Acta C* Section Editors, overlapping for one year with Paul Raithby and Larry Falvello, who retire in August 2023.

The review panel set up in 2016 has worked well and is constantly being revised to identify retired and/or non-responsive members. It is currently being expanded to include reviewers with expertise in specific areas outside crystallography. With the increased scope of material being submitted to *Acta C*, it has been recognised that many crystallographic referees do not have the necessary expertise to properly assess every aspect of a submitted manuscript. An increasing number of manuscripts report the results of DFT calculations and/or microbiological assays (being the most common) in addition to chemical synthesis and characterisation including NMR and mass spectrometry. It is hoped to build up a 'Panel of Experts' who can provide an assessment of non-crystallography content in submitted manuscripts when required. The panel of experts could be sourced from early-career researchers identified initially by Main/Associate Editors. There is a high degree of rigour in the assessment of the crystallography reported which is recognised by readers of the journal, a similar level of rigour should also be applied to the non-crystallographic content.

An Editorial Board meeting was held in February 2023. Items discussed included:

Handling of manuscripts: reviewing (identifying potential reviewers), and improving publication times.

Special Issues (suggestions included electron crystallography, crystal structure prediction, quantum crystallography).

Methods papers (e.g. Lead Articles discussing best practise in new or even commonly used techniques, e.g. micro-ED, quantum crystallography, handling disorder).

Promotion of *Acta C* as a broader chemical and structural journal (conference booths) and promotion of individual papers (social media: LinkedIn, Twitter).

Scope of the journal and having clear distinctions between *Acta E*, *Acta C* and *Acta B*.

The Main Editors would like to thank all the Co-editors and Review Board members, past and present, for their support of the journal. Finally, we wish to express our thanks to the Chester Editorial Office staff, who have maintained an outstanding professional standard throughout the recent turbulent times, and without whose hard work and dedication the journal would simply not exist.

L. R. Falvello, P. R. Raithby and J. White, Editors

Acta Crystallographica Section D

	2017	2018	2019	2020	2021	2022
No. of submissions	153	152	160	194	186	153
Rejection rate (%)	24	19	29	15	20	24
No. of published papers	105	120	112	129	146	129
Research papers	95	110	98	115	133	122
Feature articles	0	0	2	2	1	1
Topical reviews	1	0	1	1	3	2
Editorials	0	1	2	3	2	1
Commentaries	0	1	1	1	2	0
Other	9	7	8	7	5	3
No. of open-access papers	56	66	60	69	93	83
No. of pages	1030	1244	1147	1279	1623	1473
Average length (pages)	10.5	10.9	10.9	10.5	11.7	11.6

Average publication time (months)	4.9	5.6	4.9	4.7	5.4	4.9
Impact factor	3.1	3.2	5.3	7.7	5.7	
5 year impact factor	3.4	3.0	3.2	5.0	6.0	
Cited half-life (years)	7.7	8.7	9.6	>10.0	>10.0	

The *Acta D* impact factor reached 5.7 in 2022 indicating the continued impact of papers published in the journal. The five year impact factor is above 6. In 2022 there were 153 submissions, 33 lower than in the previous year. 129 of these were published, giving a rejection rate of 24%, slightly higher than for 2021 when it was 20%. Of those published, 122 were research papers compared with 133 in 2021 and 115 in 2020. As in 2021, 64% of the papers were open access. The average length of papers has gradually increased over the last few years and is now 11.6 pages.

During 2022 there was one Feature Article (*Native glycosylation and binding of the antidepressant paroxetine in a low-resolution crystal structure of human myeloperoxidase*), an introduction to the CCP4 Study Weekend virtual Special Issue, 2 Topical Reviews and 3 other papers (1 essay by C. Abad-Zapatero, an obituary of Mamannamana Vijayan and a review of the book *The secret of life: Rosalind Franklin, James Watson, Francis Crick, and the discovery of DNA's double helix*).

Special Issues continue to play a positive role for the journal, particularly those from the recurring series of annual CCP4 Study Weekends and CCP-EM symposia. As instituted last year, the timeliness of the papers is emphasised 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 papers for a Special Issue are available they are also collected into a 'virtual Special Issue'. One paper on high-pressure crystallography was also published.

The main editorial innovation introduced in 2022 is the mandatory submission, for review purposes, of data associated with new structures, to ensure IUCr journals maintain their position as a global exemplar for the FAIR publication of biological molecular structures. This initiative, led by *Acta D*, was progressed through enthusiastic collaboration with the *Acta F* and *IUCrJ* Editor teams, and will be communicated to the community at the IUCr Congress in Melbourne. New submission guidelines and more detailed descriptions of the minimum information required for publication using the major structural methods were developed and implemented in the submission portal by the Chester office.

There was a reduction in the length of time for publication from 5.4 months in 2021 to 4.9 months in 2022. We would very much like to reduce this still further, and to that end have this year shortened the standard time given to authors for submission of revised manuscripts from two months to one month.

At the launch of *Acta D*, there were fewer than 1000 structures deposited in the Protein Data Bank (PDB). Many folds were unknown and protein structure prediction was primitive, so experimental phasing methods were essential. Since that date, 99.5% of currently known macromolecular structures have been determined (thanks to structural genomics, improved methods and an expanding structural biology community) and protein structure prediction is now uncannily accurate. Many of the proteins that crystallographers would have struggled to crystallize, especially large complexes, can now be studied by cryo-EM. It is fair to say, then, that structural biology is now a relatively mature field, and that the new challenges are to be found in using it to gain an ever more sophisticated understanding of chemistry and biological processes. There are challenges in studying smaller samples, which can be achieved using more powerful synchrotron and XFEL sources. Different challenges are brought by larger samples, which can be addressed for instance using electron cryo-tomography to visualize cell sections. Dramatically improved time resolution can come from a combination of powerful sources and ultrafast detectors. At the same time, we are certain to see many advances coming from the birth of powerful machine-learning methods, such as those underpinning structure prediction algorithms like AlphaFold. We aim for *Acta D* to be at the cutting edge for reporting of these exciting developments.

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 and Editor-in-chief Andrew Allen. We are very grateful for their hard work, attention to detail and dedication.

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

	2017	2018	2019	2020	2021	2022
No. of submissions	551	506	497	438	307	269
Rejection rate (%)	15	17	20	16	7	11
No. of published papers	458	411	392	365	263	261
Research communications	456	408	392	362	262	252
Teaching and education	0	0	0	0	0	2
Editorials	0	1	0	0	0	1
Other	2	2	0	3	1	6
No. of open-access papers	458	411	392	365	263	261
No. of pages	1980	1929	1952	1875	1329	1288
Average length (pages)	4.3	4.7	5.0	5.1	5.1	5.0
Average publication time (months)	0.9	1.2	1.3	1.1	1.3	1.6

In 2022, the number of submissions decreased by approximately 12% compared to 2021 (while the number of publications has remained stable). This reduction follows the general trend of the *Acta* chemistry journals, which shows an average decrease of ca 15%. The journal continues to attract papers from across the world, and authors from 55 countries have published in *Section E* in 2022.

The top five countries were the USA (18.6%), Germany (12.1%), India (8%), Ukraine (6.3%) and Japan (5.7%). As could be expected, there was a decrease in the proportion of papers from Ukraine, which, however, remains in the top five contributors. *Acta E* remains the journal with the highest number of downloads among the IUCr journals (6.2 million out of a total of over 14.1 million; both these figures have increased compared with 2022).

The average publication time, which had increased to 1.3 months in 2021, has further slightly increased to 1.6 months. The average number of pages has gone from 5.1 to 5.0, but it remains within the trend of the past four years. Submitted papers usually describe two or more structures, often analysed with complementary techniques (UV-Vis, NMR, DFT etc.). The Section Editors identify articles that do not contain sufficient scientific discussion at the pre-screening stage; these are either transferred to *IUCrData* or resubmitted after the authors have improved the content.

Acta E is currently included in the Thomson Reuters Emerging Sources Citation Index and will receive an impact factor from summer 2023. In September 2021, a tribute Special Issue in conjunction with the *Journal of Chemical Crystallography* was dedicated to the memory of Jerry Jasinski, a long-time Co-editor for *Acta E*. The virtual issue, which was edited by David Manke and Matthias Zeller, was published at the end of 2022 and contains 19 publications.

The Special Issue on Modern Approaches and Tools for Teaching Crystallography edited by Graciela Díaz de Delgado and Sean Parkin, which has the scope of collecting papers that can be used as educational materials for young crystallographers and newcomers to crystallography, comprises to date 12 publications (see below); more submissions are expected in the next weeks.

- (1) Fábry, J. (2018). *Acta Cryst.* E74, 1344–1357.
- (2) Tan, S. L., Jotani, M. M. & Tiekink, E. R. T. (2019). *Acta Cryst.* E75, 308–318.
- (3) Clegg, W. (2019). *Acta Cryst.* E75, 1812–1819.
- (4) Spek, A. L. (2020). *Acta Cryst.* E76, 1–11.
- (5) Linden, A. (2020). *Acta Cryst.* E76, 765–775.
- (6) Parkin, S. R. (2021). *Acta Cryst.* E77, 452–465.
- (7) Foxman, B. M. (2021). *Acta Cryst.* E77, 857–863.
- (8) Zheng, S.-L. & Campbell, M. G. (2021). *Acta Cryst.* E77, 864–866.
- (9) Wouters, J. & Van Meervelt, L. (2022). *Acta Cryst.* E78, 874–879.
- (10) van Terwingen, S. & Englert, U. (2022). *Acta Cryst.* E78, 966–970.

(11) Milewski, M., Caminade, A.-M., Hey-Hawkins, E. & Lönnecke, P. (2022). *Acta Cryst.* E78, 1145–1150.

(12) Vinaya, Basavaraju, Y. B., Srinivasa, G. R., Shreenivas, M. T., Yathirajan, H. S. & Parkin, S. (2023). *Acta Cryst.* E79, 54–59.

We would like to express our thanks to our Co-editors for their dedication and their excellent work. We are looking for new candidates, keeping in mind gender balance and geographical spread, with a special focus on areas that are under-represented in the Editorial Board. In this respect, we have collected suggestions for Co-editors from South America and South Africa.

We have also discussed updating the Notes for Authors to better address the requirements of the journal. In particular, there is a need to more clearly differentiate between *Acta E* and *IUCrData*.

As always, we are grateful for the constant and excellent support that we receive from the staff in Chester, particularly Gillian Holmes, Sean Conway and Mike Hoyland, for their constant help and support, and Peter Strickland for their sound advice and expert guidance.

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

Acta Crystallographica Section F

	2017	2018	2019	2020	2021	2022
No. of submissions	196	200	122	98	97	70
Rejection rate (%)	41	34	32	26	26	29
No. of published papers	108	116	105	85	64	55
Research communications	106	113	95	76	48	48
Topical reviews	1	2	1	0	1	1
Editorials	0	1	5	3	1	0
Commentaries	0	0	1	0	1	0
Other	1	1	3	6	13	6
No. of open-access papers	22	28	16	27	23	31
No. of pages	713	824	757	623	483	422
Average length (pages)	6.7	7.1	7.4	7.5	7.8	7.9
Average publication time (months)	2.6	3.4	3.9	2.8	2.8	2.7
Impact factor	1.0	1.2	1.0	1.1	1.1	
5 year impact factor	0.7	0.8	0.9	1.1	1.1	
Cited half-life (years)	5.4	6.2	6.5	7.5	8.1	

Acta Cryst. F aims to be a fast and efficient venue for interesting structural biology communications, encompassing original research, Methods Communications and Topical Reviews about structural biology matters.

In observing the statistics, we note that last year open-access papers have increased as a proportion to over 50% of the papers published in 2022, but the total number of submissions and published papers has continued to decrease. Many other statistics have stayed constant over the last few years. The average publication time remains low at just under 3 months, thanks to efficient handling by Co-editors and quick but high-quality technical editing at the Chester office (Simon Glynn and Louise Jones). The average paper length is up slightly, but still just under 8 pages. The current impact factor remains at a similar level to the last four years at 1.1, having been at 0.5–0.7 prior to 2017. This is correlated to a rejection rate of 30% since 2015, which was around 10% before then.

No new Editors were appointed in 2022. It would be good to recruit two to three new Co-editors, including one with expertise in cryo-electron microscopy. The referee panel continues to function well. This group of about thirty experienced scientists have agreed to referee twelve papers a year each, to reply to requests promptly, and to return reports within two weeks.

For the future, we need to make more people aware of the broad structural biology subject range of the journal and attract more papers. We strongly believe that the low standard of peer review in high-volume open-access journals will lead authors back to high-quality scientific society journals, including *Acta Cryst. F*. The lowish impact factor is a barrier to attracting more authors. To improve the impact factor, John Helliwell has helped to commission Topical Reviews, and we hope to have a few more submissions of reviews in the near future. On the other hand, the expected more widespread adoption of the DORA principles (<https://sfedora.org/read/>) should lead to a waning importance of metrics like the impact factor and a higher profile of journals belonging to respected scientific societies like the IUCr.

There are also plans to increase the profile of the journal by creating poster (or other, similar) prizes to early career researchers which consist of a voucher for open-access fees for publication in *Acta Cryst. F*. We firmly believe that introducing the journal to younger researchers will cement its place in the community.

J. Newman and M.J. van Raaij, Editors

IUCrData

	2017	2018	2019	2020	2021	2022
No. of submissions	440	290	195	155	108	106
Rejection rate (%)	13	17	18	13	6	9
No. of published papers	375	243	165	139	94	95
Data reports	372	242	162	138	92	94
Raw data letters	0	0	0	0	0	2
Editorials	0	0	0	0	0	1
Other	3	1	3	1	2	0
No. of open-access papers	375	243	165	139	94	94
No. of pages	1021	688	459	405	265	291
Average length (pages)	2.7	2.8	2.8	2.9	2.8	3.1
Average publication time (months)	0.7	0.8	0.9	0.9	0.9	1.2

The number of papers submitted to *IUCrData* was virtually the same as in 2021 (106 compared with 108), as was the number of published papers (95 compared with 94 in 2021). This is the first time since the launch of the journal that there has not been a significant decline in the number of submissions compared with the previous year.

Submissions of *Data Reports* to *IUCrData* are handled by four Section Editors (Bill Harrison, Edward Tiekink, Luc Van Meervelt, Matthias Weil) and 12 Co-editors. Loes Kroon-Batenburg is the Section Editor responsible for *Raw Data Letters* and five new Co-editors have been appointed for this section: Miguel Aranda, Elena Boldyreva, Aaron Brewster, Simon Coles and John Helliwell. The average page length of a data article in 2022 was 3.1 pages and the publication time averaged 1.2 months: the highest proportion of data articles came from the USA (23%) followed by China (12%) and Germany (8%).

The plans for making a new section in *IUCrData* to accommodate the description of raw diffraction data have been effectuated. *Raw Data Letters* was officially opened with an editorial (L.M.J. Kroon-Batenburg, J.R. Helliwell & J.R. Hester) and a first *Raw Data Letter* in September. A second *Raw Data Letter* appeared in November. Official announcements were placed on the journal website and in the *IUCr Newsletter*. A *Raw Data Letter* requires the data to be archived in a repository that provides a persistent identifier (preferably a DOI). Together with the paper, an imgCIF is published that describes the (core) metadata, ensuring re-usability. Software for generating these was developed and is continuously being worked on. Importantly, in addition, tools to check for the consistency, completeness and validity of the imgCIF files, as well as the accessibility and readability of the raw data, are implemented in the journal submission workflow: the first instance of *checkCIF for raw data*.

As always, we are extremely grateful for the outstanding support that we receive from the staff in Chester, above all Gillian Holmes, and to Peter Strickland for their advice and guidance.

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

IUCrJ

	2017	2018	2019	2020	2021	2022
No. of submissions	133	138	147	151	117	105
Rejection rate (%)	34	33	38	41	41	32
No. of published papers	93	95	120	129	108	89
Research papers	52	75	94	100	79	62
Feature articles	4	1	1	1	3	0
Topical reviews	12	1	3	1	1	3
Research letters	7	5	6	8	6	5
Editorials	6	4	6	5	3	4
Commentaries	12	7	8	11	11	12
Other	0	5	2	3	5	3
No. of open-access papers	93	95	120	129	108	89
No. of pages	823	879	1133	1215	1034	791
Average length (pages)	10.8	10.5	10.7	10.8	11.2	11.0
Average publication time (months)	4.0	4.8	4.3	4.3	4.5	4.9
Impact factor	6.5	4.8	5.4	4.8	5.6	
5 year impact factor	6.6	5.4	5.7	5.8	5.4	
Cited half-life (years)	2.6	3.1	3.0	3.5	3.8	

The number of submissions to *IUCrJ* was down in 2022. However, 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.

The impact factor of *IUCrJ* increased to 5.6 in 2022. All submissions undergo preliminary screening by a panel consisting of the Main Editors (Dimitri Argyriou, Ted Baker, Richard Catlow, Henry Chapman, Gautam Desiraju, Sriram Subramaniam and Xiaodong Zou) and the Editor-in-chief (Andrew Allen), and this has helped to provide a rapid and efficient preliminary review process. 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. Such transfers are seamless and do not require any further work by the authors.

The six issues of *IUCrJ* published in 2022 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 105; a total of 89 papers were published with an average turnaround time of 18 weeks. Articles have been publicised in *IUCrJ*'s social media feeds and by other methods, with 12 articles highlighted *via* in-depth commentaries.

A total of 21 papers were published in the *Biology and Medicine* section of *IUCrJ* in 2022, representing approximately 24% of the total papers published. It is evident that the biological sciences are a major source of high-impact crystallographic publications, and it is important that this momentum should be maintained.

IUCrJ published 27 papers in the *Chemistry and Crystal Engineering* section in 2022 out of the total of 220 in this section since the inception of the journal in 2014. The contribution of this section has stabilized but we hope to encourage more papers in the MOF/COF area as well as papers in popular areas such as pharmaceutical cocrystals and polymorphs, including the events leading up to their crystallization. Submissions to the *cryo-EM* section of *IUCrJ* were slightly higher than in 2021, with 8 articles published in 2022. Cryo-EM publications continue to feature in the list of most read articles in *IUCrJ*, and are well cited.

The new section on *Electron Crystallography*, which will act as a home within IUCr journals for high-quality, high-impact papers in this field, published 6 articles in its first year.

The other sections of the journal, covering *Materials and Computation*, *Neutron and Synchrotron Science and Technology*, and *Physics and Free Electron Laser Science and Technology* have published 7, 10 and 9 papers, respectively, in 2022.

In 2022, 5 new Co-editors (Mauro Gemmi, Louisa Meshi, Peter Nellist, Jose Rodriguez and Junliang Sun) were appointed for the new *Electron Crystallography* section. Andrea Thorn (*Biology and Medicine*), Vanessa Peterson (*Neutron and Synchrotron Science and Technology*) and Garth Williams (*Free Electron Laser Science and Technology*) also joined the Editorial Board. We welcome all these new Co-editors to the journal.

The objective of *IUCrJ* remains to attract high-quality science papers of broad scientific significance from across all the scientific communities that use results obtained from diffraction methods. We hope that you will consider publishing in *IUCrJ* and, by doing so, help to further establish the journal as one of the mainstream comprehensive science journals.

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

Journal of Applied Crystallography

	2017	2018	2019	2020	2021	2022
No. of submissions	330	299	284	297	282	275
Rejection rate (%)	37	33	32	33	33	26
No. of published papers	211	201	146	188	202	175
Research papers	165	152	121	132	145	131
Short communications	4	5	4	4	7	6
Feature articles	0	1	0	0	1	0
Computer programs	18	20	21	26	23	23
Editorials	1	2	1	0	1	0
Commentaries	1	0	0	2	1	0
Other	22	21	0	24	41	15
No. of open-access papers	55	38	33	55	83	99
No. of pages	1852	1776	1468	1631	1902	1706
Average length (pages)	9.8	9.7	9.7	9.8	10.5	10.2
Average publication time (months)	5.2	5.5	5.6	5.7	5.8	6.1
Impact factor	3.4	2.9	3.0	3.3	4.9	
5 year impact factor	4.3	3.4	3.4	4.2	4.5	
Cited half-life (years)	>10.0	>10.0	>10.0	>10.0	>10.0	

Louise Dawe (Wilfrid Laurier University) joined the Editorial Board as an additional Teaching & Education Editor in early 2022, to complement the expertise of Juan-Manuel García-Ruiz in this strategically important area. As detailed in the Editorial to welcome Louise, the higher download statistics for such articles compared with those in other categories hint at their impact in the development of our future authorship. Jozef Keckes (Montanuniversität Leoben) also joined the Editorial Board following the retirement of Václav Holy (Charles University, Prague). We thank Václav and fellow retiree Dmitri Svergun for their superb editorial contributions and tireless support of the journal during the previous eight years. A search for additional Co-editors, particularly to extend the geographical reach of the journal, is ongoing.

The numbers of papers submitted to and published in the journal in 2022 are similar to the numbers over the previous three years. The publication time (~6 months) and paper length (~10.2 pages) have also remained fairly stable, while the rejection rate (~26%) has decreased somewhat. Notably, the impact factor (~4.9) has increased significantly, and the fraction of open-access papers has increased a further 16%. The rejection rate and the impact factor may be lagging indicators, but the trends hint at a general increase in quality of the published articles. It is too early to quote conclusive citation statistics for articles published in 2022, but it is notable that articles describing computer programs are those most downloaded.

Research papers and computer programs are the most numerous amongst the article types, with crystallographic techniques, instrumentation, and applications to specific materials continuing to dominate in research papers. Growing or emerging topics include coherent X-ray diffraction imaging, grain mapping using various techniques and the application of machine learning. Machine learning, which has been under consideration since 2020 as a cross-journal Special Issue, has grown considerably in the past two years, to the point that retrospective and educational articles could now be appropriate. Similar to the journal being seen as a natural home for articles on small-angle-scattering techniques, the journal is hosting an increasing number of articles on X-ray and neutron reflectometry instruments and techniques, even though reflectometry is often applied to liquid interfaces.

Editing of the virtual Special Issue on magnetic neutron scattering [Guest Editors Sabrina Disch (University of Duisburg-Essen), Sebastian Mühlbauer (Technical University of Munich) and Andreas Michels (University of Luxembourg), together with *Journal of Applied Crystallography* Co-editor Elliot Gilbert (Australian Nuclear Science and Technology Organisation)] was completed by the end of 2022, to be published in early 2023. The editing of a collection of select full-length research and software articles from the 18th International Conference on Small-Angle Scattering (SAS2022) [Guest Editors Florian Meneau (Brazilian Synchrotron Light Laboratory) and Jill Trehwella (University of Sydney), together with *Journal of Applied Crystallography* Co-editor Jan Ilavsky (Argonne National Laboratory)] is underway with publication expected in the second half of 2023.

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

Journal of Synchrotron Radiation

	2017	2018	2019	2020	2021	2022
No. of submissions	247	334	297	299	273	178
Rejection rate (%)	25	20	25	24	24	17
No. of published papers	156	222	249	209	215	169
Research papers	121	172	203	158	151	130
Short communications	6	6	10	14	9	4
Feature articles	0	4	0	0	0	0
Beamlines articles	13	17	27	23	39	19
Editorials	2	2	1	2	3	1
Commentaries	0	0	0	0	2	0
Other	14	21	6	12	11	15
No. of open-access papers	54	88	87	91	100	169
No. of pages	1300	1894	2096	1754	2002	1503
Average length (pages)	8.8	8.9	8.7	9.0	9.9	9.4

Average publication time (months)	5.6	5.6	5.7	5.3	5.3	5.3
Impact factor	3.2	2.5	2.3	2.6	2.6	
5 year impact factor	3.0	2.8	2.8	2.9	2.8	
Cited half-life (years)	7.1	8.0	7.8	8.1	8.0	

The number of published papers was 169 – down from 215 in 2021 and 209 in 2020. The number of published pages was 1503 – down from 2002 in 2021 and 1754 in 2020. Submissions were down to 178 from 273 in 2021, and the rejection rate fell to 17% from 24%. The virtual Special Issue on Actinide Physics and Chemistry with Synchrotron Radiation was finalised and the papers brought together in 2022, with the Foreword to the Special Issue published in the September issue of the journal. Proposed and developed by Main Editor Kristina Kvashnina, with help from Guest Editors Sergei Butorin, Shuao Wang and WeiQun Shi, the issue featured 20 Special Issue papers totalling almost 200 pages.

Regarding changes to the Editorial Board in 2022, Gerhard Grübel retired after 11 years on the board, and we were pleased to welcome Shelly Kelly of the Advanced Photon Source, USA, and Miguel Aranda of University of Malaga, Spain.

2022 was the year that JSR went fully open access. Thanks to all the groundwork put in during 2020 and 2021, the transition has been smooth on the whole. Submissions are down, but have been in line with Wiley's predictions for the first year of open access. There were increases in the proportion of papers from China, France and the USA, and decreases in the proportion of papers from Germany, Japan and Sweden. The top three countries for JSR were the USA (22%), France (14%) and Germany (13%).

We thank the readers of JSR for their continued interest and support, the authors for publishing in our journal, and the Co-editors for their great services to the journal and to the community.

Y. Amemiya, K. Kvashnina and D. Bhattacharyya, Editors

A2. Commission on International Tables

International Tables for Crystallography is a book series published by the IUCr in conjunction with Wiley. Nine volumes designated A (and A1) through H are currently in print. A substantial part of a tenth (I, on X-ray absorption spectroscopy and related techniques) is now available online. The *Brief Teaching Edition* has also been a part of the series; in 2021 it was replaced by a revision so extensive that it has a new name (*Teaching Edition: Crystallographic Symmetry*). The Symmetry Database is a related online resource.

While *International Tables* has long been a collection of printed books it has been transformed into an electronic resource. Parts of it became available online starting in 2006. The transition is advantageous because it allows more material to be included, makes it easier to correct or add material, and because it has financial benefits. Printed copies of some volumes (e.g., Vols. A and E) are, however, expected to remain available because so many users prefer a version that they can page through and annotate. An online version of the *Teaching Edition* is being developed.

The new style for chapters, new templates, and a new workflow developed in 2020 have allowed numerous early-view versions of chapters to be published before the volume (so far C and I) is complete. Online access to early-view material is especially appreciated by authors who complete their chapters promptly, and it helps the IUCr meet Wiley's annual target of 10% new or revised content.

The 2020–22 pandemic presented important challenges. The budgets of many institutional libraries have tightened. There is increased pressure for citations of an author's publications, which the series cannot, at least not yet, provide. The pressure on scientists to produce more "countables" has made it difficult to obtain reviews for long chapters. The suspension of in-person crystallographic meetings hindered the search for new editors. On the other hand the widespread take-up of video conferencing has allowed greater contact between editors and the Chester office.

The Chester office has been working hard to formulate how *International Tables* might evolve to meet the current challenges. Discussions with stakeholders took place starting in 2021 and continued in 2022.

During the ACA meeting in summer 2022 the Commission Chair had a long conversation with IUCr President Hanna Dabkowska about *International Tables*. The Executive Committee is very interested in the series being successful. There have been discussions of the future of the series, particularly of volumes other than those including symmetry tabulations and other reference data not conveniently available elsewhere (e.g., CIF standards).

Descriptions of activities during 2022 for the individual volumes follow:

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

In 2022 the Executive Committee decided that the 17 plane-group tables in Vol. A should become freely available because they are so important for crystallographic education. The change has been implemented. An article for the *IUCr Newsletter* was written announcing that

decision. The article also advertised for 2017 edition (the third) of Caroline MacGillavry's book *Symmetry Aspects of M. C. Escher's Periodic Drawings*, and for Danny Litvin's massive e-book compilation of magnetic (i.e., antisymmetry) groups.

Plans for the near future of Vol. A include the following.

(1) Online accessibility of the modified tables and texts of Section 1.6.4 of Vol. A; these are the so-called reflection-condition that include the "diffraction symbols" previously known as "extinction symbols". The corresponding modifications to the texts of Section 1.6.4, which were discussed in detail with the late Uri Shmueli, have also been approved.

(2) Implementation of the corrections/modifications/improvements of the texts in the online edition of Vol. A that resulted from the editing work on the *Teaching Edition*.

(3) Addition of the DOIs that appear in references in the html version of the Vol. A to the corresponding pdf versions.

(4) Possible modification of Chapter 3.1 of Vol. A on crystal lattices: Herbert Bernstein and Larry Andrews have expressed their interest in extending the discussion on lattices in Chapter 3.1. The new texts could be based on/related to the contributions to the Special Issue of *Acta Cryst. A* on crystal lattices that is currently being prepared.

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

An online version of the *Teaching Edition* is in preparation. A few sample pages are already accessible online on the *International Tables* website.

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

The work on the Symmetry Database of the online edition of *International Tables* and its *Teaching Edition* continued through 2022 within the framework of the project between the IUCr and the software company eFaber (Bilbao) and in collaboration with the Bilbao Crystallographic Server team. The teaching edition of the Symmetry Database gives access to all programs of the full database while limiting the sets of space and point groups to which the programs can be applied.

Main activities during 2022 were modifications of the contents, terminology, design, and layout of the data resulting from local checking and comments made by Ulrich Mueller. Apart from error corrections, there were some changes in a few of the Symmetry Database programs, namely:

(1) Extension of the set of possible monoclinic settings that are accessible online.

(2) Implementation of a step-by-step procedure in the programs studying the symmetry relationships between space groups.

(3) Further integration of *JSmol* (Robert Hanson, St Olaf College) for the visualization of the general-position positions and space-group diagrams.

Plans for the near future:

(1) Allow online access via the Chester servers to the updated Symmetry Database and its teaching subset.

(2) Further integrate *JSmol* to allow polyhedral representation of the general-position diagrams, especially for high-symmetry space groups; visualization of Wyckoff positions; and user introduction and visualization of symmetry operations that are not modulo lattice translations.

These improvements were discussed with Robert Hanson (*Jmol* Principal Developer) during their 2022 visit to Bilbao.

Vol. A1 (Symmetry relations between space groups; most recent online edition is dated 2011; Editor Ulrich Müller, who has retired)

Attempts to find a new Editor for Vol. A1 have not yet been successful but no revision seems to be needed at this time.

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

A major article on structure refinement by dual space iterative methods has just been accepted for Vol. B. An article on the three-dimensional pair distribution function is in the final stage of revision, as is an article on the theory of superspace.

Many of the chapters in Vol. B are timeless and so do not need revision.

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

Seven articles for the revised Vol. C (162 pages) have been put online. A substantial number of other articles are almost ready to be typeset. An article on free-electron laser science is nearing completion.

Focus is now shifting to revision of existing sections of Vol. C that have been deemed important to retain.

Vol. D (Physical properties of crystals; most recent online edition is dated 2013; Editor was the late André Authier)

Attempts to find a new Editor for Vol. D have not yet been successful but no revision seems to be needed at this time.

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

Programs that calculate layer groups and rod groups are ready to be made public. They will be accessible via the Bilbao Crystallographic Server during the first half of 2023.

A first version of software for inverse scanning tables is nearing completion. It allows the user to search for the space groups compatible with a specific layer group. The program is currently restricted to the standard settings.

The current description of the scanning tables is being reviewed with the aim of simplifying it.

The symbols of the subperiodic groups are being evaluated. The difference in the choice of axes (in layer groups the layer normal is always *c*) complicates the process of relating rod and layer groups to space groups.

A decision must be made whether to retain the scanning tables in the printed volume or to have them available electronically only.

Vol. F (Crystallography of biological macromolecules; most recent online edition is dated 2012; Editors Liang Tong, Eddy Arnold, and the late Michael Rossmann)

The Executive Committee and the staff in Chester have been working hard to find ways to get more exposure for articles written for *International Tables*. Exposure is a particular concern of the Editors of Vol. F, who find potential authors are unwilling to contribute unless their articles will be indexed by PubMed. The discussions have been delayed some by the retirement of the IUCr's main contact at Wiley.

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

Material relating to the current syntax, dictionary and dREL standards is essentially complete, and conformance of dictionary content to the DDLm standards is under review.

Revisions to the content of individual dictionaries will be made with the involvement of COMCIFS and relevant dictionary maintenance or development groups.

New material is being commissioned for the parts in which applications of the CIF standards in the fields of software, publishing and databases are discussed.

Technical editing of some chapters has begun. It is hoped that an inspection copy of a large portion of the volume will be available in time for the Melbourne Congress.

Vol. H (Powder diffraction; new volume in 2019; Editors Henk Schenk, who has retired, Chris Gilmore, who has also retired, and Jim Kaduk)

A new Co-editor has been identified but not yet appointed.

Plans have been made to fill several gaps in coverage and to replace a few weaker chapters.

Vol. I (X-ray absorption spectroscopy and related techniques; new volume; Editors Chris Chantler, Federico Boscherini and Bruce Bunker)

During 2022 articles for the new Vol. I were put online regularly (79 as of the last count). (The number is very large because articles in Vol. I are mostly much shorter than those in other volumes.) The editors of Vol. I have met to discuss how to tie up loose ends so that the volume can be completed.

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 home pages for the individual volumes (e.g., <http://it.iucr.org/A/>).

International Tables could not be the resource that it is without the talent and dedication of the staff in Chester. The skill of Nicola Ashcroft and Simon Glynn in turning authors' texts, and their often complicated tables into attractive pages in two formats (html and pdf) is remarkable. Nicola is also very effective in helping authors edit their texts for clarity, and in interacting with the volume editors. In addition they are an important part of the group that discusses the future of the series. The need to find a way to increase the exposure of articles written for the series has been discussed for years, but the matter became pressing in 2022 in connection with the revision of Vol. F. Developments have also shortened the timeline for making decisions about which volumes should remain available in print. Other staff in Chester also make important contributions to the series, but those of Simon and, especially, of Nicola are key.

C. P. Brock, Chair

A3. Commission on Aperiodic Crystals

The Commission (the CAC) continued to actively promote aperiodic crystallography, in organizing, supporting and promoting meetings, workshops and educational activities worldwide. It is worth noting a return to normality for the Commission in 2022 after the long pandemic episode; this recovery has resulted in the organization of the following recurring events that are a crucial part of the CAC's life.

The 5th International School on Aperiodic Crystals was held in Kutna Hora (Czech Republic), 23–27 May 2022. This International School is our central educational activity, with the objective of providing an overview of aperiodic order, of the basics of the mathematical description

of both modulated structures and quasicrystals, and of the physical properties and chemical understanding of aperiodic crystals. The number of participants (66, an in-person meeting) is a measure of the success of this edition.

The CAC also supported regular workshops, including the series of *ad hoc* workshops on *JANA2020* which continued to be organized by the Institute of Physics of Prague, Czech Republic; since the beginning of the pandemic, virtual workshops have been held.

In June 2022, the 10th edition of the conference on aperiodic crystals, Aperiodic2022, took place in Sapporo. Originally planned for 2021, it was postponed to 2022 due to the COVID-19 epidemic. Despite access restrictions to Japan leading to the conference to be organized in hybrid mode, Aperiodic2022 was a real success with around 150 participants. The International Congress on Quasicrystals (ICQ) originally planned for Tel Aviv in 2022 was postponed to June 2023 to avoid unfortunate overlap with Aperiodic2022. The next edition of the conference on aperiodic crystals, Aperiodic2024, is expected to be held in Caen (France) in 2024.

Finally, an important event in 2022 was of course the 33th European Crystallographic Meeting (ECM33), Versailles, France, 23–27 August 2022. The meeting had good coverage of aperiodic crystals, with two microsymbiosia directly related to aperiodic crystals.

O. Perez, Chair

A4. Commission on Biological Macromolecules

The Commission (the CBM) aims to support structural biology and macromolecular crystallography worldwide through scientific exchange, training, and promoting policies that encourage generating and disseminating knowledge and technologies.

(1) The activities of CBM representatives Diana Tomchick, Andrea Dessen, and Atsushi Nakagawa related to the IUCr Congress Programme Committee were described in the previous report. Our representatives worked diligently to curate the best possible programme for the upcoming IUCr Congress in Australia. Unfortunately, their work, as well as the continued efforts of the CBM Chair, continued until the end of March 2023. Several individuals declined invitations to be session Chairs, necessitating some persuasion to encourage participation in Australia. The number of abstracts submitted to each session ranged from 89 to 4, making it necessary to reallocate some abstracts to less popular sessions. The abstract review process was time-consuming, prompting our proposal for the IUCr to adopt the Oxford system for abstract submission in the future, as it has proven to be effective and user-friendly for abstract submitters. The CBM Chair expresses concern that cryo-EM and AlphaFold2 did not receive a substantial number of abstracts, and the low attendance from North America does not adequately reflect the region's contributions to the field of structural sciences.

(2) Efforts are underway to improve the impact factors (IFs) of the IUCr's journals. Scientists now have equally easy access to *Acta Cryst. D*, *IUCrJ*, *Nucleic Acids Research*, and journals like *Nature* or *Science*. The CBM Chair has been in contact with several authors who submitted hot papers to bioRxiv and had to wait for one year for their publication. Unfortunately, it appears that the IF of a journal still holds more importance than the timely publication of hot papers. Two important papers remained in bioRxiv for a year before being published in a peer-reviewed journal. A recent analysis of the top 100 cited papers reveals that the impact factor of a journal does not necessarily determine the number of citations. As previously discussed, two critical factors are the time between paper submission and publication, and the careful selection of keywords. The publication time has improved, especially for the IUCr journals. Keywords should be reviewed diligently not only by reviewers but also by the paper's Editor. Authors should be encouraged to use modern and engaging ways to share their results, such as presenting structural results using rich internet applications [e.g., Porebski *et al.* (2020). *Protein Sci.* **29**, 120–127]. Additionally, authors should inform their respective institutions' press release offices about papers that may be of interest to the public. The IUCr should further promote TV/radio interviews and notes in the popular press about significant structural achievements.

(3) Another issue of concern is the large discrepancy between the title of a paper and the title of the corresponding Protein Data Bank (PDB) deposit, which can be misleading for biomedical researchers searching the PDB. Commission members and other crystallographers interested in data depositions have been engaged in discussions about standards for the PDB that would make the information more understandable for non-structural biologists who use the PDB. The COVID-19 pandemic accelerated the development of quality standards, as several groups have been closely monitoring the quality of COVID-19-related structures [Croll *et al.* (2021). *Biophys. J.* **120**, 1085–1096]. Classification of common problems in macromolecular structures was described by Grabowski *et al.* [*IUCrJ* (2021), **8**, 395–407]. It is worth noting that the classification may vary depending on the viewer's perspective, e.g. whether a crystallographer or a biologist. For example, non-standardized cell placement should be avoided as it can make comparing two or more similar structures challenging for scientists without a crystallography background. Additionally, the occupancies of water and metals should be carefully examined as they can mislead biomedical researchers.

(4) Following the suggestions from CommDat and the CBM, since September 2021 the PDB has implemented a policy to include the structure PI/Contact Author (aka Depositor-of-Record) name, e-mail address, and ORCID ID in the metadata of the deposited structure in the public PDBx/mmCIF files. Providing the ORCID ID etc. for the PI/Contact Author (aka Depositor-of-Record) has been mandatory since 2018 (providing ORCID IDs for other entry authors remains optional). Approximately 99.99% of PDB structures deposited in 2022 comply with PI/Contact Author information requirements. The CBM and the IUCr should encourage all authors of manuscripts and PDB deposits to provide their respective ORCID IDs.

(5) The IUCr should advertise resources like Proteopedia as a great resource for undergraduate, graduate students, and biologists. The Proteopedia page on the lifecycle of SARS-CoV-2, created by Raimond Ravelli and Kévin Knoops, provides a detailed description of the virus's lifecycle and the role of its proteins. 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). A very nice animation was also put together by PDB.

Meetings, workshops, and other outreach activities

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

W. Minor, Chair

A5 Commission on Crystal Growth and Characterization of Materials

In the summer of 2022 two meetings which were awarded support by the IUCr through recommendation by our Commission (the CCGCM) were held. These were the Third European School on Crystal Growth (ESCG3, 20–23 July) and the Seventh European Conference on Crystal Growth (ECCG7, 25–27 July) held in Paris, France. These meetings saw good participation by members of the CCGCM with participation at all levels. A meeting of the IOCG was also held during the above conference, with many attendees.

The members of our Commission were called upon to put forward suggestions for microsymbiosia (MS) to be included in the IUCr 2023 Congress in Melbourne, and many suggestions were forthcoming. Geetha Balakrishnan, as Chair of this Commission, represented it at the International Programme Committee (IPC). The IPC met in April 2022, with the meeting being a hybrid one, with participants based in-person in Prague/Melbourne, as well as online (by Zoom). Of the several MS put forward by our Commission, 3 were chosen for inclusion in the programme:

MS41: Crystal growth for emerging technologies – from medicine to semiconductors;

MS 42: Quantum materials; and

MS43: Crystal growth and characterization of biominerals and biomimetics.

Our Commission also put forward several suggestions for Plenary as well as Keynote speakers, and I am glad to report that one of our members, Dr Elias Vlieg, was chosen as a Keynote speaker for the IUCr 2023 Congress.

The Commission received a number of requests from conference and workshop organisers for financial support for early career researchers. Positive recommendations for support from our members were recorded and submitted to the IUCr for sponsorship for Hot Topics in Contemporary Crystallography 5 (HTCC5), Croatia, April 2023; The International Conference on Biological Crystallisation (ISBC 2023), Granada, May 2023; and The International Conference on Crystal Growth and Epitaxy (ICCGE-20), Naples, July–August 2023.

The members and consultants of the Commission have not met in person since before the COVID-19 pandemic and we look forward the upcoming meetings and conferences, which will enable us to meet. The main events in which members of our Commission will be actively participating at all levels (as organisers as well as delegates) are the ICCGE-20 in Naples, Italy, the 18th International Summer School on Crystal Growth in Parma, Italy, followed by the IUCr 2023 Congress, Melbourne, Australia. We intend to hold a meeting of the Commission members and consultants in Melbourne, to discuss our way forward and our plans for hosting and organising events for our community in the immediate future.

G. Balakrishnan, Chair

A6. Commission on Crystallographic Computing

In 2022, the Commission had no changes in membership. The Commission was involved in preparing the programme for the 2023 IUCr Congress in Melbourne. Our member of the Programme Committee is Santosh Panjekar. In 2022, the Commission started organizing a computing school, which will take place at the Australian Synchrotron in Melbourne, 19–22 August 2023, as a satellite to the IUCr Congress. The school organizers are Santosh Panjekar, Yogesh Khandokar and Martin Lutz. The school is intended for method developers and programmers in all fields of crystallography. During the IUCr Congress the Commission will also have a Software Fayre, where software authors can give tutorials and show the latest features of their programs. The Software Fayre will run in parallel to the microsymbiosia and will be chaired by Santosh Panjekar and Martin Lutz.

M. Lutz, 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 Chair of the IUCr/OUP Book Series Committee, the Chair of the Commission on Crystallographic Teaching, the Chair of the Committee for the Maintenance of the Crystallographic Information File Standard, and both the IUCr President and General Secretary. In 2022 the number of members was 51. There were also two appointed consultants.

Nomenclature Problems. The Commission's web page invites crystallographers to bring nomenclature problems to the attention of any Commission member. No new matters were brought forward in 2022.

Online Dictionary of Crystallography (the ODC); Editor 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.

The ODC has been a continuing source of frustration. Only a few people seem to be interested in contributing to it. Attempts to get the IUCr Commissions to submit definitions have, with a very few exceptions, been unsuccessful. There is some disagreement about how authoritative the ODC should be considered to be. Although the ODC is run as a wiki, it is clear that the role of its Editor in maintaining its quality is very important.

Other. During 2022, when responding to a question about terminology, the ideas of starting a section of the CCN web page giving answers to Frequently Asked Questions was proposed. Examples of such questions are:

Why are two settings with different unique axes given for many of the monoclinic space groups?

Why are two different sets of axes given for the rhombohedral space groups?

What is the difference between a chiral space group and a Sohncke space group?

This idea, which has been discussed with several people, will be considered further during 2023.

C. P. Brock, Chair

A8. Commission on Crystallographic Teaching

The CCT spent most of its time this year preparing for the IUCr 2023 Congress and reviewing proposals for workshops. New members and consultants were added, and the CCT submitted multiple letters of support for workshops. The CCT did not meet virtually in 2022; communications were via e-mail and the IUCr listserv. The CCT will jointly host some sessions at the Congress in Melbourne.

O. A. Asojo, Chair

A9. Commission on Crystallography in Art and Cultural Heritage

The CrysAC Commission continues to pursue the mission of spreading crystallographic knowledge related to artworks and ancient materials.

6th CrysAC Workshop: Micro- and nano-diffraction for cultural heritage

Continuing the successful series of the CrysAC Workshops, the Commission organized the 6th Workshop as a satellite event to the 33th European Crystallographic Meeting (ECM33) in Versailles, France (<https://www.ecm33.fr/satellite-meetings>). The workshop (<https://www.ecm33.fr/crysacworkshop>), chaired by Gilberto Artioli of CrysAC and Partha Pratim Das of Nanomegas, focused on the more recent advances in micro- and nano-diffraction of applications to cultural heritage materials. Some of the leading scientists in the field were invited and contributed to an extremely lively and dynamic workshop, held in the lecture room of the C2RMF laboratories of the Louvre, Paris. The workshop really showed how state-of-the-art diffraction techniques, including electron diffraction and use of the new generation of synchrotron beamlines, may open new perspectives in cultural heritage research.

The workshop was attended by about 30 people. F. Vanmeert and co-workers, Silvie Švarcová and Patrick Ravines of CrysAC contributed to the meeting with excellent presentations.

33rd European Crystallographic Meeting (ECM33)

The CrysAC Commission played an active role at the ECM33 Meeting held in Versailles, France, 23–27 August 2022. The meeting was the first time in person after the pandemic period of 2020–2021.

MS-43 Crystallography for cultural heritage materials (<https://hopscotch.key4events.com/schedule-overview.aspx?e=281&agenda=1&date=20220827>) was co-chaired by Silvie Švarcová (ALMA Laboratory, Czech Republic, and CrysAC member) and Victor Etgens (IPANEMA, France). K. Janssens of CrysAC contributed an invited paper.

First training courses for applications of synchrotron light in archaeology and cultural heritage studies

This event, held in Istanbul, Turkey, 18–19 March 2023, was organized by TENMAK (Türkiye Enerji, Nükleer ve Maden Araştırma Kurumu: Turkish Energy, Nuclear and Mining Research Council), see <https://www.tenmak.gov.tr/giris-introduction.html>. The audience of about 100 people were half on site, half attending remotely, most being Turkish archaeologists and heritage workers. The programme encompassed presentations from beamline staff (SESAME, ELETTRA, ESRF) and from senior archaeologists and expert synchrotron radiation (SR) users. Time was also dedicated to training future users in carrying out SR experiments and writing proposals. The main objective was to make heritage workers from Turkey more aware about the capabilities offered by SR facilities.

43rd International Symposium on Archaeometry

Several contributions from CrysAC members were presented at the 43rd International Symposium on Archaeometry (ISA 2020/2022) held in Lisbon, Portugal, 16–20 May 2022 (<https://www.isa2020-lisboa.pt>). This is a very important meeting for the archaeometric community, involving both archaeology and conservation.

International Symposium: Crossroads: data-driven talks on ancient materiality at the interface of archeology, science and engineering

Gilberto Artioli delivered an invited seminar titled “An Integrated Diagnostic and Valorization Project for UNESCO Sites: The Case of the Terme del Sarno, Pompei” at this International Symposium, held at the Museo Egizio, Torino, Italy, 3 June 2022.

Molecular Transformations in Oil Paint

At this event, held 16–17 June 2022 in Paris, France, Silvie Švarcová (ALMA Laboratory, Czech Republic, CrysAC) delivered a lecture, and Marine Cotte (ESRF, France, CrysAC), Frederik Vanmeert (University of Atwerpen, Belgium – Koen Janssens' group) and their co-workers presented work within the Historical Materials BAG (block allocation group) and numerous results from the investigation of Dutch painted artworks.

Structure 2022 – The colloquium of the Czech and Slovak Crystallographic Association (CSCA)

Silvie Švarcová (ALMA Laboratory, Czech Republic, CrysAC) presented a lecture “XRPD as a powerful tool for study of painted artworks” and attended the assembly of the CSCA, 20–23 June 2022, Tábor, Czech Republic.

Exhibition: Rises and Falls of Portrait Miniature

This event, held in Chomutov, Czech Republic, 25 June – 24 September 2022, was organised by the ALMA Laboratory and presented to the public results of the scientific project focusing on non-destructive analysis of portrait miniatures from the Czech collections. The impact of the detailed material investigation on authentication of these subtle pieces of arts was documented by numerous examples. An illustrative film ‘Technique and history of miniature paintings’ complementing the exhibition is available at <https://www.iic.cas.cz/homepage/video/>.

School of XFEL and Synchrotron Radiation Users

Silvie Švarcová (ALMA Laboratory, Czech Republic, CrysAC) delivered an invited lecture “XRPD and EDS for analysis of paintings”, 6–10 November 2023, Liptovský Ján, Slovakia.

Quasicrystals: State of the art and outlooks

Emil Makovicky presented a lecture at the Quasicrystals conference at Accademia dei Lincei, Rome, Italy, 18 November 2022, titled “Quasicrystals and Art: Interesting new facts”.

The Historical Materials BAG event

Following the workshop organized in January 2020 at the ESRF for the cultural and natural heritage community, access to a ‘historical materials BAG’ was discussed (<https://www.esrf.fr/BAG/HG172>). After one year of operation, it was important to get scientific feedback from the BAG partners and to discuss ways to further improve this process. The 2-day event, held in Grenoble, France, 5–6 December 2022, was a clear success. 23 persons attended, most of them being PhD students from all over Europe. The first day was dedicated to scientific presentations (PhD students and beamline scientists). On the second day, a training course on the *FullProf* software was given by Gilles Wallez, Chimie Paris, and was very well received by the participants.

ERASMUS+ project 'Building Power Skills through ART'

Alicia Rafalska of CrysAC participated in the Erasmus Action: Cooperation partnerships in higher education.

26th Congress and General Assembly of the IUCr, Melbourne, 2023

The Commission at present is actively involved in the organization of microsymbiosia and keynote lectures for the 26th Congress and General Assembly of the International Union of Crystallography, 22–29 August 2023, Melbourne, Australia.

CrysAC website

The Commission is responsible for updating the CrysAC website at <http://www.iucr.org/resources/commissions/crysac>.

G. Artioli, Chair

A10. Commission on Crystallography of Materials

Organizing conferences and symposia

Yury Gogotsi organized the 23rd Annual Conference on Materials Science, <https://www.mrs-serbia.org.rs/index.php/youcomat/youcomat-2022>, Herceg Novi, Montenegro, 29 August – 2 September 2022. Number of participants: ~160.

Changqing Jin was a Committee Member of Nature Conference “Frontiers of High Pressure Research Science under Extreme Conditions”, 21–23 November 2022, a hybrid of online and on-site attendance, Shanghai, China. Number of participants: 300.

M. Fantini organized “X-rays of oral vaccines”, Brazilian Workshop of Engineer Physical Science, Lorena, SP, Brazil, 9–11 November 2022. Number of participants: ~100. They also organized the Workshop XVII Reunion of the Argentinian Crystallography Association, Cordoba, Argentina, 2–4 November 2022. Number of participants: ~120.

Disseminating knowledge and technical skills

Yury Gogotsi organized the MXene Course – a 5-day online workshop, offered twice in 2022, <https://nano.materials.drexel.edu/mxene-course/>. Number of participants: ~60 in each session.

Artem Oganov: “Modern Trends in Computational Materials Discovery” (Isfahan, Iran, 17–21 November 2022): <https://qsm.iut.ac.ir/workshop-iutuspe>. Number of participants: ~80. Also “Computational Materials Discovery and Thermoelectric Materials”: https://uspexteam.org/en/uspex/online_courses, 3 October – 8 November 2022.

A. Abakumov: VII International School–Conference of Young Scientists in Topical Issues of Modern Electrochemistry and Electrochemical Materials Science, Skoltech, Moscow, 18–22 November 2022, <https://crei.skoltech.ru/cest/conference-of-young-scientists-2022/>. Number of participants ~50.

Changqing Jin, Chair

A11. Commission on Diffraction Microstructure Imaging

This year (2022) was the first full year of operations for the Diffraction Microstructure Imaging (DMI) Commission. This year saw advances on several fronts. First was the formation of sub-committees associated with physical standards for DMI techniques, code standards for data reporting, and outreach for increasing the inclusiveness and size of the DMI community. The physical standards committee has begun fabricating test specimens to be circulated across instruments around the world, the code standards committee has begun developing a best-practices document, and the outreach community has developed a web platform for young researchers to ask questions and connect with more senior practitioners.

Also during 2022, the DMI Commission hosted a hybrid workshop on 25–26 June in Washington DC, USA. The workshop had in-person and virtual attendees from around the world. Over 50 attendees heard 8 invited talks (with focuses on machine learning, coherent techniques, and high-pressure) and 8 contributed talks, along with discussions of Commission business. The workshop also had a special session that provided young DMI practitioners with the opportunity to give invited talks that were selected by the outreach sub-committee. Maintaining momentum is a goal of next year. A major Commission goal for the upcoming year is to develop a DMI ‘taxonomy’ giving a broad overview of DMI techniques and developing a standardized nomenclature.

D. Pagan, Chair

A12. Commission on Electron Crystallography

The major goals of the Commission on Electron Crystallography (the CEC) are the teaching, promotion and development of electron crystallography science.

During our meetings in 2022 most of the discussion was focused on the organization of the next IUCr Congress in Melbourne. The CEC endorsed H. Xu for the organization of an electron crystallography school in Melbourne as a side event of the IUCr Congress. The CEC also discussed the issue of CIF standardization of electron diffraction data and agreed to open a discussion about that within the IUCr.

The CEC called for and collected nominations for the Gjønnnes Medal in Electron Crystallography 2023. The Chair set up a committee for the evaluation of the nominations, which successfully selected the winner, Jian-Min Zuo, by the end of the year.

Activity in workshops and schools for teaching electron crystallography

Several members and consultants of the CEC participated in the organization of the Electron Crystallography School, 29 August – 1 September 2022, a satellite to ECM33 held in Caen, France, and proposed by Philippe Boullay. The school covered diverse theoretical and practical aspects of the 3D electron diffraction technique (3DED/microED) and its application to structure determination of nano/microcrystalline materials of different classes – from inorganic, to organic and biological compounds. The school was attended by 47 students.

Ute Kolb (consultant) gave a lecture on “3DED crystal structure solution of Ca-acetate hemihydrate from marble relief corrosion” at the 6th CrysAC workshop on “Micro- and nano-diffraction for cultural heritage”, C2RMF, Porte des Lions, Palais du Louvre, Paris, France, 23 August 2022. This was a satellite event of ECM33, attended by 40 participants, and included lectures by scientists from research institutions, museums and conservation bodies in order to illustrate state-of-the-art applications of diffraction techniques to cultural heritage problems.

Mauro Gemmi (Chair) gave a lecture on 3D electron diffraction at the Summer School on Neutron, Electrons and X-ray Techniques, held at the Universidad de Almeria, Spain, 20–22 July 2022. Around 50 students participated in the school, which was organized by the Spanish Society on Neutron Techniques.

Tatiana Gorelik (member) gave a lecture on “Crystallographic structure analysis with X-rays and electrons – common concepts, major differences” at VINCI – Interdisciplinary International Silesian Summer School, 4–22 July 2022, University of Silesia in Katowice, Poland.

Joke Hadermann (consultant) gave a lecture on "Conventional electron diffraction and 3DED" at the 6th Stanisław Gorczyca European School on Electron Microscopy and Tomography, 12–15 July 2022, Krakow, Poland.

Karla Balzuweit (member) participated with Rodrigo Prioli Menezes, Paula Mendes Jardim, Daniel Baptista Lorscheiter and Mauro Gemmi (Chair) in the organization of X Micromat (<https://www.sbpomat.org.br/20encontro/flyer/download.php?id=1060>), a symposium of the Brazilian Materials Society Meeting (SBPMat), where Kayla Nguyen gave an invited lecture about the new EMPAD detector with high dynamic range and its application in electron diffraction. The event was part of the XX Brazil MRS Meeting held in Iguassu Falls, Paraná, Brazil, 25–29 September 2022.

M. Gemmi, Chair

A13. Commission on High Pressure

In 2022 the Commission on High Pressure (the CHP) participated in the following activities.

(1) The CHP has taken part in the work of the Melbourne IUCr 2023 Congress International Programme Committee. Two keynote lectures and three microsymbiosia proposed by the CHP were accepted: High-Pressure Quantum Crystallography (co-sponsored by the Commission on Quantum Crystallography), High-Pressure Diffraction in Designing and Understanding Functionality, and Diffraction Studies in Dynamic Compression Experiments. The CHP also co-sponsored four microsymbiosia proposed by other Commissions.

(2) The 56th Course of the International School of Crystallography was held in Erice, Italy, 3–11 June 2022, under the title “Crystallography under extreme conditions: the future is bright and very compressed”. The CHP Chair was one of the co-directors of the School, while several CHP members (Stephen Moggach and Narcizo Marques Souza-Neto) and consultants (Agnès Dewaele, Andrzej Katrusiak and Yongjae Lee) were among the lecturers and tutors. An extensive report of the School was published in the *IUCr Newsletter*, see https://www.iucr.org/news/newsletter/etc/articles?issue=155020&result_138339_result_page=19.

(3) The 2022 IUCr High-Pressure Workshop was held 6–10 December 2022 at Argonne National Laboratory, USA. The local team consisted of Vitali Prakapenka (GSECARS/University of Chicago), Stella Chariton (GSECARS/University of Chicago), Dongzhou Zhang (University of Hawaii/GSECARS) and Yanbin Wang (GSECARS/University of Chicago). The workshop attracted more than 200 participants, including almost 100 on-site attendees. A detailed report of this workshop will be published soon.

(4) The CHP has maintained close ties with the IUCr Committees CommDat and COMCIFS, especially in the initiative of the high pressure CIF dictionary.

K. Dziubek, Chair

A14. Commission on Inorganic and Mineral Structures

As face-to-face meetings and workshops began to return in the aftermath of the pandemic, members and consultants of the Commission (CIMS) were active across their national and related international communities. Of particular relevance is that 2022 was proclaimed the International Year of Mineralogy (IYM) by the International Mineralogical Association (IMA), and this was supported by the United Nations and formally approved by UNESCO. It was celebrated as part of the UN International Year of Basic Sciences for Sustainable Development, IYBSSD2022.

Michele Zema was a member of the Steering Committee for IYM, and is chairing a microsymbiosium at the 26th IUCr Congress on “The Future of Mineralogy: events and outcomes of the Year of Mineralogy 2022”.

Anna Gaġor was one of the organisers of the 63th Polish Crystallography Meeting, which took place 29 June – 1 July 2022. It was an online meeting, free of charge for all participants, with 21 lectures (10 male and 11 female speakers) and 69 poster presentations. This year the conference was accompanied by a workshop on powder diffraction.

Màrius Ramírez Cardona was a member of the Organizing Committee of the XI National Congress of the Mexican Society of Crystallography (SMCr), 30 November – 2 December 2022, held at the UAEH Mineralogy Museum to celebrate the International Year of Mineralogy.

K. Byrappa was elected Vice President of the Indian Crystallographic Association from 2023.

Emma McCabe is chairing a microsymbiosium at the 26th IUCr Congress and taught at the British Crystallographic Association Physical Crystallography Group’s 2022 Intensive Postgraduate Summer School.

Giovanni Ferraris and Roberta Oberti coordinated the official iYBSSD meeting “Mineralogical sciences and materials for a sustainable development”, held at the Accademia delle Scienze in Turin, Italy, 24–25 May 2022. Roberta Oberti edited a book derived from this meeting, which is presently in press as *Quaderno dell’Accademia delle Scienze di Torino*, Vol. 41, and will also be distributed as an e-book.

Giovanni Ferraris and Roberta Oberti are members of the Organising Committee for the meeting “Minerals as treasure trove for scientific discoveries” at the Italian National Academy of Lincei, Rome, Italy, 15–16 February 2024.

Isabella Pignatelli proposed two symposia at IMA2022 (Lyon, France, 18–22 July 2022): “Haüy 200 Years On: What News In Gem Research?” (chairing three sessions) and “Serpentinites and Beyond”.

Massimo Nespolo taught at the school “Analyse Structurale par Diffraction des Rayons X sur Monocristal et Applications” (France, 3–7 July 2022), the tenth “Training Course in Symmetry and Group Theory” (Tsukuba, Japan, 22–26 August 2022) and the 2022 “Spring Festival Crystallographic School and Workshop on Crystal-Field Applications” in Beijing, China (an online event).

Isabella Pignatelli and Massimo Nespolo are organising the fourth IUCr Summer School on Mathematical Crystallography to be held in Nancy, France, in June 2023.

Chris Ling is a member of the International Programme Committee for the 26th IUCr Congress (Melbourne, Australia, August 2023).

C. Ling, Chair

A15. Commission on Magnetic Structures

Preparations for the 2023 IUCr Congress in Melbourne

The IUCr Commission on Magnetic Structures has contributed actively to the organization of the 2023 IUCr Congress in Melbourne, Australia, in sponsoring or co-sponsoring ten microsymbiosia and one keynote address (Oksana Zaharko, Switzerland), where topics will include methods of magnetic structure determination, magnetic symmetry, topological magnetic materials, functional magnetic materials, molecular magnets, geometrically-frustrated magnets, magnetic diffuse scattering and short-range magnetic order, aperiodic magnetic structures, and van der Waals magnetism. We have also identified and advertised for six additional sessions with magnetism-centric themes. Capable session Chairs have secured outstanding invited speakers for each session and put together an impressive programme. Commission members invested considerable time and effort during the year to advertise the Congress programme widely amongst magnetic-structure researchers around the world, with particular effort being devoted to reaching out to scientists in parts of the world with less IUCr representation. We particularly thank Maxim Avdeev (ANSTO, Australia) for the extensive effort and patience required to represent the Commission on the Congress International Planning Committee.

Standard and data development

The Commission has continued to discuss a number of high-priority projects, which include the following: (1) Update of the magCIF standard to accommodate the new system of unified (UNI) magnetic-space group symbols and associated magnetic superspace-group symbols [*Acta Cryst.* (2022), A78, 99–106] and other recent developments. (2) Establish a minimal unambiguous description for a magnetic structure. (3) Develop a CIF standard for the symmetry-mode description of a magnetic structure. (4) Expand, complete, and maintain the MAGNDA-TA database of magnetic structures. (5) Promote the use of a new infrastructure for presenting magnetic structures, including the magCIF standard itself, new symmetry data and descriptors, and software tools and databases that employ them correctly.

Meetings

A combination of scientific meetings, schools, and workshops supported by the Commission and its members included the following:

HERCULES School, 28 February – 1 April 2022, Grenoble, France (tutorials on the use of *JANA2020* for crystal and magnetic structures, lecturers: Vaclav Petricek and Margarida Henriques).

JANA Workshop on Magnetic Structures, 25–28 April 2022, Prague, Czech Republic (hybrid format, organizers/lecturers: Vaclav Petricek and Margarida Henriques, lecturers: Manuel Perez-Mato and Branton Campbell).

American Crystallographic Association Meeting, 29 July – 3 August 2022, Portland, USA, "A unified (UNI) system of magnetic space-group symbols" (presenter: Branton Campbell, co-authors: J. Manuel Perez-Mato and Juan Rodríguez-Carvajal).

EPDIC17, 31 May – 3 June 2022, Šibenik, Croatia, microsymbiosium on "Magnetic structures and neutron scattering" (organizer/Chair: Maria Teresa Fernandez-Diaz).

Workshop on Magnetic Structure Determination from Neutron Diffraction Data (MagStr), 3–7 October 2022, Oak Ridge National Laboratory, USA (organizer/lecturer: Ovidiu Garlea, lecturers: Juan Rodríguez-Carvajal, Manuel Perez-Mato, Margarida Henriques, Vaclav Petricek and Branton Campbell).

Workshop on Topology in Magnetic Materials, 22–24 November 2022, Herzberg, Switzerland, "Magnetic symmetry for multi-k structure models" (lecturer: Vladimir Pomjakushin).

B. J. Campbell, Chair, and J. M. Perez-Mato, Secretary

A16. Commission on Mathematical and Theoretical Crystallography

International schools and workshops organized by MaThCryst Commission members

2022 Spring Festival Crystallographic School and Workshop on Crystal-Field Applications, 1–14 February 2022, Beijing University of Science and Technology, Beijing, China. Local organiser: Zhen Song (Beijing), MaThCryst advocate: M.I. Aroyo, lecturers: M.I. Aroyo (Bilbao), M. Nespolo (Nancy), L. Suescun (Montevideo), Zhen Song (Beijing). Participants: 65 students online; 1000 watches of recorded videos. (<http://ustb.cc/zh/2022crystallographyschool/>.)

Crystallographic Symmetry of Quantum Materials, 11–22 July 2022, Nanjing University of Aeronautics and Astronautics, Nanjing, China. Online Summer Lecture Program 2022. Local organizer: Yanda Ji (Nanjing), MaThCryst advocate: M.I. Aroyo, lecturers: M.I. Aroyo (Bilbao), G. de la Flor (Karlsruhe), E. Tasci (Ankara). Participants: 16 undergraduate students in physics, chemistry and materials, 4 graduate students in physics.

Crystallography Online: Workshop on the use and applications of the structural and magnetic tools of the Bilbao Crystallographic Server, 27 June – 1 July 2022, University of the Basque Country (UPV/EHU), Leioa, Spain. Local organizers: J. Lago, J. Igartua, MaThCryst advocate: M.I. Aroyo, lecturers: M.I. Aroyo (Bilbao), G. de la Flor (Karlsruhe), J. Igartua (Bilbao), J.-M. Perez-Mato (Bilbao), E. Tasci (Ankara). Participants: 11 participants in person, 25 participants online. (https://www.cryst.ehu.es/cryst/BCS_Bilbao2022_program_final.pdf.)

Training course on symmetry and group theory, Sokendai Interdisciplinary Lecture. Tenth Basic Course: 22–26 August 2022, Tsukuba, Japan. Organizer, MaThCryst advocate and lecturer: M. Nespolo. (<https://crm2.univ-lorraine.fr/mathcryst/TrainingCourseJapan.php>.)

International seminar series

Materials Innovation Factory (MIF++) Seminars: 20+ seminars running from January 2022 to December 2022, University of Liverpool, Liverpool, UK. Local organizer and MaThCryst advocate: Vitaliy Kurlin. MaThCryst speakers: V. Kurlin, R. Tomiyasu and G. McColm, including two open tables with MaThCryst members. (<http://kurlin.org/MIFplusplus.php>.)

Meetings

3rd meeting MACSMIN as a hybrid satellite of ECM33 in Liverpool, UK. Organizers and MaThCryst advocates: V. Kurlin and M.I. Aroyo. MaThCryst speakers: B. Souvignier, V. Kurlin, K. Tomiyasu, G. McColm. (<http://kurlin.org/ECM33MACSMIN2022crystal-lattice-classifications.html>.)

Editorial work

M.L.A.N. De Las Peñas acted as a Co-editor for *Acta Crystallographica Section A*.

Vladislav Blatov is preparing the Topology CIF Dictionary (https://www.iucr.org/resources/cif/dictionaries/cif_topology).

V. Kurlin and M.I. Aroyo are acting as invited Co-editors for a Special Issue on Crystal Lattices to be published in *Acta Crystallographica Section A*.

Software and educational material

An interactive program to visualize the 2D Fourier transform (<https://github.com/bstoeger/xfft>), developed by Berthold Stöger, was presented at ECM33.

An English book that introduces mathematical ideas with real applications in crystallography, mainly for students on courses in mathematics, was written by Ryoko Tomishasu to be published in the series SpringerBriefs.

Planning and sponsorship

Planning for activities during 2023 has been ongoing.

The 7th MaThCryst School in Latin America to be held in Goiania, Brazil, and organized by Hamilton Napolitano has been discussed. The school should be held before the end of 2023.

Three microsymbiosia and a workshop are being organized by MaThCryst members for the IUCr 2023 Congress and General Assembly to be held in Melbourne, Australia.

L. Suescun, Chair

A17. Commission on Neutron Scattering

The Commission (the 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.

The major neutron facilities have continued operation.

The construction of the European Spallation Neutron Source (ESS) in Sweden is progressing and will be ready to deliver neutrons to 8 instruments by 2025. Although the Orphée reactor at the Laboratoire Léon Brillouin (LLB) in France has been shut down, the LLB is still the neutron scattering center for French users involved in different outstations at the ILL, PSI or building 5 instruments at the ESS. To face these challenges, a League of advanced European Neutron Sources, LENS, was created: it is a not-for-profit consortium working to promote cooperation between European-level neutron infrastructure providers offering transnational user programmes to external researchers. It should also be noted that numerous groups have been working on alternative sources to compensate for the loss of neutrons for research in Europe.

Great efforts are currently being made to enable a relaunch of the German neutron source FRM II in Garching near Munich towards early 2024. Many colleagues used their time in 2022 to focus on publishing their data, e.g. at conferences like the ICNS in Argentina, to organize workshops, e.g. a neutron workshop at the German Crystallography Conference (DGK2022) in Munich or the JCNS Workshop on machine learning/AI aspects of data from neutron experiments in Tutzing, and to strengthen their cooperation with members of other institutions.

The Spallation Neutron Source (SNS) in the USA continued operation at 1.4 MW providing more than 4500 neutron production hours annually. Progress continues on the Proton Power Upgrade (PPU) project for SNS, which will be complete in 2025. The PPU project will double the power capability of the SNS accelerator from 1.4 to 2.8 MW, to facilitate new types of experiments and discoveries. The High Flux Isotope Reactor (HFIR) in the USA continued operation at 85 MW, providing more than 3900 neutron production hours annually.

The operation of J-PARC MLF in Japan is also continuing with 800kW beam power, and the beam power will be upgraded step by step every year. The Japanese Research reactor (JRR-3) is also continuing operation. The Chinese Spallation Neutron Source (CSNS) provided 5262 hours of user operation in 2022, and reached 140 kW in October 2022. The number of instruments is increasing. Four instruments are currently open to users, five are under commissioning, and two more will be completed in 2024. The phase-2 project with 500 kW power has been approved and the construction will be finished in five years and six months, with an additional nine instruments to be constructed.

The Australian Centre for Neutron Scattering (ACNS) is continuing with a number of upgrade projects. The new improved Koala Laue Diffraction instrument took its first diffraction pattern in early February 2023 and is expected to be returned to the user programme soon. A shutdown of the OPAL reactor is planned for 2024 during which the Cold Neutron Source will be replaced. The OPAL long shutdown in 2024 will run from 18 March to 5 July 2024. Some ACNS instruments will also be unavailable for users in July 2024 as performance measurements for the new Cold Neutron Source are undertaken after the reactor returns to normal operations. As a consequence of the reduced days, the proposal rounds will be adjusted with the 2023-2 round running from 1 August 2023 to 17 March 2024 and the 2024-2 round running from 1 August 2024 to 31 January 2025.

Our Commission members were also involved in organizing several meetings and schools, not only for neutron but also for quantum beam (synchrotron, neutron and ion radiation etc.) joint use that took place in 2022. In J-PARC (Japan), the 6th Neutron and Muon School, 12–16 December 2022, was held in a hybrid style, with lectures online and on site and hands-on training on site with 175 students for lectures and 18 for practicals from 20 countries. The Australian Centre for Neutron Scattering (ACNS) held the ANSTO-HZB Neutron School, ANBUG-AINSE Neutron Scattering Symposium (AANSS 2022), the ANSTO Powder Diffraction School and the ANSTO Small-Angle Scattering Workshop, all face-to-face events. At BARC, Mumbai (India), the 19th School on Neutrons as Probes of Condensed Matter was held 14–19 November 2022, attended by ~50 students who also performed experiments at the Dhruva reactor. The Xth International Meeting of the Spanish Society on Neutron Techniques (SETN), University of Almeria, 18–20 July 2022, and the XXIII Summer Course UAL on Neutrons, Electrons and X-Ray Techniques, University of Almeria, 20–22 July 2022, were held in Spain.

Commission members also were involved in planning activities for several important neutron-related conferences and schools in 2023.

T. Ishigaki, Chair

A18. Commission on NMR Crystallography and Related Methods

In addition to participation at the triennial IUCr Congresses, the Commission on NMR Crystallography and Related Methods works towards several outreach objectives. Examples of such activities include coordination and sponsorship of themed sessions on NMR crystallography at annual meetings of the American Crystallographic Association and the SMARTER conferences.

Commission member Professor Yaroslav Khimiyak is serving as our representative on the International Programme Committee for the IUCr Congress to be held in Melbourne in 2023. Professor Khimiyak and Commission Chair Professor David Bryce have proposed three microsymposia for this Congress and have put forward the names of keynote speakers. The microsymposia currently planned include “Structural Chemistry at the Interface of Diffraction, Nuclear Magnetic Resonance and Other Spectroscopic and Computational Tools”, “Polymorphism, Functional Materials and Structural Transformations: Understanding Properties and Disorder” and “NMR Crystallography Approaches to Biomolecular Structure Determination”. The first two of these build on the strengths of the Commission’s previous contributions to IUCr Congresses, while the third represents a concerted effort to further involve the biomolecular NMR community in the Commission and in the IUCr Congress.

Members of the Commission continue to contribute to the broader NMR crystallography community via a range of initiatives. For example, Commission member Professor Steven Brown is the Chair of the Steering Group of the Collaborative Computing Project for NMR Crystallography (CCP-NC), which has added and updated several useful tools for NMR crystallography over the past year (<https://www.ccpnc.ac.uk/>). The CCP-NC has also launched a series of meetings and an online discussion platform this year. Finally, plans are underway for a Royal Society of Chemistry Faraday Discussion on NMR Crystallography in the coming years, and a new textbook on the topic, edited by Professor Bryce.

D. Bryce, Chair

A19. Commission on Powder Diffraction

Following the COVID-19 pandemic, the Commission for Powder Diffraction’s activities started normalizing. Most significant was the extremely successful running of the EPDIC 17 in Sibenik, Croatia, 31 May – 3 June 2022, following 2 years of postponement. For many of the delegates this was their first face-to-face meeting after an extend lockdown period.

The CPD did however support the following meetings:

ePCCr3 2023, Nairobi, Kenya;

International School of Crystallography: Fundamentals of X-Ray Powder Diffraction in Manizales, Caldas, Colombia, 11–15 September 2023.

Following a successful programme at the Prague Congress and General Assembly, focus also shifted to the 2023 Melbourne Congress and General Assembly and the CPD, represented on the International Programme Committee (IPC) by Angus Wilkinson (USA) and Antonia Neels (Switzerland), successfully motivated for a number of microsymposia, many jointly with other Commissions.

The CPD is also pleased to confirm that the 59th International School of Crystallography in Erice will be devoted to powder diffraction and has been scheduled for 31 May to 8 June 2024 (with David Billing, Matteo Leoni and Dubravka Sisak as co-directors), and the 3rd Southern African Powder Diffraction Conference and Workshop organized under the auspices of the CPD is scheduled for 16–21 April 2023 in Namibia (see 2023sapdc.com). Sponsorship for more than 25 students and young researchers has been secured.

The CPD has also made some progress with revitalizing and modernizing the use of pdCIF, mostly in conjunction with the IUCr journal editors and representatives.

The Commission on Powder Diffraction maintains close links with the ICDD, and has initiated discussions about how this relationship can possibly be developed into something more substantive and of mutual benefit.

D. G. Billing, Chair

A20. Commission on Quantum Crystallography

In April 2022, a representative of the Commission on Quantum Crystallography (QCr), Paulina Dominiak, participated in a hybrid meeting (Prague/Melbourne/online) of the International Programme Committee of the 26th Congress and General Assembly of the International Union of Crystallography (IUCr 2023). After a very lively discussion during the meeting and some adjustments made throughout 2022, it was decided that one candidate of the QCr Commission was accepted for a plenary lecture, and three candidates for keynote lectures, and six microsymposia will be (co)organized by the Commission.

In June 2022, the first post-pandemic conference organized on site by our community took place. It was the 9th International Charge Density Meeting (ICDM9) held in Aarhus, Denmark, and was organized by Anders Ø. Madsen and Jacob Overgaard. We had the opportunity to listen to many excellent lectures, have in-person discussions and welcome many new students and young researchers. Discussion of a common platform for all QCr software was continued, and decisions about new schools and the place for the next ICDM were taken.

In September 2022, Nicolas Claiser and Mohamed Souhassou organized the Robert Stewart School 2: Spin and Charge Densities Modelling at University of Lorraine, Nancy, France. The school was a satellite to the 33rd European Crystallographic Meeting (ECM), Versailles, France. At the ECM our community was represented by one keynote lecture by Paulina Dominiak and four microsymposia (co)organized by the Special Interest Group SIG-02 on Quantum Crystallography.

Throughout the whole of 2022, the Distinguished Lectures on Quantum Crystallography and Complementary Fields continued online. The series is organized jointly by the QCr Commission and the European Crystallographic Association SIG-02 on Quantum Crystallography, with the support of the University of Warsaw (Poland) and the Crystallography Committee of the Polish Academy of Sciences. Fifteen lectures were broadcast in 2022, with more than 650 registered participants, and 80–170 people attending each lecture. The lectures are recorded and posted on the website (<https://qcrwebinar.chem.uw.edu.pl>); each recording already has 60 (up to 230) viewers.

In 2022 the Commission recommended that the IUCr support the 12th International Conference on Inelastic X-ray Scattering (IXS2022) organized by Arun Bansil, Wolfgang Caliebe, Yoshiharu Sakurai and others in Oxford, UK; and the First Masuku Remote Crystallography OpenLab organized by Jean Jacques Anguile and Adam Bouraima in 2023 at the University of Science and Technology of Masuku, Gabon.

P. Dominiak, Chair

A21. Commission on Small-Angle Scattering

Commission activities, meetings, and communication

Members co-organized SAS 2022 in Campinas, Brazil, and at least 10 different workshops and microsymposia related to SAS at other venues. SAS2022, the major topical conference on small-angle scattering, brought together the worldwide SAS community both in person and virtually.

The Commission (CSAS) assisted in proposing 11 microsymposia at the IUCr2023 Congress, helping to select topics and suggest Chairs and speakers.

Preparation for SAS2024 in Taipei, Taiwan is underway, spearheaded by Dr Jeng and supported by CSAS members.

Educational activities

Members organized and taught at a three-day summer school on BioSAXS (Dr Jeng) and a solution scattering school for young students (high school, Dr Surayama), and gave lectures on the fundamentals of SAS, bioSAXS, polymers, food science, and other SAS topics (Dr Gilbert, Dr Ilavsky and many others). Members have been organizing seminars and courses for young scientists on the theory of SAS, GISAS, and reflectometry, as well as on applications of SAS in different fields. Most members have served as supervisors and advisors to students (MS, PhD, post graduate). Dr Allen is preparing a meeting of IUCr journals Co-editors and an authors' workshop for the IUCr2023 Congress.

Community-building activities

Members serve as Editors and Co-editors of IUCr journals such as *Journal of Applied Crystallography (JAC)* and *Journal of Synchrotron Radiation (JSR)*. Dr Ilavsky and Dr Meneau are serving as Co-editors of open-access Special Issues of the *Journal of Applied Crystallography* associated with the SAS 2022 meeting in Campinas, Brazil. Dr Gilbert is Guest Co-editor for the Special Issue of *JAC* dedicated to "Magnetic small-angle neutron scattering – from nanoscale magnetism to long-range magnetic structures". Dr Allen (consultant) is Editor-in-chief of the IUCr journals. CSAS members in collaboration with the SAS2022 team have administered the Guinier prize and other prizes and competitions for SAS2022.

Consultant activities

Most members serve on International Advisory Boards, Proposal Review Committees, and other advisory bodies for facilities, instruments, major grant agencies, conferences, workshops, schools, etc. Many serve as Chairs of these bodies.

Technical activities summary

Members of CSAS spearheaded round-robin experiments where small-angle X-ray scattering (SAXS) and small-angle neutron scattering (SANS) measurements of five standard proteins in solution using 12 SAXS and four SANS instruments demonstrate reproducibility and yield consensus scattering profiles that provide a foundation benchmarking set to evaluate approaches to scattering profile prediction from atomic coordinates [*Acta Cryst.* (2022). D78, 1315–1336]. CSAS supported and members participated in a round-robin experiment in data analysis (“The human factor: results of a small-angle scattering data analysis round robin”, submitted to the IOP journal *Measurement Science and Technology*). Other standards are being developed or maintained: the existing NIST SRM 3600 (absolute intensity standard), a future SAXS q-calibration standard, and NIST Reference Materials RM8012 and RM8013, partially based on SAXS measurements.

An updated template for the reporting table based on the 2017 publication guidelines for biomolecular SAS and 3D modelling has been presented that includes standard descriptions for proteins, glycosylated proteins, DNA and RNA, and some reorganization of data to improve readability and interpretation. A specialized template also has been developed for reporting SAS-contrast variation (SAS-cv) data and models that incorporates the additional reporting requirements for these more complex experiments (*Acta Cryst.* D79, <https://doi.org/10.1107/S2059798322012141>).

Members advise, maintain, and develop the widely used SAS software (*ATSAS*, *Irena*, *sasView*, *AUCSASv3.0*, etc.) and contribute to development of data formats (canSAS, Nexus).

J. Ilavsky, Chair

A22. Commission on Structural Chemistry

The Commission on Structural Chemistry (the 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 Commission last met in person at the 2017 Hyderabad Congress and there agreed to focus on:

- (i) support for appropriate crystallographic conferences and schools, in particular those which aim to expand crystallography to under-represented regions such as South America and Africa;
- (ii) support for IUCr journals, through encouraging submission of excellent scientific results to *IUCrJ* and other journals, and
- (iii) building relations with other Commissions and external bodies such as IUPAC and the CCDC.

In the past year the CSC lent support to the following conferences and schools, which draw on crystallographers in the structural chemistry sphere:

British Crystallography School, Durham, UK, March/April 2023.

MOF School 2023, Como, Italy, June 2023.

Hot Topics in Contemporary Crystallography 5 (HTCC5), Dubrovnik, Croatia, April 2023. The organisers were also advised to approach the Commission on Macromolecules, since the focus of the meeting was largely macromolecular.

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 Sub-committee on the Union Calendar.

It is apparent that most conferences are now being planned as in-person physical meetings, with far fewer online or hybrid meetings being planned than was the case in 2021 or 2022.

Members of the Commission are looking forward to the IUCr Congress in 2023 in Melbourne, Australia. The CSC representatives on the International Programme Committee (IPC), Delia Haynes, Tomoji Ozeki, and Christian Lehmann, provided an excellent liaison between the IPC and the Commission, and have ensured that there will be a strong structural chemistry programme at the Congress.

S. Bourne, Chair

A23. Commission on Synchrotron and XFEL Radiation

Synchrotron radiation and free electron laser facilities

Following the beginning of operations of the first “4th generation” storage ring, MAX IV in Sweden, many synchrotron facilities have been planning to upgrade or build new rings. For example, the ESRF completed a major upgrade of its accelerator in 2020 and beamlines have

been upgraded since 2021. The APS upgrade was approved and user operation will cease in April 2023. Following in the footsteps of these two hard X-ray facilities, Spring-8 is also planning significant upgrade programmes based on these new designs. In addition, SIRIUS, the 4th generation Brazilian facility, has most of the beamlines under commissioning and the 6 GeV High Energy Photon Source (HEPS) is being built near Beijing, China. Many other facilities have plans to adapt the new high-brightness designs.

There are now 5 hard X-ray FELs open to users worldwide: the European XFEL in Germany, SACLA in Japan, PAL-XFEL in South Korea, SwissFEL in Switzerland and the LCLS in the USA. The first hard X-ray FEL based on superconducting accelerator technology, the European XFEL, started operation in 2017. A major upgrade is ongoing for the LCLS with the installation of a 4 GeV continuous wave (cw)-mode superconducting accelerator and a new suite of soft X-ray instruments. SwissFEL is continuing to increase the instrument portfolio. In addition, SHINE, a new 8 GeV cw-mode superconducting accelerator FEL facility, is under construction in Shanghai (China).

Supported meetings, schools and workshops

During 2022, the effects of the COVID-19 pandemic kept impacting these events. No support letters were requested via the form on the IUCr website, as required by the current procedure. The Commission on Synchrotron and XFEL Radiation (the CSXR) has mainly focused on activities concerning the IUCr Congress in Melbourne in 2023.

Here we should highlight that we are contributing to the organization of four microsymbiosia:

- (1) X-ray Ptychography: Recent Developments and Applications. Chairs: Ana Diaz (SLS/Paul Scherrer Institute) and Cameron M. Kewish (ANSTO).
- (2) Data-Driven Science: Current Status and Outlook. Chairs: Nicholas Schwarz (Argonne National Laboratory) and Andrew Goetz (ESRF).
- (3) Room-Temperature Serial Snapshot Micro-Crystallography: Highlights from XFELs and Synchrotrons. Chair: Dominik Oberthür (CFEL, DESY).
- (4) In Vivo Crystallography and Synchrotron Radiation. Chairs: Leo Chavas (Synchrotron Radiation Research Center) and Fasseli Coulibaly (Monash University).

CSXR member and consultant activities

The members of the Commission are active in key synchrotron and crystallography communities and conferences. For example, Miguel A. G. Aranda is currently a member of the Scientific Advisory Committee of ELETTRA, and gave an invited talk at the ALBA industrial meeting, 17 June 2022, titled “Industrial usage of ALBA synchrotron: what is it for?”.

M. A. G. Aranda, Chair

A24. Commission on XAFS

International Tables for Crystallography Volume I

International Tables Volume I, X-ray absorption spectroscopy and related techniques, is a very significant volume for the community, and we expect it to become a reference book for scientists performing spectroscopy and related techniques. All three Editors have been working diligently towards the volume, and good progress has been made, with chapters regularly being made available online. 79 of the 150 chapters prepared by international experts can already be found online at <https://it.iucr.org>, and most of the contributions have now been accepted, having passed the review process and moved into preparation of proofs. The majority of the ten sections that form the volume are now close to completion.

We expect to be in a position to advertise the volume at the Quantity and Quality for XAFS 2023 (Q2XAFS2023) conference in Melbourne (Australia) in August 2023.

Support for the XXVI General Assembly and Congress of the International Union of Crystallography

The Commission on XAFS (CXAFS) has participated very actively in the preparation of the scientific programme for the XXVI Congress in Melbourne in 2023, proposing several microsymbiosia and keynote speakers.

As part of the Congress, the Commission on XAFS is organizing a one-day XAFS workshop with international invited tutors. The workshop will take place on 22 August, and will cover the fundamentals of XAFS and its applications to materials science. The workshop will also include a hands-on session, where the basis of XAFS data analysis will be covered.

In addition, and as a satellite of the main event, CXAFS, together with the International XAS Society, are working towards the organization of the Quality and Quantity for XAFS 2023 (Q2XAFS2023) conference. The conference will be held at the Australian Synchrotron in Melbourne (Australia), 17–19 August 2023. The conference aims to bring together experts in the field of X-ray absorption spectroscopy to discuss aspects of the technique that affect data quality in XAFS experiments.

Round-robin activities

Preparations for the planned first inter-laboratory round-robin test of XAFS results were finished in 2022. The exercise aims to test the reproducibility and comparability of XAFS spectra measured at different facilities, and to compile a catalogue of essential metadata needed to describe the experiments and understand possible differences between spectra. The first three samples, titanium, copper and molybdenum metal foils, have been sent to more than 20 (synchrotron) facilities worldwide. The XAFS beamlines involved in the tests use undulators,

wigglers or bending magnets as X-ray sources, and are in operation in 3rd and 4th generation storage rings. Bench-top XAFS instruments have also been included in these tests. The first results will be presented and discussed during the Q2XAFS2023 satellite meeting to the IUCr Congress in Melbourne, Australia, in August 2023.

S. Diaz-Moreno, Chair, V. Briois, Secretary, and G. Aquilanti, Secretary