international union of crystallography

FOUNDATIONS ADVANCES

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Report of the Executive Committee for 2020

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1. Meetings

The IUCr sponsored the following meetings that were held during 2020:

4th International Workshop on X-ray Crystallography in Structural Biology, The Islamia University of Bahawalpur, Pakistan, 25–27 February 2020.

4th International Symposium on Halogen Bonding (ISXB4), Stellenbosch, South Africa, originally planned for 23–27 March 2020, held online 2–6 November 2020.

3rd LACA School on Small Molecule Crystallography, Universidad Nacional Autónoma de México, Mexico, originally scheduled for 26–29 March 2020, held as a two-part virtual meeting in November and December 2020.

The Executive Committee met virtually in March and August. The Finance Committee met virtually in March and August, to prepare its advice and recommendations on finances, establishment and staff matters.

The most important items of business dealt with by the Executive Committee at its meetings, and in e-mail ballots, were:

editorial policy, pricing policy and subscription rates, approval of appointments of Editors and Co-editors, Wiley contract renewal, journals development, Journals Management Board meeting, Special Issues, Plan S and open access, and other matters concerning the IUCr journals;

approval of audited accounts for the previous year;

status of membership subscriptions;

investment policy;

sponsorship and financial support for meetings, young scientists' support, Visiting Professorship Scheme, gender balance of programmes;

progress with Volumes A, A1, B, C, D, E, F, G, H and I of *International Tables* and development of associated software;

IUCr Newsletter;

World Database of Crystallographers;

Online Dictionary of Crystallography; and

promotional activities.

Other items dealt with in this way were:

consideration of publications, jointly with Oxford University Press, in the IUCr/OUP Book Series;

outreach and education, LAAAMP;

Crystallography in Africa;

review of activities of Commissions, formation of a new Commission;

provision of services to and review of activities of Regional Associates;

review of reports of IUCr Representatives on other bodies;

updates from the Committee on Gender Equity and Diversity and an updated Diversity Statement;

arrangements for the Prague Congress; and

Swiss registration and taxation.

Items concerning the Chester office were:

staffing requirements in the IUCr office in Chester;

office premises;

risk analysis; and

office technology.

2. Publications

Volume 76 of *Acta Crystallographica*, Volume 53 of *Journal of Applied Crystallography* (*JAC*), Volume 28 of *Journal of Synchrotron Radiation* (*JSR*), Volume 7 of *IUCrJ* and Volume 5 of *IUCrData* were published.

3. Adhering Bodies

A list of Adhering Bodies of the Union, with names and addresses of the Secretaries of the National Committees for Crystallography, was published as Appendix D to the Report of the Twenty-Fourth General Assembly and International Congress of Crystallography [*Acta Cryst.* (2020), A**76**, 217–224].

4. Work of the Commissions

4.1. Commission on Journals

4.1.1. *IUCrJ*

IUCrJ had a strong year in 2020, with a record number of articles published and continuing to establish itself within the wider scientific communities that use results obtained from diffraction methods. Impressions from authors, readers, referees and commentators are very positive with a number of papers receiving high downloads and citations in line with high-impact publications.

The journal impact factor increased to 5.4 in 2020. All submissions undergo preliminary screening by a panel consisting of the Main Editors (Dimitri Argyriou, Ted Baker, Richard Catlow, Gautam Desiraju, John Spence and Sriram Subramaniam) and the Editor-in-Chief (Andrew Allen), and this has helped to provide a rapid and efficient review process. Where appropriate, any articles that do not meet the journal's requirement for broad scientific significance are usually 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 2020 featured papers from a wide variety of areas including biology, chemistry, crystal engineering, cryo-EM, materials, physics and free-electron lasers (FELs). The number of articles submitted to the journal was 151; a total of 129 papers were published with an average turnaround time of 15 weeks. A number of papers have been highlighted in each issue via an in-depth commentary in a manner similar to other comprehensive journals such as *Nature* and *PNAS*.

The Biology and Medicine section of *IUCrJ* continues to attract a wide variety of papers, with 41 research articles and 6 commentaries/letters in 2020. Most report novel biological structures, with an emphasis on the binding of ligands and drug-related molecules, but innovative methods for obtaining structural data from biological systems continue to appear. These latter include new variations on serial crystallography, to better capture the dynamics of biological reactions, and approaches that further push the boundaries of crystallography, such as *in situ* imaging of cells. Other sections of the journal (*e.g.* the Cryo-EM, Neutron/Synchrotron and Physics/FELs sections) also address biological systems, making this a strong focus for the journal. Importantly, the current COVID-19 pandemic has galvanized structural biology to generate an outpouring of COVID-related structures. Most are not yet published, but we expect to be publishing many papers on this topic in the coming years; some outstanding examples have already appeared in *IUCrJ* and more are in the pipeline.

In 2017, we introduced a new section in *IUCrJ* to provide a forum for rapid publication of important results in the cryo-EM field. This section publishes papers reporting both methodological advances as well as new biologically relevant findings that emerge from the use of cryo-EM and related techniques. In 2020, papers in the cryo-EM section featured prominently among the most downloaded articles in *IUCrJ*. The establishment of *IUCrJ* as a venue for publication of high-quality articles of relevance to technical and biological findings in cryo-EM, along with *IUCrJ*'s continued maintenance of a high and competitive impact factor, bode well for the future.

The Chemistry and Crystal Engineering section of the journal has continued to make progress. There were 35 submissions of which 28 articles were voted for review. A total of 23 articles were accepted for publication. These numbers are satisfactory, but one might have expected around 50 submissions every year in this section (one per week). The present Co-editors of the Chemistry and Crystal Engineering section of the journal are M. Eddaoudi, P. Lightfoot, L. R. MacGillivray and C.-Y. Su. This number appears to be satisfactory given the number of submissions.

The 19 papers published in the Materials and Computation section of *IUCrJ* in 2020 illustrate well the challenges posed by structural problems in the science of materials and the key role that computation can play in this and related fields in structural science. They demonstrate the continuing developments in techniques and instrumentation and the increasingly complex structural problems which these developments now make accessible.

The other sections of the journal, covering Neutron and Synchrotron Science and Technology, and Physics and Free Electron Laser Science and Technology published 9 and 11 papers, respectively, in 2020 and have illustrated the rapid advances that are being made in these fields.

We hope that you will consider publishing in *IUCrJ* and, by doing so, help to establish the journal as one of the mainstream comprehensive science journals.

D. Argyriou, **E. N. Baker**, **C. R. A. Catlow**, **G. R. Desiraju**, **J. C. H. Spence** and **S. Subramaniam**, Editors

4.1.2. *Acta Crystallographica Section A*

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 2020 (based on number of downloads and/or citations) were:

The quaternion-based spatial-coordinate and orientation-frame alignment problems by A. J. Hanson [*Acta Cryst.* (2020), A**76**, 432–457], which was highlighted by the Scientific Commentary *Quaternions: what are they, and why do we need to know?* by B. K. P. Horn [*Acta Cryst.* (2020), A**76**, 556–558];

pinkIndexer – a universal indexer for pink-beam X-ray and electron diffraction snapshots by Y. Gevorkov *et al.* [*Acta Cryst.* (2020), A**76**, 121–131];

The atomic structure of the Bergman-type icosahedral quasicrystal based on the Ammann–Kramer–Neri tiling by I. Buganski *et al.* [*Acta Cryst.* (2020), A**76**, 180–196];

Cluster-mining: an approach for determining core structures of metallic nanoparticles from atomic pair distribution function data by S. Banerjee *et al.* [*Acta Cryst.* (2020), A**76**, 24–31]; and

Refinement of organic crystal structures with multipolar electron scattering factors by B. Gruza *et al.* [*Acta Cryst.* (2020), A**76**, 92–109].

Like many of the other IUCr journals, the number of open-access papers we publish has been increasing. We have found that open-access articles are around four times as likely to be viewed, and almost twice as likely to be cited, as articles that are not open-access. Other factors that boost readership and citations are featuring the article in a scientific commentary (which we find to 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).

Back in 2017 our impact factor peaked at 7.9, after the publication of two particularly highly cited articles, on *SHELX* and *OLEX2*, in 2015. As these articles passed out of the 'window' for inclusion in the impact-factor calculation, the impact factor has dropped back down to 2.0. This prompted us to carry out an in-depth analysis of why, when we are publishing many excellent articles in the Advances section, the impact factor was not higher. We found that while our Advances papers were doing very well, a significant number of articles had a very low number of downloads and were uncited within the required window. One reason for this might be that new methods take time to be adopted by the community, so articles describing these might not start to gather citations immediately. However, there were also a number of articles where little effort had been made to explain to potential readers why the work described in the article might be of interest to them. As a result, in an Editorial published in January 2021 [*Acta Cryst.* (2021), A**77**, 1] we reminded our readers of the great history of the journal and the wide range of articles that it accepts, but also outlined some simple steps that authors could take to help maintain its prominence and impact as the premier journal for foundational work in crystallography. 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. We strongly feel that this is important for maintaining the relevancy, vibrancy and broader impact of the journal at a time when, whether rightly or wrongly, journals are often judged by their impact factor rather than their long-term worth to the scientific community.

In 2020 we welcomed four more new Co-editors: Mois Aroyo, Irene Margiolaki, Lukas Palatinus and Amit Singer, along with Commissioning Editor Thomas Proffen, whose role is to attract new articles on materials, methods and instrumentation to the IUCr journals. Werner Kuhs, Laurie Marks, Kenji Tsuda, Henk Schenk and Jean-Guillaume Eon retired from the Board and are thanked for their dedicated service and all their hard work for the journal.

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

4.1.3. *Acta Crystallographica Section B*

During 2020 *Acta Crystallographica Section B* continued to publish six issues per year, the numbers of articles (pages) published during the year being 117 (1147). The numbers tend to depend on the number and size of Special Issues published in the year.

In 2020 the rejection rate was 31% and the average article length was 10.5 pages. The average time between submission and publication (4.6 months) previously rose and fell in response to the number of Special Issues published, but now appears more stable. There has been a slight increase in the number of open-access papers in 2020.

The journal's base impact factor is around 2.0 but can be considerably higher when we publish very highly cited feature articles. Despite a strong programme of invited articles and Special Issues, it has not yet been possible to achieve a sustained increase in the impact factor. We look forward to working with the new Commissioning Editor, Professor Elena Boldyreva, in part to address this issue.

Future Special Issues include those on *Quantum crystallography* (Guest Editor: Piero Macchi), *Structure correlation and dynamics in crystals* dedicated to H.-B. Bürgi (Guest Editors: Simon Grabowsky and Mark Spackman) and a virtual Special Issue on *High-pressure crystallography* across *Acta B*/*C*/*D*, *JAC* and *JSR* (Main Guest Editor: Elena Boldyreva). A Special Issue on *Crystal growth* is in the early planning stage. We record our thanks to all Guest Editors for their efforts in

bringing about the Special Issues. Importantly, Special Issues represent a source of additional articles in the journal: they do not redirect or reclassify submissions that the journal would receive anyway. Invited articles are regularly sought from prominent scientists, including keynote lecturers at IUCr Congresses and Regional Associate Meetings.

Among the Chester staff who have contributed to the work of *Acta B*, we particularly appreciate the many contributions of our Managing Editor Amanda Berry and her predecessor Jill Bradshaw, from editing articles and advising on technical issues to generally supporting the work of the Section Editors.

We are grateful to two Co-editors (Michal Dusek and Pierre Bordet), who were due to retire in 2020 but who have agreed to serve until the Prague Congress. The Editorial Board has not been sufficiently well balanced in terms of gender and geography and we are pleased to welcome several new Co-editors to the Board: Tatyana Bekker (Russian Federation), Karah Knope (USA) and Olga Yakubovich (Russian Federation). Crucially, these appointments also add significantly to the aggregate expertise available on the Board. *Acta B* is aiming to strengthen and emphasize its role as a route to publication for papers on crystal growth related to the scope of the journal (structural science, crystal engineering and materials) and some of the new appointments are in support of this initiative.

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

4.1.4. *Acta Crystallographica Section C*

This year has been difficult for *Acta Crystallographic Section C* in terms of submissions. The number of articles received by the journal has been affected by the pandemic and there was a fall in the number of submissions. The Editorial Board and review panel were contacted to let them know of the situation and to ask them to support the journal if possible. There was a general consensus that the drop in papers was directly attributable to the pandemic and we expect to see a rise in submissions once normal working conditions are resumed.

The 2019 impact factor showed a rise to 1.09 from 0.93 in 2018. The increased impact factor should be maintained in 2020 with an estimated impact factor of 1.1.

The journal has continued to try to strengthen its readership within the chemistry community through the publication of feature articles and topical reviews on areas of particular research interest that we have identified. We have plans to publish further feature articles and reviews in late 2021 and early 2022, and are grateful to Professor Elena Boldyreva, in her role as Commissioning Editor, for her support in moving these ideas forward. There will be a particular focus in attracting feature articles relating to work involving the Cambridge Structural Database and knowledge mining using small-molecule data sets.

Commentaries are seen as an important addition to the range of article types in *Acta Crystallographica Section C* and two commentaries appeared in 2020. We plan to continue this programme of publishing commentaries highlighting high-quality structural papers.

A Special Issue on *Non-covalent interactions based on the sigma hole*, organized by Jonathan White with Guest Editors Lee Brammer, Thomas Roseveare and Anssi Peuronen, is currently being planned with a publication date early in 2022.

The Review Board of referees set up in 2016 of 50-plus members provides Co-editors with a dedicated panel of reviewers from which to obtain rapid and focused reviews. New members were added in 2020 and retiring Co-editors are given the opportunity to join the panel of referees.

The *Acta Crystallographica Section C* Editorial Board was strengthened with the appointment of nine new Co-editors. These were appointed to replace outgoing Co-editors who have now retired. The Co-editors leaving the journal, Phillip Fanwick, Maciej Kubicki, Vratislav Langer, Helena Shepherd, Bernie Santarsiero, Hidehiro Uekusa and Dmitry Yufit, are thanked for their many years of excellent work. The current board has 22 Co-editors. We are very grateful to all our Co-editors, old and new, for their outstanding service.

The current Section Editors, Paul Raithby, Larry Falvello and Jonathan White, are extremely grateful to our Co-editors and to the whole team at Chester Editorial Office for their outstanding support over this difficult year. Their dedication and professionalism is much appreciated.

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

4.1.5. *Acta Crystallographica Section D*

There are encouraging signs that *Acta D* is gradually recovering from the effects of the impact factor having dropped in 2014 from over 7 to 2.7, when several highly cited methods papers disappeared over the limited horizon of the impact-factor calculation. The number of submissions increased significantly to over 190 in 2020, with 115 of these papers in the research category, the highest number since 2016. The impact factor for 2019 of 5.3 (announced in 2020) is a notable improvement on the 2018 value of 3.2, and is very good relative to the historic range of 2 to 3. The average rejection rate dropped in 2020, and the highest number of papers since 2016 were published. This was perhaps partly because of the number of Special Issue papers that were published. Three Editorials were published covering COVID-19 and the new members of the Editorial Board. Around 69% of all papers published in 2020 were open access, an increase from 60% in 2019.

Special Issues continue to play a positive role for the journal, particularly the recurring series of annual CCP4 and (more recently) CCP-EM symposia. The timeliness of the papers was improved by the decision in 2020 to publish them 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 now collected in a 'virtual Special Issue'.

One new Section Editor (Charlie Bond, July 2020) and three new Co-editors (Kristina Djinović-Carugo, Ana González and K. R. Vinothkumar, May 2020) were approved and appointed during the year. The addition of these new Co-editors will cover an expansion into different areas of struc-

tural biology, particularly metalloproteins, integrative structural biology techniques that combine a variety of methods, cryo-electron microscopy and the use of XFELs.

Publication times have decreased in 2020 to an average of 4.7 months – it is important to note that this is driven largely by the time required for refereeing and manuscript revision, rather than by the technical editing or typesetting, which are both highly efficient thanks to the excellent work by 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

4.1.6. *Acta Crystallographica Section E*

In the last few years, the quality of the submitted papers has increased, and the range of structures is far broader. Many papers now report two or more structures, and discuss complementary techniques and include extra tables and figures to illustrate their results. We are increasingly receiving papers describing measurements using synchrotron radiation, powder diffraction analyses and Hirshfeld surface analyses, energy frameworks and the results of complementary techniques such as DFT calculations. 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.

The number of submissions and of published papers has decreased in recent years, with a low for 2020, which, however, is probably due to the difficulties related to the global health emergency. On the other hand, the average length of the papers has increased, reflecting the more detailed discussion of the underlying science in the submitted papers. The average publication time remains close to a month, thanks to the efforts of our Co-editors. In 2020, the number of downloads for *Section E* articles was 7.4 million, by far the largest number of the IUCr journals.

In July 2020, six new Co-editors were appointed, namely: Dr Andrei Batsanov, Durham University, UK; Professor Alexander Briceno, Venezuelan Institute of Scientific Research, Venezuela; Dr Danielle Grey, University of Illinois Urbana-Champaign, USA; Professor Vojtech Jancik, Universidad Nacional Autónoma de México; Dr Joseph Reibenspies, Texas A&M University, USA; and Professor Carola Schulzke, Ernst-Moritz-Arndt-Universität Greifswald, Germany.

Following the suggestion of publishing Topical Reviews, the Section Editors have been actively trying to commission papers that will be widely read and highly cited. The series continued in 2020 with papers on *checkCIF* [A. L. Spek, *checkCIF validation ALERTS: what they mean and how to respond*, *Acta Cryst.* (2020), E**76**, 1–11] and tips and tricks for obtaining the best results [A. Linden, *Obtaining the best results: aspects of data collection, model finalization and interpretation of results in small molecule crystal structure determination*, *Acta Cryst*. (2020), E**76**, 765–766] and has been recently enriched by an educational paper on twinning [S. R. Parkin, *Practical hints and tips for solution of pseudo-merohedric twins: three case studies*, *Acta Cryst*. (2021). E**77**, 452–465].

As well as the commissioning of individual articles, plans are well in hand to produce a number of Special Issues over the next few years with a particular focus on teaching, education and outreach.

As always, we are extremely grateful to our Co-editors for the excellent work they have done and cannot thank them enough. We are also extremely grateful for the 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 to Peter Strickland for his sound advice and expert guidance.

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

4.1.7. *Acta Crystallographica Section F*

Acta Cryst. F is the home for short and rapid structural biology communications, welcoming manuscripts covering a range of techniques, including crystallography, cryo-electron microscopy, NMR spectroscopy, SAXS and computational approaches. Preliminary results, such as crystallization notes, will only be accepted if the system studied is novel, and the method also has new aspects that may be useful for researchers working on other systems.

In 2020, the journal published 85 papers. This number has continued to fall in recent years and represents a large decrease in the number of papers submitted – we need to attract more authors. The overall number of pages has also decreased to 623, but the average paper length has increased slightly to 7.5 pages, probably owing to the extra scientific requirements for publishing in *Acta Cryst. F*. The average publication time has dropped to an average of 2.8 months. Accepted papers undergo prompt final editing and usually appear published online in a matter of days, thanks to the efficient handling in Chester.

No new Co-editors were appointed in 2020 but the current team of Co-editors has good geographical and subject diversity, and hopefully should be sufficient for 2021 and beyond. The referee panel continues to function well. This group of about thirty experienced scientists have each agreed to referee twelve papers a year, to reply to requests promptly and to return reports within two weeks.

The strengths of the journal include the fast but high-quality scientific and technical editing, its standing in the crystallographic community and its goodwill, by virtue of it being a scientific society journal. However, the impact of the journal and its familiarity to non-crystallographic structural biology communities need to be increased further. The 2019 impact factor (announced in 2020) was similar to previous years at around 1.0.

Three Editorials (including one on COVID-19) and four papers in the recently added Methods Communications section were published in 2020. One communication from the

International Symposium on Diffraction Structural Biology (ISDSB) with a methods orientation was also published.

It will be important to continue to grow the journal in terms of quantity and quality of papers, but also to maintain the philosophy of short and rapid communications, to distinguish it from *Acta Cryst. D* and *IUCrJ*. One focus of the journal is to communicate its wide scope more effectively within the structural biology community. Commissioning more Topical Reviews and Special Issues would help to achieve this goal, together with continued attention to the quality of the Research and Methods Communications.

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

4.1.8. *Journal of Applied Crystallography*

The promotion of Andrew Allen to Editor-in-Chief of IUCr Journals in 2018, the transition of Thomas Proffen to be the new IUCr Commissioning Editor for Materials, Methods and Instrumentation and the retirement of several highly valued Co-editors of the *Journal of Applied Crystallography* triggered the appointment of several new Co-editors in 2020 to ensure that *JAC*'s Editorial Board spans all topics within the scope of the journal. Helen Brand (Australian Synchrotron, ANSTO), Jan Ilavksy (Argonne National Laboratory), Arthur Haozhe Liu (Harbin Institute of Technology and HPSTAR), Stephen Moggach (University of Western Australia) and Taku Sato (Tohoku University) are all now contributing expertly to the journal. We thank the retiring Co-editors, Gilles Renaud (CEA, Grenoble) and Satoshi Sasaki (Tokyo Institute of Technology), who stepped down in 2019 and 2020, respectively, for their valuable and tireless support of *JAC* over many years. We especially thank Gernot Kostorz, who finally retired in 2020 after many years of outstanding service to IUCr Journals in the following roles: Editor-in-Chief, IUCr Journals (2005–2012); Editor, Journal of Applied Crystallography (1999–2006); and Co-editor, Journal of Applied Crystallography (1979–1988, 2012–2020).

It was pleasing to see that the numbers of papers submitted to and published in the journal increased in 2020, reversing the trend of recent years. There was also an increase in the fraction of open-access papers in 2020, which may be due in part to changing policies of research funding agencies. Research Papers and Computer Programs continue to be the mainstay of article types, while we need to encourage more Feature and Lead Articles on emerging subjects to attract a wider readership. The rejection rate (just over 30%), impact factor (∼3), publication time (∼5.5 months) and paper length (∼9.8 pages) remain stable.

All articles in the Special Issue on ptychographic software and technical developments, with Guest Editors Stefano Marchesini and David Shapiro from Lawrence Berkeley National Laboratory, and Filipe Maia from Uppsala University, were published in the second half of 2020, with an Editorial closing the issue to appear in April 2021. A cross-journal Special Issue on machine learning is advancing slowly.

K. Chapman, **J. Hajdu** and **G. J. McIntyre**, Editors

4.1.9. *Journal of Synchrotron Radiation*

The number of papers published dropped from 249 papers in 2019 to 209 in 2020, the high in 2019 probably due to the majority of papers for two virtual Special Issue papers being published in that year. The number of pages published also dropped – from a high of 2096 in 2019 to 1754 in 2020. The number of submissions remained about the same (299), as did the rejection rate (24%). Publication times reduced slightly to 5.3 months (5.7 in 2019).

Two virtual Special Issues were finalized in 2020 – though, as mentioned above, the majority of papers were published throughout issues in 2019 (30 papers on X-ray Free-Electron Lasers and 17 papers from the PhotonDiag2018 Workshop). *JSR* is continually looking to publish such themed issues of selected papers from workshops or meetings because as well as providing an important service to the synchrotron-radiation community they are a good way for the journal to expand into new areas and to attract new authors and readers.

Regarding changes to the Editorial Board in 2020, we gratefully acknowledge the work of Main Editor Ilme Schlichting, who retired in 2020, as did Co-editors Aldo Craievich, Piero Pianetta and David Reis. Dibyendu Bhattacharyya joined the board as Main Editor and Kristina Kvashnina was promoted from Co-editor to Main Editor. The Editorial Board now comprises four Main Editors and 13 Co-editors.

The number of open-access papers increased slightly to 91, *i.e.* over 40% of published papers, which has been one of the factors in deciding to make *JSR* fully open access from January 2022.

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, **D. Bhattacharyya**, **K. Kvashnina** and **I. Lindau**, Editors

4.1.10. *IUCrData*

The number of papers submitted to *IUCrData* has dropped significantly by some 65% over the past four years from 440 (2017) to 155 (2020) and the number of published papers shows an even larger decline from 517 to 139 (–73%) over the same period. Whether this decline correlates with difficulties associated with the global COVID-19 pandemic, the increase in the open-access fee to USD 300, competition from the deposition service with the Cambridge Structural Database or other reasons is not clear.

Submissions to *IUCrData* are handled by five Section Editors (Bill Harrison, Jim Simpson, Edward Tiekink, Luc Van Meervelt, Matthias Weil) and 16 Co-editors. The average length of a Data Article in 2020 was 2.9 pages and the publication time averaged 0.9 months: the highest proportion of Data Articles came from the USA (30%) followed by Germany (14%) and India (14%).

The steep decline in submissions noted above is of serious concern and plans to make *IUCrData* a more general 'data

journal' as part of the Open Digital Academic Publishing initiative are being investigated as a priority.

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 his advice and guidance.

W. T. A. Harrison, **J. Simpson**, **E. R. T. Tiekink**, **L. Van Meervelt** and **M. Weil**, Editors

4.2. 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. Parts of a tenth (I, on X-ray absorption spectroscopy and related techniques) are now available online. The *Brief Teaching Edition* of Vol. A (*Space-group symmetry*) is also part of the series; a revised edition will be sent to the printers in early 2021. The *Symmetry Database* is a related online resource.

While *International Tables* has long been a collection of printed books, parts of it became available online starting in 2006. The transition to electronic access is expected to continue because it allows more material to be included, makes it easier to correct or add material, and is advantageous financially. Printed copies of some volumes (*e.g.*, Vols. A and E), however, are expected to remain available; printed versions of the revised Vol. A (dated 2016; 400 copies sold) and the new Vol. H (dated 2019; 200 copies sold) have performed well. So far there has been no online version of the *Brief Teaching Edition*.

The 2020 pandemic presented both opportunities and challenges. Editors and authors may have had more time for projects of this type but budgets of institutional libraries appear to have tightened. The support staff in Chester have been very busy adapting to working remotely. The suspension of in-person crystallographic meetings hindered the search for new Editors.

During 2020 a new style for chapters, new templates and a new workflow were developed that allow early view versions of chapters to be published online even before the order of the chapters is known. 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.

Descriptions of activities during 2020 for the individual volumes follow.

Volume A (*Space-group symmetry*; most recent online edition is dated 2016; Editor Mois Aroyo). During 2020 a proposal for the modification of the reflection-condition tables of Chapter 1.6 by the Subcommittee on International Tables of the Commission on Electron Crystallography was approved after considerable discussion with all the interested parties. The tables will be updated online in 2021.

Symmetry Database server of the Online Edition of *International Tables* (updated continuously; Editor Mois Aroyo). A *Teaching Edition* of the Symmetry Database is being developed. The full-version programs and databases are being adapted to the limited set of data that will be accessible in that new edition.

Work is well under way to allow interactive visualization of the space groups using *JMol*.

Activities in 2020 also focused on bug-fixing and improvements to the databases and programs including: (i) renewal of the navigation style and layout presentation; (ii) new design and contents of the help pages for group–subgroup relations calculations and graph-related results; and (iii) development and implementation of validity checks for group–subgroup and/or group–supergroup relationships.

BTE (*Brief Teaching Edition* of Vol. A; current edition is dated 2010; Editor Mois Aroyo; being renamed *Teaching Edition of International Tables for Crystallography*, with subtitle *Crystallographic Symmetry* and the abbreviation TE). Work continued on the TE, which will introduce Vols. A1 and E of *International Tables*, magnetic symmetry and the *Symmetry Database* as well as Vol. A. The expanded coverage prompted the name change. The TE also includes other new material designed specifically for people new to the field.

Parts 1 and 2 of the TE were typeset and proofed; material for the preliminaries is undergoing a final check. The new version should go to press very early in 2021.

During 2020 it was decided that the TE should give access to all current programs of the *Symmetry Database* while limiting the sets of space and point groups to which the programs could be applied.

Because of the current switch to online crystallographic meetings and schools, the possibility for an online edition of TE will be considered.

Volume A1 (*Symmetry relations between space groups*; most recent online edition is dated 2011; Editor Ulrich Müller). Editor Ulrich Müller is retiring; a search for a new Editor is underway. The expansion of Vol. A1 (or possibly Vol. E) to cover the subperiodic groups remains under consideration.

Volume B (*Reciprocal space*; most recent online edition is dated 2010; Editor Gervais Chapuis). Two new articles, one on the use of the 3D pair-distribution function in the analysis of diffuse scattering and the second on crystal structure determination by dual-space iterative algorithms, are under review. An article on structure determination by electron diffraction is planned.

Ted Janssen completed a revision of his article on modulated structures (currently Chapter 9.8 of Vol. C) before his passing in 2017 but the revision has not yet been reviewed. The plan is to combine that article with Chapter 4.6 of Vol. B (*Reciprocal-space images of aperiodic crystals*). Efforts are underway to find somebody willing to take responsibility for this material.

Volume C (*Mathematical, physical and chemical tables*; online edition is dated 2006; Editor Richard Welberry). Many of the articles for this essentially new volume have been completed and are awaiting typesetting. Early view articles from this volume will start to appear during 2021.

Volume D (*Physical properties of crystals*; most recent online edition is dated 2013; Editor was André Authier, who

has since retired). Attempts to find a new Editor for Vol. D have been unsuccessful so far but it seems that there is no immediate need for a revision.

Volume E (*Subperiodic groups*; most recent online edition is dated 2010; Editor Danny Litvin). Danny Litvin is retiring as Editor. Several possible successors have been identified.

As interest in two-dimensionally periodic materials like graphene increases, interest in Vol. E is expected to grow. Suggestions for extensions have been received; they include adding tables of penetration rod groups, allowing searches for all space groups for which a specific layer group is a sectional layer group, and revising the text to make it more accessible to readers who are less expert in mathematics.

Volume F (*Crystallography of biological macromolecules*; most recent online edition is dated 2012; Editors Liang Tong, Eddy Arnold and the late Michael Rossmann). Preparations for the third edition of Vol. F are currently on hold because of the pandemic and other considerations. Activities will resume once instructions to proceed are received from the IUCr office.

Volume G (*Definition and exchange of crystallographic data*; online edition is dated 2006; Editors Brian McMahon and James Hester). New Volume G chapters and sections covering the updated CIF syntax, dictionary and dREL standards were finalized and reviewed in 2020. Other chapters in this part of the volume covering unchanged standards have also been reviewed and updated by the original authors. Work progressed on new automated typesetting routines for CIF dictionaries. Authors of new dictionary chapters are expected to have those chapters submitted by mid-2021.

Volume H (*Powder diffraction*; new volume in 2019; Editors Henk Schenk, Chris Gilmore and Jim Kaduk). Vol. H, which appeared in 2019, has already sold well (200 copies so far). A review will appear in *J. Appl. Cryst.* A list of suggested corrections and possible additions and improvements is in hand. Jim Kaduk and Chris Gilmore will continue as Editors; they have identified a replacement for Henk Schenk, who is retiring.

Volume I (*X-ray absorption spectroscopy and related techniques*; new volume; Editors Chris Chantler, Federico Boscherini and Bruce Bunker). Vol. I has now published online the first set of fourteen chapters. A large number of additional chapters will be added in 2021.

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/).

Three Editors are retiring: Ulrich Müller (Vol. A1), Danny Litvin (Vol. E) and Henk Schenk (Vol. H). All three helped create their volumes; Vol. A1 first appeared in 2004, Vol. E in 2002 and Vol. H in 2019. All three Editors have served the IUCr in a variety of ways for many years. We are particularly grateful for all their work on behalf of *International Tables*.

This year it is especially important to thank the staff in Chester and, above all, Nicola Ashcroft, for all they have done. They adapted seemingly seamlessly to working from home even as they had to develop numerous new procedures, monitor uncertain financial conditions, and forego in-person contact with Editors and with each other. They continued to perform at a very high level while keeping any stress they felt to themselves. While there have been some delays in typesetting there have also been technical advances, such as developing templates for 'early view' articles on the web and working out guidelines for modifying the *Symmetry Database* to allow limited free access. Bravo!

Carolyn P. Brock, Chair

4.3. 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.

The CAC has supported regular workshops and schools, including the Workshops on Structural Analysis of Aperiodic Crystals in Bayreuth, Germany (local organizer Professor Sander van Smaalen). These provide young scientists with an overview of the methods of structural analysis of incommensurately modulated crystals and composite crystals. The 10th edition scheduled for March 2020 had to be cancelled owing to the COVID-19 pandemic.

The series of *ad hoc* workshops on *JANA2006* continued to be organized by the Institute of Physics of Prague, Czech Republic; since the beginning of the pandemic, virtual workshops have been held.

The International Schools on Aperiodic Crystals are 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 physical properties and chemical understanding of aperiodic crystals, as well as a working knowledge of structural analysis of aperiodic crystals. The fifth edition is expected to take place in Prague in 2022.

Finally, the 1st International School on Hypermaterials (ISH2021), organized by Professor Hiroyuki Takakura (Hokkaido University, Japan), will be held online, 21–25 June 2021. The objective of this school is to provide students with a basic understanding of the structure and properties of hypermaterials.

The 10th edition of the International Conference on Aperiodic Crystals, planned for Sapporo in 2021, has been postponed to 2022 owing to the COVID-19 pandemic.

The next edition of the International Conference on Quasicrystals is expected to be held in Tel Aviv (Israel) in 2022, but is under discussion owing to the probable overlap with the 10th edition of the International Conference on Aperiodic Crystals.

The series of workshops Open Space Between Aperiodic Order and Strong Electronic Correlations, which aim to explore the frontiers between aperiodic order and strongly correlated electron systems, and bring together specialists of the two communities to explore the open space between aperiodic order and strong electronic correlations to promote the exchange of ideas, led in 2020 to the formation of an international research network 'Aperiodic'; its objective is to foster collaborations between the aperiodic crystal community and those who work on chemical and physical properties of materials.

O. Perez, Chair

4.4. Commission on Biological Macromolecules

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

The Commission (the CBM) has been working with the Committee on Data (CommDat) on three issues:

(1) The CBM and CommDat submitted a memorandum to the IUCr Executive Committee and proposed a mechanism for making the results of diffraction experiments publicly available. The goal of this action was to achieve better reproducibility of scientific discoveries and ensure that the structures and subsequent publications are of the highest possible quality. A paper that was jointly authored by the Editors of all crystallographic journals and the Chairs of the Committee on Data and the Commission on Biological Macromolecules that encourages researchers to deposit diffraction images was published by all relevant crystallographic journals [*e.g.* Helliwell, J. R. *et al.* (2019). *IUCrJ*, **6**, 341–343]. Thus, IUCr Journals are taking the lead by encouraging authors to provide a digital object identifier (DOI) for their deposited original raw diffraction data when they submit an article describing a new structure or a new method. An extensive discussion of the issues is available in Grabowski *et al.* [*Acta Cryst.* (2016). D**72**, 1181–1193], Kroon-Batenburg *et al.* [*IUCrJ* (2017). **4**, 87–99], Meyer *et al.* [*Nat. Commun.* (2016). **7**, 10882], Baker [*IUCrJ* (2017). **4**, 1–2] and Grabowski *et al.* [*Struct. Dyn.* (2019). **6**, 06430].

(2) CommDat and the CBM jointly addressed the long-standing and growing issue of deposits that have the phrase 'To be published' as their primary citation. As of 12 June 2020, there were over 26 000 'To be published' deposits in the Protein Data Bank (the wwPDB), and over 9000 deposits have held this status since 2010, *i.e.* for up to twelve years. When a researcher is working on a similar structure, they may often need additional information that is impossible to get from the PDB deposit alone. It was proposed that every PDB deposit should have the e-mail address of the senior author at their work institution included in the metadata of the deposit. This suggestion has been approved by the wwPDB and awaits full implementation. Currently, the PDB provides the ORCID number, which in some cases has alleviated the problem. More than 30 senior crystallographers, including Nobel Laureates and US National Academy members, supported this initiative.

(3) The Commission Chair discussed with some CommDat members better ways to filter PDB deposits that describe non-standard experiments and metadata needed to fully describe some types of experiments. Discussion on the High Pressure Macromolecular Crystallography (HPMX) metadata was initiated between Wladek Minor (the CBM), John Helliwell (CommDat), Kamil Dziubek (Commission on High Pressure Secretary) and specialists in the field. In May 2021, at the online kick-off meeting, a working group consisting of Kamil Dziubek, Nathalie Colloc'h (Université de Caen Normandie, France) and Julia Lieske (Center for Free-Electron Laser Science, DESY, Germany) was formed and mandated to work on the topic of standardizing high-pressure descriptors in the macromolecular CIF dictionary and relevant annotations in the PDB. The group is currently working on a proposal to be submitted to the wwPDB, aimed at creating common standards of pressure-related metadata in X-ray crystallography and NMR deposits. The parameters under consideration are the pressure value, calibration method and description of the experimental techniques (including the type of a pressure vessel).

There is an ongoing discussion with the Executive Managing Editor of IUCr Journals about a mechanism that would improve the impact factor (IF) of the journals. The IF of *IUCrJ* is now ∼5.4. The IF of *Nucleic Acids Research* is ∼11.5. Currently, scientists have equally easy access to *Acta Cryst. D*, *IUCrJ*, *Nucleic Acids Research* and *Science*. Two issues are critical: the time between paper submission and publication and the careful selection of keywords. Keywords should be carefully reviewed not only by reviewers but also by the Editor of the paper. One of the questions that reviewers should answer is 'Are the keywords reflecting the contents of the paper?'

It is essential that manuscripts submitted to IUCr journals, and to *IUCrJ* in particular, be processed promptly. The CBM Chair's personal experience is very good, but there are reports that manuscripts might linger with the Editors for months without being reviewed or that the publication of a non-problematic manuscript could take almost a year from submission to publication. Another issue that is critical for structural biology is that information about papers should be published in PubMed within 24 h. Authors should be encouraged to use more modern ways, like presenting structural results using rich internet applications [Porebski *et al.* (2020). *Protein Sci.* **29**, 120–127]. The ambitious goal is to double the IF for *IUCrJ* in the next five years and increase the IF of our other biological journals, *Acta Cryst. D* and *Acta Cryst. F*.

The Commission members and other interested crystallographers have continued to discuss standards of PDB and data depositions that would help *consumers of the PDB who are not structural biologists* receive information that is easier to understand. The COVID-19 pandemic sped up the process of developing quality standards due to several groups who were carefully watching the quality of COVID-19 related

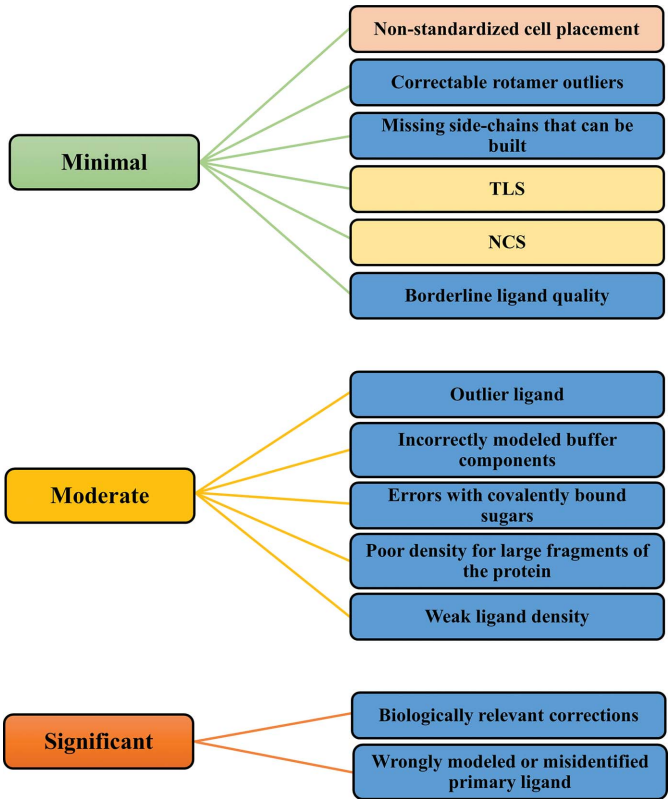

Figure 1
Classification of problems noted in various macromolecular structures.

structures [Croll *et al.* (2021). *Biophys. J.* **120**, 1085–1096]. A classification of common problems that occur in macromolecular structures can be visualized as shown in Fig. 1 [Grabowski *et al.* (2021). *IUCrJ*, **8**, 395–407]. These problems, which do not represent an exhaustive list, may be difficult or even impossible to correct. Some criteria are case- and resolution-dependent, such as NCS and TLS (indicated in a different colour in Fig. 1). For example, the use of NCS may be critical for low-resolution structures due to the decreased number of parameters. The classification may depend on who is looking at the structure, *i.e.*, a crystallographer or a biologist. Non-standardized cell placement should be avoided because it makes it more challenging to compare two or more similar structures (also indicated by colour) by scientists without a crystallographic background.

Meetings, workshops and other outreach activities. The CBM has recommended support from the IUCr for a number of meetings and workshops that could play an important role by providing resources for teaching or major dissemination of results obtained through macromolecular crystallography.

W. Minor, Chair

4.5. Commission on Crystal Growth and Characterization of Materials

The work of the Commission in 2020 was strongly reduced owing to the pandemic.

The Commission recommended that the IUCr supported the following events:

7th International School on Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials (ISC2020), Granada, Spain, 24–29 May 2020;

2020 Crystal Engineering Gordon Research Conference (GRC), Newry, Maine, USA, 21–26 June 2020; and

ISCoC 'Molecular Crystal Engineering', Erice, Italy, 28 May – 5 June 2021.

I would like to express my great honour and pleasure to chair this Commission, and hope I am making my own contribution to all the work done up to now by the Commission to bring more understanding of the role of crystals and their influence on many aspects of life and technology.

A. Zappettini, Chair

4.6. Commission on Crystallographic Computing

Commission members: M. Lutz (Chair), R. Giordano, B. Gopal, P. Mercier, C. Millan, L. Palatinus, S. Panjikar, T. Proffen and A. Thorn. Consultants: H. R. Powell, R. I. Cooper, K. Diederichs, M. Fodje, Y. Yamada, G. Shields, J. Hester and A. L. Spek.

Activities of the Commission in 2020 included: organization of a Computing School as a satellite to the IUCr Congress in Prague, which was postponed to 2021 because of the COVID-19 pandemic; preparation of microsymposia for the IUCr Congress in Prague; and organization of a Software Fayre at the IUCr Congress in Prague (also postponed to 2021).

Martin Lutz, Chair

4.7. 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 for Crystallography*, 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 CIF Standard, and both the IUCr President and General Secretary. In 2020 the number of members was 54. 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. The only issue considered during 2020 was the definition of a *crystal* in the *Online Dictionary of Crystallography* (the *ODC*). Chair C. P. Brock and Consultant A. M. Glazer worked with M. W. Senechal, former member of the Commission on Aperiodic Crystals (the CAP), to draft an extension to the current *ODC* definition of *crystal*; the extra material would make the definition more accessible to beginning students and other non-experts. The proposal for the new definition retains, essentially unchanged, the current definition, which was developed by the CAP after much discussion. The proposal will be presented to the full CCN in early 2021.

Online Dictionary of Crystallography (the *ODC*); the Editor is Gervais Chapuis. The CCN is responsible for main-

taining 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. Snapshots of the *ODC* were published in paperback form in 2014 and 2017 (*i.e.*, on the occasion of the two most recent IUCr Congresses).

The number of new entries in 2020 was 19, which brings the total to 335. The number of authors who created new entries or revised existing definitions remained very small.

It is noteworthy that progress on the IUPAC dictionaries (the Color Books including the Gold Book) is also very slow. The Chair of the CCN is a member of the IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols (the ICTNS) and so sees all the meeting minutes and correspondence.

Other matters. Consultant Massimo Nespolo contributed an interesting article on nomenclature to the first issue of the 2020 Newsletter, entitled *Not so elementary, my dear Wyckoff*. The article discusses the use of term crystallographic *orbits*, a term unfamiliar to many because it was first introduced in 1979. Nespolo's article was highlighted in the issue's Editorial written by Newsletter Editor and CCN Consultant Mike Glazer.

Carolyn P. Brock, Chair

4.8. Commission on Crystallographic Teaching

Members: Oluwatoyin Asojo (Interim Chair), Annalisa Guerri, Tsuyoshi Inoue, Pavel Kashkarov, Diego G. Lamas, Sol Lopez-Andres, Jarugu Narasimha Moorthy and Manfred Weiss. Consultants: Mois Aroyo, Alexander (Sandy) Blake, Elena Boldyreva, James Britten, JuanMa Garcia Ruiz, Saulius Grazulis, S. Krishnaswamy, Edward Michalski, Claudine Mayer, Claudia Rawn, Miriam Rossi, Nivaldo Speziali, Michele Zema, Shao-Liang Zheng and Katherine Kantardjieff (Past Chair). The Vice Chair, Toyin Asojo, has served as Interim Chair of the Commission (the CCT) since 2020 and will do so until the rescheduled Congress.

Overview of activities. Action items from the last report have been addressed, specifically the reorganization and updating of web resources are ongoing and CCT web pages are now current. The CCT met via Zoom in December 2020 and April 2021, and communicated regularly via e-mail. Planning is underway on educational and crystallography teaching activities in the age of COVID-19.

Social media and web resources. The Commission Twitter account (@IUCrTeach) has only 275 followers, while the Facebook page (http://www.facebook.com/IuCrCommission OnCrystallographicTeaching) has 1154 followers. Social-media accounts are currently owned and managed by the Past Chair, and efforts to transfer the account ownership have stalled during the COVID-19 pandemic. Online meetings are now directly advertised in a timely fashion on the CCT's web page.

Review of applications for workshops and schools. Members reviewed applications for multiple workshops and summer schools. All reviews were completed via e-mail. Documents were shared among the members both via Google Drive and e-mail. The CCT continues to use standardized rubrics and an evaluation form, described in the previous report, to facilitate clarity, objectivity, transparency and timely writing of evaluation letters. The number of applications dipped in 2020 because of postponement and cancellation of meetings. The CCT strived to improve our response time for providing informative letters of evaluation for all reviewed applications to the applicants, the Subcommittee on the Union Calendar and the Executive Committee within one month of receipt of the complete application package. Plans to develop instructions and a tip sheet for applicants on the website will be developed after the Congress in Prague.

IUCr Congress. The CCT is sponsoring the following sessions at the 2021 Congress:

MS-202 Machine Learning in Biological and Structural Sciences;

MS-117 Social Media and New Frontiers for Spreading Crystallographic;

MS-116 Crystallography Schools to Promote Interdisciplinarity in Science;

MS-205 Online Crystallography: Tools, Apps and Web Services; and

Special session: Using Crystallography for Education During the Pandemic.

O. A. Asojo, Interim Chair

4.9. Commission on Crystallography in Art and Cultural Heritage

The Commission (CrysAC) continues to pursue the mission of spreading crystallographic knowledge related to artworks and ancient materials. However, 2020 was a difficult year because of the COVID-19 pandemic, the severe restrictions on travelling and the cancelling of most of the meetings. We hope that the IUCr Congress in Prague will mark the restart of activities. CrysAC is involved in the preparation and chairing of two microsymposia at the Prague meeting.

Despite the situation, publication activity continued and a few lectures were delivered, mostly online.

Conferences, sessions and lectures. Marine Cotte organized the Cultural And Natural Heritage Workshop, ESRF, Grenoble, France, 22–24 January 2020. The following CrysAC members and consultants contributed to the workshop:

'Basic principles of X-ray spectroscopy' (M. Cotte);

'Scopes and objectives of the workshop' (M. Cotte);

'Cultural heritage & synchrotron radiation: Quo vadis?' (Koen Janssens); and

'Complementary use of SR and neutrons for heritage study at the NRC 'Kurchatov Institute" (Elena Tereschenko).

A workshop on the Chemistry of Lead in Oil Paintings was organized at the Rijksmuseum Ateliergebouw, Amsterdam, 20–21 February 2020. The following CrysAC members and consultants contributed to this:

'Tracking the chemical fate of Pb-containing pigments in works of art at different length and time scales' (Koen Janssens);

'The reactions of PbO with oil studied with X-ray and infrared microscopy' (Marine Cotte); and

'The reactivity of lead-based pigments versus the reactivity of oils in model paints' (Silvie Švarcová).

Gilberto Artioli delivered a keynote lecture on 'The contribution of materials analysis to archaeological research' at a school of advanced training on Analysis of Materials in Archaeology and Cultural Heritage, University of Trento, and delivered a seminar on 'Mineralogy, crystallography, art and archaeology: Science and passion' within the frame of 'UniPadova Incontra' for high-school students, Piazzola sul Brenta, in February 2020.

Sebastian Bette delivered a seminar on 'Calcium acetate hydrates: simple salts with surprisingly complex crystal structures' at the Joint Polish–German Crystallographic Meeting, Wroclaw, 25 February 2020.

Gilberto Artioli delivered an invited lecture at the Raw Materials University Day on 'Alpine copper: exploitation since prehistory to recent times', Università di Trento–KIC Raw Materials, November 2020, available from https://geo.geoscienze.unipd.it/cristalli/video/Raw%20Materials%20University%20Day%202020%20-%20Trento%20-%20Zoom-1_ga.mp4, and also delivered a seminar at the National Academy on 'Mineralogy and cultural heritage: fatal attraction', Accademia Nazionale dei Lincei, Rome, in December 2020, available from https://www.lincei.it/it/videoteca/11122020-la-mineralogia-ed-i-beni-culturali-video.

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

Gilberto Artioli, Chair, and **Alicja Rafalska-Lasocha**, past-Secretary

4.10. Commission on Crystallography of Materials

The Commission website is at https://www.iucr.org/iucr/commissions/crystallography-of-materials.

Members: Changqing Jin (Chair, China), B. Albert (Germany), E. Antipov (Russia), Wenhui Duan (China), V. Blatov (Russia), M. Eremets (Germany), Y. Gogotsi (USA) and M. Petrukhina (USA). Consultants: Tian Cui (China), V. L. Solozhenko (France), A. R. Oganov (Russia/USA), H. Maynard-Casely (Australia), O. Yaghi (USA), S. Qiu (China), Nan Zhang (China) and Y. Sugawara (Japan).

Conferences and symposia

3–5 August 2020, MXene Conference 2020, https://mxeneconference.coe.drexel.edu. Conference Chairs: Michel Barsoum, Yury Gogotsi. Online: 2400 registered participants.

11–14 October 2020, 3rd International Conference on MXenes, Ningbo, China, https://nano.materials.drexel.edu/2020/10/3rd-international-conference-on-mxenes/. Conference Chairs: Qing Huang, Yury Gogotsi. Hybrid – on site and online: 500 registered participants.

The IUCr Congress in Prague, Czech Republic, was rescheduled for 2021.

Organization of workshops to disseminate knowledge and technical skills

11–13 November 2020, 19th Online USPEX Workshop Crystal Structure Prediction with the USPEX Code. Organizers: Vladimis S. Baturin, Artem R. Oganov (Skoltech, Russia; Stony Brook University, USA). No. of participants: more than 200 researchers worldwide.

Last week of July 2020, last week of February 2021 and last week of March 2021, three one-week online courses on MXenes (https://nano.materials.drexel.edu/mxene-course/). Organizer: Yury Gogotsi. Ten instructors from Drexel University lectured to about 60 participants in each session.

Changqing Jin, Chair

4.11. Commission on Electron Crystallography

The major goals of our Commission (the CEC) are teaching and promotion of the electron crystallography science. Although COVID-19 has prevented us from meeting in person, we tried to continue our activities using online platforms, as indicated below.

Workshops/schools on electron crystallography

3D Electron Diffraction Across Nanocrystallography, GE3C Online Congress, 20 January 2020 (webinar). More than 100 participants. CEC members and consultants gave lectures.

Christmas (online) Workshop on Electron Crystallography, 17 December 2020. No. of participants: registered ∼600, actually present ∼300. The workshop was organized by CEC members and consultants as well as endorsed by the CEC. It was organized in order to fill the information gap due to the cancellation/rescheduling of the major crystallographic events. This one-day online event comprised a collection of reports from the most prominent research groups related to 3D electron diffraction.

The 39th Ad Hoc Workshop on Program *Jana* – Electron Diffraction (online), 14–15 January 2021. No. of participants: 30. Organized by CEC members. Lectures and tutorial introducing structure analysis from 3D electron diffraction data using programs *PETS2* and *Jana2020*.

Low-Dose Electron Crystallography: Fast, Easy and Powerful, 15 January 2021 (webinar organized by the Institute of Structural Biology, Grenoble, France). No. of participants: 50. CEC consultants organized and served as lecturers, and presented a 3D electron diffraction method for beam-sensitive materials.

Louisa Meshi, Chair

4.12. Commission on High Pressure

Since the IUCr General Assembly and the 25th Congress in Prague were postponed to 2021 because of the COVID-19 pandemic, the major activities of the Commission (the CHP) in this year, which were to include two dedicated high-pressure science sessions and five joint sessions with other

Commissions at the Congress, as approved by the International Programme Committee in 2019, did not happen.

In July 2020, three CHP committee members, Haozhe Liu, Kamil Dziubek and Boris Zakharov, held a long Zoom meeting with Professor Elena Boldyreva, who will be the Chair of the Local Organizing Committee for the 2021 IUCr High Pressure Workshop. After discussing all the possibilities including hybrid modes, the committee members decided to hold the upcoming workshop via Zoom at Novosibirsk, Russia, in February 2021. It was not an easy decision to make, and we also understood that it would be disappointing for many peers who were looking forward to enjoying winter time in the heart of Siberia. It seemed, however, the most sensible solution in this situation. We proposed a five-day meeting window, which would allow the remote contributors from all over the world to participate during convenient hours, considering the different time zones. This proposal was supported by the whole CHP.

Although there was no regular workshop organized by the CHP in 2020 because of international travel bans, two small related workshops/summer schools were held. CHP member Professor Natalia Dubrovinskaia organized a workshop for the IUCr/DGK (German Society of Crystallography) International Summer School on Novel Methods of Atomic and Electronic Structure at High Pressure at Bayreuth, Germany, 31 August – 4 September 2020. This school was attended online via Zoom by 25 participants from seven countries, and co-organizers included Dominique Laniel, Thomas Meier and Leonid Dubrovinsky. A detailed report of this summer school can be found in the *IUCr Newsletter* at https://www.iucr.org/news/newsletter/volume-28/number-4/the-iucrdgk-international-high-pressure-summer-school-2020-bayreuth-germany. CHP consultant Professor Andrzej Katrusiak organized the 13th Frolic Goats Workshop on High Pressure Diffraction (https://frogo.home.amu.edu.pl/#) at Poznan, Poland, 19–21 April 2020. This is an ongoing effort from Professor Andrzej Katrusiak's group with the primary goal of disseminating practical skills, allowing newcomers to perform high-pressure experiments in an X-ray lab, and then to outline possibilities for further studies at dedicated high-pressure beamlines at synchrotrons and neutron sources worldwide.

The CHP website at https://www.iucr.org/resources/commissions/high-pressure is updated and maintained by the Secretary of the CHP, Dr Kamil Dziubek.

Haozhe Liu, Chair

4.13. Commission on Inorganic and Mineral Structures

Members and consultants of the Commission (CIMS) discussed various issues via e-mail. Other forms of communication usually take place through participation at occasional meetings or conferences. However, owing to the COVID-19 global pandemic, almost no discussions took place in the period from March 2020 until May 2021.

The CIMS website is kindly maintained by M. Nespolo (CIMS member) at http://www.crystallography.fr/cims/.

The Commission on Structural Chemistry (the CSC) and CIMS maintained their links. P. Mercier (CIMS Chair) is the liaison person representing the CSC in CIMS and vice versa.

CIMS also maintains strong links with the new IUCr Commission on NMR Crystallography and Related Methods. J. Rocha (CIMS consultant) is the liaison person and also a consultant for that Commission.

P. Mercier (CIMS Chair) continued to remain available to act as liaison officer of CIMS with the *IUCr Newsletter*; however, there were no communications from the *IUCr Newsletter* during the last year.

Strong links remain between CIMS and the European Crystallographic Association. Marie Colmont (CIMS member) is Chair of the Special Interest Group SIG-05, Sergey Krivovichev (CIMS consultant) is Vice-Chair and Oleg Siidra is Secretary.

There are very good relationships between CIMS and the European Mineralogical Union (EMU, http://eurominunion.org/); R. Oberti (CIMS member) is Commissioning Editor of the *EMU Notes in Mineralogy*.

M. Nespolo (CIMS member) is Book Review Editor for the IUCr journals, member of the IUCr/OUP Book Selection Committee, Editor-in-Chief of the SpringerBriefs series for crystallography, and a consultant on two IUCr Commissions (Crystallographic Nomenclature; Mathematical and Theoretical Crystallography).

C. Ling (CIMS member) was President of the Society of Crystallographers in Australia and New Zealand (SCANZ) in 2019 and Past Secretary of the Asia-Oceania Neutron Scattering Association (AONSA). They were also Chair of Crystal-33, the 33rd meeting of SCANZ, held in early 2020. They are a member of the Australian Synchrotron's User Advisory Committee and BRIGHT Advisory Committee, and a member of the Australian National Committee for Crystallography (ANCCr).

P. Mercier (CIMS Chair) was Chair of the Canadian National Committee for Crystallography between August 2015 and December 2020.

R. Oberti (CIMS member) was elected as Corresponding Member of the Accademia Nazionale dei Lincei in Rome. They are a member of the committee on the participation of the Consiglio Nazionale delle Ricerche (CNR) to IUCr.

P. Mercier (CIMS) represented CIMS interests at the International Programme Committee meeting held in May 2019 in Prague, Czech Republic. They remained available for discussion with the IUCr Congress organizers during the last year while the Congress was being rescheduled to take place in 2021.

CIMS received no applications for funding by the IUCr in the period between January 2020 and May 2021.

The current list of CIMS members is: P. Mercier (Chair, Canada), P. C. Burns (USA) (resigned February 2019), M. Colmont (France), F. Hatert (Belgium), V. Kahlenberg (Austria), M. Nespolo (France), R. Oberti (Italy), M. Wolcyrz (Poland), A. Yoshiasa (Japan) (resigned February 2019) and N. Zubkova (Russia). A gender-balanced list of new candidates for members for the next triennium has been proposed.

It is understood that a Chair shall be elected among the new members, either prior to or at the next IUCr Congress in 2021.

Current consultants: C. Cahill (USA), G. Ferraris (Italy), J. B. Parise (USA), I. Pignatelli (France), D. Pandey (India), S. V. Krivovichev (Russia), K. Byrappa (India), J. Rocha (past Chair, Portugal), R. Carbonio (Argentina), T. Gesing (Germany), C. Ling (Australia) and M. Welch (UK). This list of consultants will be revised prior to the next IUCr Congress.

Patrick H. J. Mercier, Chair

4.14. Commission on Magnetic Structures

Preparations for the IUCr Congress in Prague

The scientific programme of the 2021 IUCr Congress in Prague will include 15 sessions with magnetic structure themes or components, among which nine microsymposia and three keynote lectures were sponsored or co-sponsored by the Commission. In preparation for the Congress, the Commission was very active during the first months of 2020 in advertising for these sessions. We reached out to the international magnetic structure community through website adverts, major mailing-list subscriptions, the IUCr World Directory of Crystallographers, attendees of past Commission-organized workshops and schools, instrument scientists at magnetic scattering beamlines, and personal contacts in developing nations.

Owing to the worldwide public health situation in 2020, the Congress was postponed until 2021, so that it was necessary to duplicate the advertising effort the following year. We are grateful that the vast majority of session Chairs and invited speakers were able to translate their involvement forward by one year. Oksana Zaharko, our representative to the International Programme Committee (IPC), deftly managed all of the required changes.

Standard development

The magCIF working group actively discussed a variety of revisions to the standard magCIF dictionary established by the Commission in 2016: improvement of the descriptions of tags related to magnetic moments and incommensurate magnetic modulations; addition of a tag for the magnitude of a magnetic moment; and creation of a new category for rotational moments (applicable to the pivot points of rigid units) that is highly analogous to that for magnetic moments.

In 2018, Branton Campbell and Harold Stokes presented a proposal for an international-standard magnetic space-group symbol, and in 2020, Juan Rodriguez-Carvajal presented a related proposal for Hall symbols for magnetic space groups. Both proposals were discussed and debated by the Commission, and improved by the feedback received. The magnetic Hall symbol concept appeared in *J. Appl. Cryst.* (2021). **54**, 338–342.

Educational/reference materials

Structure and Magnetic Neutron Diffraction (2020, 169 pp.) by Alexander N. Pirogov and Mikhail A. Semkin, Ural University Publishing House, Ekaterinburg, provides a new Russian-language source of tutorial materials for students who are new to magnetic neutron diffraction.

Scientific meetings

Most in-person research meetings were cancelled during 2020 owing to the COVID-19 pandemic. Virtual meetings supported by the Commission included the Virtual Workshop on Magnetic Structures Determination, 28 September – 2 October 2020, Oak Ridge National Laboratory, USA (co-organizer: O. Garlea; lecturers: O. Garlea, B. Campbell, J. Rodriguez-Carvajal, J. Manuel Perez-Mato, Margarida Henriques), and Workshop La Diffusion des Neutrons pour Sonder la Structure de la Matière et au-delà, 12–16 September 2020, Sete, France (lecturer: Margarida Henriques).

Branton J. Campbell, Chair, and **J. Manuel Perez-Mato**, Secretary

4.15. Commission on Mathematical and Theoretical Crystallography

Owing to the COVID-19 pandemic, activities planned by the Commission (MaThCryst), as well as most of the IUCr-sponsored activities for 2020, were cancelled or postponed. One that was held online and those that were postponed are listed below.

H. Napolitano and L. Suescun co-organized and lectured at the 3rd LACA School: Small Molecule Crystallography – Virtual Edition, UNAM, Mexico City, DF, Mexico (Part 1: 23–27 November 2020; Part 2: 7–11 December 2020; originally organized for 23–30 March 2020). Organizers: V. Jancik, N. Alvarez, F. Di Salvo, J. Ellena, H. Napolitano, M. de J. Rosales Hoz and L. Suescun. Lecturers: M. de J. Rosales Hoz, L. Suescun ('Symmetry and *International Tables for Crystallography* Volume A'; 'Symmetry of the diffraction pattern'), F. Di Salvo, J. Ellena, H. Napolitano ('Methods for structure determination'), V. Jancik, B. Noll, D. Martínez-Otero, G. Alvarado and N. Alvarez. The school had 65 students from 13 countries (including 30 from Mexico). This event was sponsored by the IUCr (https://www.iquimica.unam.mx/LACA/).

IUCr Congress and General Assembly

Discussions of lists of speakers and keynotes for the IUCr Congress in Prague (Czech Republic, planned for August 2020 but postponed until 14–22 August 2021) were held by e-mail, moderated by the International Programme Committee representative for the Commission, M. L. A. N. De Las Peñas. Thanks to the hard work and very successful and efficient negotiations of our representative, the Commission is responsible for a keynote lecture (D. Gratias) and for the organization of three microsymposia (MS-111 Graphs, Tilings and Crystal Structures; MS-112 Generalizations of Crystallographic Groups and their Applications; and MS-114 Beyond Pure Point Diffraction: Theory and Application of Diffuse Scattering), and co-sponsored another three (MS-53, MS-66 and MS-95).

Other events postponed to 2021

(i) The International School on Fundamental Crystallography (Seventh MaThCryst School in Latin America), which was planned for November 2020 at Universidad Nacional Mayor de San Marcos, Lima, Peru, organized by J. Quispe with M. I. Aroyo, M. Nespolo, L. Suescun (Commis-

sion members), A. Pentón-Madrigal and E. E. Estevez-Rams (Commission consultant) as lecturers, was postponed to November 2021 at the same location. If problems persist there the School will take place in 2022 in Goiás, Brazil, organized by H. Napolitano (Commission member) (https://www.crystallography.fr/mathcryst/lima2021.php).

(ii) SIAM Conference on Mathematical Aspects of Material Science, 17–28 May 2021, Bilbao, Spain. M. I. Aroyo, MaTh-Cryst Interim Co-chair, is a co-organizer of minisymposium MS25: Computational Geometry, Topology and Symmetry meet Material Science (MaThCryst contributors: M. L. A. N. De Las Peñas and M. I. Aroyo).

(iii) Crystallography Online: Workshop on the Use and Applications of the Structural and Magnetic Tools of the Bilbao Crystallographic Server, University of the Basque Country (UPV/EHU), September 2021, Leioa, Spain. Organized by M. I. Aroyo, MaThCryst Interim Co-chair.

L. Suescun, Commission member

4.16. 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.

In the last four years, there were significant changes in some facilities. Unfortunately, two reactor neutron sources were shut down: the Orphée reactor of the Laboratoire Léon Brillouin (LLB) in France and the BER I reactor of the Helmholtz Zentrum Berlin (HZB) in Germany. Note that the LLB remains the centre for neutron science in France with a compact accelerator-driven neutron source (CANS) project on site (SONATE). On the other hand, a spallation neutron sources was started [The Chinese Spallation Neutron Source (CSNS) in China] and one is under construction [the European Spallation Neutron Source (ESS) in Sweden; the first three instruments will be dedicated to structural measurements: a diffractometer, DREAM; a SANS instrument, LOKI; and an imaging station, ODIN]. A European association for CANS called ELENA (European Low Energy accelerator-based Neutron facilities Association) has been set up and there are several important CANS projects under test: SONATE in France with the LLB, HBS in Germany, ARGITU in Spain and LvB in Hungary. The first diffractometer is under construction at Saclay, France.

Major neutron facilities have stayed operational except for some temporary closures and/or suspension of user operations in some facilities due to the COVID-19 pandemic. Remote experiments and a rapid-access programme were widely introduced in many facilities during the pandemic.

The construction of ESS in Sweden is progressing. The first beam will be delivered in 2023, and the user programme will start in 2024 with four instruments.

The CSNS started operation in 2018 with three instruments.

The operation of J-PARC MLF in Japan is also continuing with 500 kW to 600 kW beam power; the power will be upgraded step by step every year.

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 the 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 FRM II reactor of the Heinz Maier-Leibnitz Zentrum (MLZ) in Germany resumed standard operation from January 2020.

The Japanese Research reactor (JRR-3) has relaunched operation from February 2021 after a ten-year shutdown.

The High Flux Isotope Reactor (HFIR) in the USA continued operation at 85 MW, providing more than 3900 neutron production hours annually.

On 23rd March 2020 ANSTO moved to an essential and critical operations mode with all scientific research infrastructure being shutdown, including the Australian Centre for Neutron Scattering (ACNS). ACNS recommenced user operations on 23rd June 2020 with a focus on clearing the backlog of proposals unable to be run because of COVID-19 travel restrictions and the ANSTO shutdown, and the recently approved 2020–2 round proposals, initially using mail-in services and then progressively to Sydney-basin users and interstate users. Since then the OPAL reactor has continued to operate, with the long shutdown scheduled for June 2020 now postponed to June 2021. Unfortunately international borders have not opened and are not planned to until early 2022. However, recently (April 2021) a travel bubble between Australia & New Zealand has opened up, allowing New Zealand researchers to visit ANSTO to undertake measurements. The ACNS provided additional support to early-career researchers (ECRs) in 2020/2021, and prioritized discretionary beam-time proposals to backfill COVID experiment cancellations, undertaking 51 discretionary proposals supporting ECRs.

The ACNS opened the Spatz neutron reflectometer to the user community in 2020. The BioRef neutron reflectometer was transferred from the BER-II reactor in Berlin to ANSTO in February 2017 and renamed ‘Spatz’, which is German for ‘sparrow’. Spatz adds significant capability and capacity to the existing suite of neutron-scattering instruments at the OPAL reactor, and is ideally suited to the investigations of soft matter, biomedicine, energy and materials science.

Our Commission members were also involved in organizing several meetings, not only for neutron but also for quantum beam (synchrotron, neutron and ion radiation *etc*.) joint use. In 2020, we also planned many meetings, including various annual meetings of regional crystallographic associations. However, most of these were postponed or cancelled, and some are now virtual meetings owing to the COVID-19 pandemic.

Several neutron schools at many facilities and crystallographic seminars were supported by Commission members in each year in many countries or regions. In 2020, some of these schools and seminars were held in virtual classrooms. These included the annual Powder Diffraction Workshop held jointly by the ACNS and the Australian Synchrotron. The annual Small Angle Scattering Workshop organized by the ACNS with the Australian Synchrotron was also held remotely in 2020.

Commission members were involved in planning activities for several important neutron-related conferences and schools in 2021. Owing to the still-rampant pandemic, many conferences, workshops and schools will be held in virtual classrooms.

T. Ishigaki, Chair

4.17. Commission on NMR Crystallography and Related Methods

The Commission was created at the 2014 Montreal Congress of the IUCr. At the Prague Congress in 2020, the Commission was to have ended its second triennium. In deference to, and not to compete with the programme of the Prague Congress, many of the annual activities of the Commission were put on hold, as was done in anticipation of the Hyderabad Congress in 2017. 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. The global pandemic coincided with this planned pause, although made it worse in some ways.

We anticipate that much of the planned programme content regarding NMR crystallography will be in place for the hybrid format of the Prague Congress in 2021. Because of the year-long interruption in 2020, we anticipate it will not be until 2022 when the activities of the Commission resume their normal, pre-pandemic pace.

M. Mehta, Interim Chair

4.18. Commission on Powder Diffraction

Perhaps not unexpectedly, the COVID-19 pandemic has impacted significantly on the activities and planning of the Commission on Powder Diffraction (the CPD). This has resulted in the postponement and in some cases cancellation of meetings and workshops while members focused on more immediate crises impacting on them personally and professionally.

Unfortunately the pandemic that started in 2020 also resulted in the 17th European Powder Diffraction Conference (EPDIC17) in Croatia as well as the 25th Congress and General Assembly of the IUCr being rescheduled (the Prague meeting to 2021 and EPDIC17 to 2022). Professor Brendan Kennedy continues as the CPD representative on the International Programme Committee for the IUCr Prague Congress.

The CPD is 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 – 8 June 2024.

The 3rd Southern African Powder Diffraction Conference and Workshop is also in the early planning stages and provisionally scheduled for 2023.

It has proven rather challenging to make progress with a number of projects, mostly this is understood to be because of limited resources and the already-high demands on their time from their primary employers experienced by most members. It might be worthwhile approaching some retired ex-CPD members for this, possibly as commissioned work for which funding can be sought.

Ongoing CPD projects include:

Recommended practice and publication guidelines: Most members are concerned about the poor quality of data published in many journals and the fact that this is generally exacerbated by poor reporting and/or poor interpretation of the data.

QPA Round Robin. After approximately 20 years the Commission has decided to put together another Quantitative Phase Analysis Round Robin, to assess the current state of this traditionally very important part of powder diffraction, particularly the impact that improved instrumentation, software and methodologies might have had on the field. The project will be coordinated by Dr Matthew Rowles from Curtin University in Australia. This is a considerable undertaking and will require the hiring of a temporary assistant. To cover this as well as the operational expenses, the CPD hopes to raise financial support from suppliers and other interested parties. Dr Rowles will put together a more detailed project plan and budget.

Powder CIF project. It appears that this project has become dormant in the last triennium and it is necessary to reconsider an appropriate course of action once we have clarity of its current status.

Commission publications: It is hoped that the *Guidelines* as well as the Call and subsequent results from the QPA Round Robin will all be published in IUCr Journals.

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

D. Billing, Chair

4.19. Commission on Quantum Crystallography

The members of the Commission on Quantum Crystallography (QCr) were particularly eager to attend the IUCr meeting in Prague and were looking forward to the micro-symposia co-organized with other Commissions. The rapid spread of COVID-19 decided otherwise and forced us to change our plans. The Commission thus decided by a large majority to organize an online meeting. This was seen as an opportunity to propose an alternative to traditional events and to pave the way for a new kind of scientific gathering. Rather than a succession of plenary speeches, emphasis was placed on

the possibility of free exchange of ideas and opinions. The aims of this Quantum Crystallography Online Meeting 2020 (QCrOM2020) were to increase the size of the community and broaden the scope of the topic itself. Particular care was taken to encourage attendance by the youngest researchers, the oldest researchers, and those with physical disabilities and/or with financial difficulties. From very early on it was decided that we should offer this meeting for free. The last-minute organization hampered efficient communication, yet we were quite happy to welcome close to 120 registrations (from more than 20 countries).

As promised, most activities of the three-day meeting (27–29 August) were dedicated to poster sessions and open discussion meetings (How do scattering and spectroscopy methods combine in quantum crystallography?; Quantum crystallography at the crossroad: the challenge of becoming popular; What is hot in quantum crystallography, what needs to be solved?). Each day a new poster session was organized during two different time slots so that participants from extreme time zones could always easily attend. The discussion meeting was during the GMT+2 lunchtime, which suited most of the attendees. Additionally, each day between two and four plenary talks were organized and recorded for replay. Finally, for each poster session, a jury nominated a recipient for a best poster presentation award with gift certificates offered by one of our sponsors, World Scientific Publishing Co.

To encourage newcomers to the QCr community, a satellite conference day (26 August, called 'Day 0') was proposed with three introductory talks by prominent scientists with great pedagogical skills.

The entire meeting was held online, on a website specially designed for this very purpose by four students (Sara Delahaie, Antoine Marras, Nizar Melk and Hugo Julien) from CentraleSupelec School (France). They also served as the local organizing committee, helping the participants to register, collect the abstracts and fix remote connection issues. They guided the presenters and the attendees to their (virtual) poster rooms or the (virtual) hall for the plenary talks.

All the feedback collected from the participants was extremely enthusiastic and many suggested that when the situation goes back to normal such an enriching meeting could be held again as a useful addition to the traditional conferences.

It was also decided that the appointment of a new Commission Chair would be postponed by one year, and would take place during the IUCr meeting in Prague in 2021.

Jean-Michel Gillet, Chair

4.20. Commission on Small-Angle Scattering

This report was prepared by U-Ser Jeng, Chair, together with members David Babonneau, Kristina Djinovic Carugo, Elliot Gilbert, Duncan McGillivray, Jan Ilavsky, Eleonora Shtykova and Masaaki Sugiyama, and consultants Andrew Allen, Javier Pérez, Daniel Clemens, Pete Jemian, Jill Trewhella, Dmitri Svergun, Iris Torriani and Florian Edouard P. Meneau.

For 2020, the business of the Commission (CSAS) was conducted totally via e-mail, as personal meetings at national and international conferences were not possible owing to the COVID-19 pandemic. The pandemic resulted in the postponement of the 2020 IUCr Congress (and the planned SAS 2021 Conference) by a full year, and extension of the usual IUCr triennium to four years. The pandemic restricted many activities for all CSAS members and consultants. Nevertheless, what follows is a summary of activities for 2020.

Commission activities, meetings and communication

Andrew Allen served as CSAS representative, throughout 2020, on the International Programme Committee (IPC) for the IUCr 2020 Congress, now planned for August 2021 as a hybrid conference with participation in Prague, Czech Republic, for some and as a virtual conference for others. Andrew continues to serve as a member of the IPC both as CSAS representative and as IUCr Journals Editor-in-Chief. As CSAS representative, Andrew is hopeful that the several previously negotiated SAS-related microsymposia and SAS-related keynote talk will proceed as part of the overall IUCr Congress programme.

U-Ser Jeng served as CSAS Chair, recommended an IUCr2020 Workshop on GISAXS-GIWAXS by Eva Herzig, R. Joseph Kline and U-Ser Jeng, and updated the CSAS website, including the historical data about SAS conferences. U-Ser Jeng also wrote to the organizer of the SAS-2021 triennial conference (Dr Florian Edouard P. Meneau) to say that CSAS recommended a postponement of the SAS-2021 triennial conference at Campinas, Brazil, to 2022 (now rescheduled to 11–16 September 2022), to avoid competing with the rescheduled IUCr2021 Congress and ongoing conflicts between the IUCr Congresses and SAS triennial meetings. Dr Meneau indicated that the organizers of SAS-2022 might be interested in producing a Special Issue of *Journal of Applied Crystallography*, depending on the conference budget. Dr Meneau was also appointed as a new consultant for CSAS.

U-Ser Jeng also worked with the Chair/Co-chairs of the two SAS workshops and six SAS-related microsymposia at the 25th IUCr Congress to promote them, and organized funding from the NSRRC for the workshops.

Educational activities

Andrew Allen worked with IUCr Editorial Office staff in initial planning of IUCr Journals Author Workshops and other activities for the postponed Congress, and at least one virtual meeting/workshop for prospective and existing IUCr journal authors is planned.

U-Ser Jeng arranged a three-day exhibition on BioSAXS applications in the annual exhibition of Future Tech 2020, Taiwan.

Eleonora Shtykova, with the help of Maxim Petoukhov, has been running a weekly online seminar on processing and interpretation of small-angle X-ray scattering data for students, postgraduates and young scientists at educational and scientific institutions in Moscow. Eleonora was also involved, with Vladimir Volkov, in a summer workshop on small-angle X-ray scattering methods for fourth- and fifth-year

students of the Physics Faculty of Moscow State University, and gave a lecture for students of the Faculty of Bioengineering and Bioinformatics of Moscow State University on the use of small-angle scattering in the study of biological objects and modern nanomaterials as part of the course Selected Physicochemical Methods in Biology. For an online seminar jointly conducted by the Department of Physicochemical Methods of Research and the Center for Collective Use 'SKIF' of the Institute of Catalysis of the Siberian Branch of the Russian Academy, Eleonora gave an invited talk 'Introduction to small angle scattering and structural nanodiagnostics'.

Jan Ilavsky maintains the APS SAXS Special Interest Group page at https://small-angle.aps.anl.gov/.

Elliot Gilbert gave an invited lecture at the Institute of Physics Food Physics conference on 'Exploiting neutron scattering to reveal the structure of food materials'.

Elliot also served on a panel highlighting opportunities for nuclear techniques, including SAS, to investigate food materials in the Women for Nuclear Science Education and Communications (W4NSEC) conference – a continuing education programme for female university science teachers and science communication professionals – hosted by the International Atomic Energy Agency and ANSTO. In addition, Elliot gave three lectures at the EMBL Online Lecture Course on Solution Scattering from Biological Macromolecules (May–June 2020), an online introductory lecture at the P12 Users Meeting 2020 (17 November 2020), an online lecture at the INSTRUCT theoretical and practical course Integrative Structural Biology in Latin America (24 November 2020) and an online lecture at the Predoctoral Course of the EMBL (28 November 2020).

Liubov Dadinova, a young scientist from the group of Eleonora Shtykova, as part of the International Youth Scientific Forum Lomonosov-2020, gave an invited talk 'What do you need to know to overcome bacterial resistance?' as an example of the possibilities of small-angle scattering for studying complex biological objects.

Community-building activities

During 2020, Andrew Allen served as Editor-in-Chief of IUCr Journals. As such, Andrew continues to encourage negotiations between the (now) SAS 2022 Conference organization and IUCr Journals for an open-access Special Issue of the *Journal of Applied Crystallography* to be created, associated with the conference. While some uncertainties remain due to the effects of the pandemic in Brazil, as elsewhere, it is hoped these will be resolved during 2021.

Jan Ilavsky became a Co-editor for the *Journal of Applied Crystallography* in April 2020.

Elliot Gilbert continues to serve as a Co-editor for the *Journal of Applied Crystallography* and on the Editorial Board of *Food Structure*.

D. Svergun continued as a Co-editor of the *Journal of Applied Crystallography* and as a member of the Associate Editorial Board of *Frontiers in Molecular Biosciences*, section Structural Biology.

U-Ser Jeng continued to serve as Co-editor for the *Journal of Synchrotron Radiation*.

Jill Trewhella continued community-building work with the biomolecular structure community in the role of Chair of the Protein Data Bank (PDB) Small-Angle Scattering Validation Task Force (SASvtf) and as a member of the Hybrid and Integrative Methods Validation Task Force (IHMvtf). Jill continued as a Co-editor (Biology and Medicine section) for *IUCrJ*, as an Editorial Board member for *Biophysical Journal* and as an International Advisory Board member for *Protein Science*.

Consultant activities

Andrew Allen continued to provide informal input for drafts for ISO standards on the use of small-angle scattering, specifically SAXS for particle characterization. Some revision was completed for the existing ISO standard on particle size determination using SAXS, and significant progress was made in 2020 on the new ISO standard being drafted to cover surface area measurement using SAXS methods. As previously reported, critical aspects of characterizing particle size distributions (not just mean size), and particle shape, are now being incorporated into the new standard as key issues in relating surface area measurements (using Porod scattering *etc.*) to particle size and volume fraction.

Eleonora Shtykova and Vladimir Volkov participated as consultants in a federal program for the development of a high-brilliance biological SAXS/WAXS beamline at the Russian SSRS-4 facility.

Jan Ilavsky serves as Chair of the Beamtime Proposal Review Committee for ORNL SANS instruments and has served as a reviewer for NIST SANS instruments as well as the SSRL SAXS instrument. Jan is a member of the Diamond X-ray source for nano-focused X-ray investigations for Soft-Condensed Matter (X4SCM) beamline User Working Group to provide technical and scientific advice. X4SCM will provide monochromatic and high-flux 'pink' X-ray modes for a multi-purpose X-ray beamline enabling time-resolved studies that will simultaneously cover the USAXS/SAXS/WAXS range. Jan is also a member of International Advisory Committee for SAS2021 (now SAS2022) in Campinas, Brazil.

Elliot Gilbert serves as a reviewer for the Swedish government research and development agency in 'Industrial pilot projects for utilization of large scale infrastructures for neutron- and photon-based techniques'.

D. Svergun continued to serve on the Scientific Advisory Committee (SAC) of the National Synchrotron Radiation Research Center, Taiwan. Owing to the pandemic, no SAC meeting took place in 2020.

Jill Trewhella continues to serve as a member of the Protein Data Bank Advisory Committee, providing expert input on small-angle scattering and its role in integrative/hybrid structure determination.

Daniel Clemens is a member of the Scientific and Technical Advisory Panel of the European Spallation Sources for future instrumentation for neutron reflectometry and small-angle neutron scattering. Daniel also serves as a member of the

Neutron Science Advisory Council of The Pennsylvania State University.

Organizational activities

D. Svergun was a co-organizer of an EMBL Online Lecture Course on Solution Scattering from Biological Macromolecules, together with Melissa Gräwert and Al Kikhney from D. Svergun's group. The course was run on Tuesdays and Thursdays from 5 May to 2 June 2020 in the form of online lectures followed by discussion, and was aimed at young biochemists/biophysicists and researchers active in related structural methods but with little or no experience in solution scattering. The course covered basics of SAXS, instrumentation, sample preparation, modelling techniques and complementary use with other methods. Participants sent their questions/comments through the text chat during/after the lectures. There were a total of nearly 600 registrants for the course, and its materials including the lectures and videos are available at https://www.embl-hamburg.de/biosaxs/courses/embl2020/.

D. Svergun's group also conducted a P12 Virtual User Meeting on 17–19 November 2020 (organizers: Clément Blanchet, Melissa Gräwert and Dmitri Svergun). P12 is a SAXS beamline run by the group at the Petra-3 storage ring in Hamburg, and the User Meeting stimulated information exchange between the group and the user community. Recent beamline developments were presented and the users reported SAXS results as poster presentations, flash talks and selected oral presentations. The meeting had over 150 registrants (https://www.embl-hamburg.de/biosaxs/courses/users2020/).

David Babonneau continued to serve as Chair of the Peer Review Committee 3: Matter and Material Properties: Structure, Organization and Characterization, Elaboration for beam-time allocation at the SOLEIL synchrotron, France.

International activity

Eleonora Shtykova took part in the International Taiwan–Russia NSRRC–JINR webinar Bi-lateral Scientific Cooperation in Physics, Chemistry and Bio-Medicine on 10 September 2020, where a small-angle scattering section was organized. (U-Ser Jeng participated from the NSRRC side.)

David Babonneau will be a Co-chair of MS-180, Integrative Methodologies for Novel Thin Film Structures, at the 25th IUCr Congress in Prague, Czech Republic.

Technical activities

During 2020, Andrew Allen continued to provide technical support to users of the NIST Standard Reference Material (SRM) SAXS Intensity Standard: NIST SRM 3600, and continued to encourage development of a SAXD q-Calibration Standard NIST SRM.

Eleonora Shtykova reports that the new programs *BILMIX* and *ELLLIP* (developed by Maxim Petoukhov and Petr Konarev) have been included in the latest release of the *ATSAS* program suite available for academic users at https://www.embl-hamburg.de/biosaxs/software.html.

Jan Ilavsky is lead instrument scientist for the USAXS/SAXS/WAXS instrument at the Advanced Photon Source, ANL, USA. Jan also maintains the software packages *Irena* and *Nika* used widely by the materials science SAS community for data reduction and analysis. Two updates to the packages were released in 2020, and the total combined number of unique installations in 2020 was over 1000.

Elliot Gilbert is beamline scientist for the QUOKKA SANS instrument at the OPAL facility in Australia and continues to have a focus on the development of novel sample environments to generate increased utilization and demand for SANS.

U-Ser Jeng continued to lead a team operating a SAXS beamline at the Taiwan Light Source of the NSRRC. The advanced BioSAXS beamline at the 3.0 GeV Taiwan Photon Source has been opened for users since November 2020, after five years of planning and construction. U-Ser Jeng gave invited talks on the new BioSAXS beamline during the annual meeting of TWNSS neutron society.

D. Svergun's group continued to maintain and curate the Small Angle Scattering Biological Data Bank (https://www.sasbdb.org/; main curators A. Kikhney and C. Jeffries), which presently contains over 1900 data sets and over 2500 models. The *ATSAS* program package developed by the group is presently at version number 3.0.3, and, as of 2020, *ATSAS* has been downloaded over 110 000 times and is utilized in over 50% of publications on biological SAS.

D. Svergun was involved in collaborative research at the beamline P12 in Hamburg with the biotechnology company BioNTech to support development of anti-COVID mRNA vaccines (https://www.embl.org/news/science/biontech-uni-mainz-embl-hamburg/). Three collaborative papers were published with this company in 2020.

In another COVID-related collaborative project, SAXS at P12 was used for screening and characterization of synthetic mini-antibodies called sybodies, which are able to bind to SARS-CoV-2 and prevent it from infecting human cells (https://www.embl.org/news/science/sybody-against-sars-cov-2/).

Jill Trewhella notes that the *2017 Publication guidelines for structural modelling of small-angle scattering data from biomolecules in solution: an update* by Trewhella *et al.* in *Acta Cryst. Section D* continues to attract strong readership with more than 100 citations and over 11 600 downloads since going online, and increasing uptake in the community of the recommended tables for presentation of methods and results as well as data deposition.

Jill Trewhella, in her capacity as Chair of the PDB SASvtf, is continuing as the lead coordinator for the initiative that aims to generate a set of SAS data sets that can be used to benchmark different approaches to predicting SAS profiles from atomic coordinates (see https://sas.wwpdb.org/?q=node/25 for full details and participants). The effort included CSAS consultants Javier Pérez and Dmitri Svergun, and has grown to include 41 structural-biology and SAS experts from across Europe, Asia and the Americas. During 2020, data analysis has been progressing for the 150 SAXS data sets and more than 70 SANS data sets submitted from 12 SAXS facilities and four SANS facilities, including SEC-SAXS and batch SAXS, SEC-SANS and batch SANS in H_2O and D_2O. The analysis so far shows a strong consensus in the results obtained in terms of

overall conformational parameters as well as in the detailed shapes of the scattering profiles. A draft paper is in progress for submission to *Acta Cryst. Section D* and work is proceeding toward deposition of a set of data suitable for benchmarking methods for SAS profile prediction.

Masaaki Sugiyama developed a laboratory-based size exclusion chromatography SAXS system in Kumatori, Japan.

Daniel Clemens provides technical support in the handover process of HZB neutron scattering instrumentation to international partner institutes in Germany, Poland, the Netherlands, France, Switzerland, Hungary, Argentina and the USA.

U-Ser Jeng, Chair

4.21. 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 Commission on Inorganic and Mineral Structures and the Commission on Crystallographic Teaching, as well as with important external bodies such as the Cambridge Crystallographic Data Centre (CCDC).

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 that aim to expand crystallography to underrepresented regions such as South America and Africa; (ii) support for IUCr journals, through encouraging submission of excellent scientific results to *IUCrJ* and the other journals, and (iii) building relations with other Commissions and external bodies such as IUPAC and the CCDC. In considering the future composition of the Commission, it could also be of value to include a member or consultant to represent relevant industries.

Since our last annual report, the CSC lent support to the following conferences and schools, which draw on crystallographers in the structural chemistry sphere:

Gordon Research Conference on Crystal Engineering, USA, June 2020. Organizing committee contact: Jennifer Swift.

SARX, Puebla, Mexico, November 2020. Organizing committee contact: Javier Martínez Juárez.

3rd Pan-African Crystallography Conference, Nairobi, Kenya, January 2021. Organizing committee contact: Dickson Andala.

Zurich Crystallography School, Zurich, Switzerland, June 2021. Organizing committee contact: Tony Linden.

ICCOSS XXV, Ohrid, Macedonia, June 2021. Organizing committee contact: Panche Naumov.

6th Conference of the Bangladesh Crystallographic Association, Dhaka, Bangladesh, January 2021. Organizing committee contact: Altaf Hussain.

International School of Crystallography on Molecular Crystal Engineering, Erice, Italy, May 2021. Organizing committee contact: Annalisa Guerri.

International School on Advanced Porous Materials 2, Como, Italy, June 2021. Organizing committee contact: Simona Galli.

In each case, the CSC members and consultants 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 played a role in the degree of support that was expressed to the IUCr Calendar Committee.

Unfortunately, the COVID-19 pandemic has played havoc with conference organization in 2020 and 2021, with the following effect on conferences which the CSC supported:

Cancelled: SARX, Puebla, Mexico, November 2020.

Moved to online/virtual:

4th International Symposium on Halogen Bonding (ISXB-4), Stellenbosch, South Africa, March 2020, held online in November 2020.

3rd LACA School on Small Molecule Crystallography, Mexico City, Mexico, March 2020, held online in November 2020.

6th Conference of the Bangladesh Crystallographic Association, Dhaka, Bangladesh, held online in January 2021.

International School of Crystallography on Molecular Crystal Engineering, Erice, Italy, held May 2021.

Postponed:

6th European Crystallography School (ECS), Budapest, Hungary, July 2020, postponed to July 2021.

International School on Advanced Porous Materials 2, Como, Italy, June 2020, postponed to September 2021, and to be held online (to be confirmed).

AICS Italy Crystallography School, Parma, Italy, September 2020, postponed to September 2021.

Gordon Research Conference on Crystal Engineering, USA, June 2020, postponed to July 2022.

3rd Pan-African Crystallography Conference, Nairobi, Kenya, January 2021, postponed to January 2023, with a virtual e-PCCr planned for January 2022.

Zurich Crystallography School, Zurich, Switzerland, June 2021, postponed to June 2022.

ICCOSS XXV, Ohrid, Macedonia, June 2021, postponed to July 2022.

A further casualty of COVID-19 was the IUCr Congress 2020 in Prague, Czech Republic, which has also been postponed by one year, and will be held in hybrid mode. We look forward to a successful IUCr-25 in Prague in 2021, which will include a strong chemical crystallography programme.

Susan Bourne, Chair

4.22. Commission on Synchrotron and XFEL Radiation

The mission of the Commission on Synchrotron and XFEL Radiation is to promote access and awareness of crystallographers worldwide to the world's synchrotron radiation

(SR) and X-ray free-electron laser (XFEL) facilities. To this end, the Commission promotes the development of crystallographic instrumentation, technology and standards, and the synergies between storage-ring-based and LINAC-based next-generation XFEL sources. The bulk of the Commission's work is carried out via e-mail, with occasional face-to-face meetings held at selected conferences attended by a sufficient number of Commission members.

The current members (with year appointed) are P. Grochulski (Canada) (2008), Chair; M. A. Garcia-Aranda (Spain) (2011); Y. Murakami (KEK, Japan) (2011); S. Pascarelli (France, then Germany from 2019) (2011); J. Smith (USA) (2011); T. Tschentscher (Germany) (2014); E. Granado (Brazil) (2014); M. Kozak (Poland) (2017); S. Ramaswamy (India) (2017); and T. Hatsui (Japan) (2017). The consultants are R. Garrett (Australia) (previous Chair), D. Fritz (USA), S.-I. Adachi (Japan), M. Suchomel (USA), M. K. Sanyal (India), N. Zatsepin (Australia) and Lisa Keefe (USA).

Synchrotron radiation and free-electron laser facilities

Following the beginning of operations of the first 'fourth-generation' storage ring, MAX IV in Sweden, many synchrotron facilities have been planning to upgrade or build new rings. For example, the ESRF has announced the completion of a major upgrade, and officially started operation on 25 August 2020. The APS upgrade was approved in December 2018, and replacement of the ring will start in 2022. 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 fourth-generation Brazilian facility, was erected in 2018. The first loop of electrons of this 518 m storage ring was achieved on 22 November 2019. Other facilities will also adapt the new high-brightness designs including: the 6 GeV High Energy Photon Source (HEPS) to be built near Beijing, China, and the 3 GeV facilities SLiT-J (Tohoku, Japan) and SPS-II (Thailand).

There are now five 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 late 2017, with all three SASE FELs at the European XFEL now operational. 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 its instrument portfolio and in 2020 started the operation of their soft X-ray FEL and instruments. In addition, with SHINE, a new 8 GeV cw-mode superconducting accelerator FEL facility is under construction in Shanghai (China).

Supported meetings, schools and workshops

The Commission provided letters of support and endorsement for the following meetings in 2020:

RapiData 2020 at the SSRL course on automated data collection. The Commission has endorsed this annual event for many years, and did so again for the school held at the Stanford Synchrotron Radiation Lightsource in March/April 2020.

Conference on X-ray Absorption Fine Structure (XAFS 2021), Sydney, Australia, July 2021.

XVII Latin American Congress of X-ray Applications (SARX 2020), and X National Congress of Crystallography.

16th School on Synchrotron Radiation, organized by the Italian Radiation Society in collaboration with Elettra, 13–24 September 2021.

In general, the Commission has strongly supported IUCr sponsorship for the purpose of assisting attendance by young researchers and scientists from developing countries.

The European XFEL organized with various partners several major events for the FEL community in 2020. Owing to the COVID-19 pandemic, all were organized as fully remote meetings. In early August the 'Science at FELs' conference, hosted by DESY and the European XFEL, and co-organized with the FELs of Europe consortium, was held as a fully remote conference, including tutorials, lectures and posters. This meeting was attended by more than 400 participants. The European XFEL and DESY also organized an annual collaboration meeting of the Hard X-ray FEL facilities as a remote event. In addition to the five member facilities (LCLS, SACLA, PAL-XFEL, the European XFEL and SwissFEL) collaborators from SHINE were also invited.

Activities of Commission members and consultants

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

Miguel A. G. Aranda was Chair of the ESRF Council 2018–2020, and gave an invited (online) talk: 'Quantitative analysis of building materials by synchrotron X-ray ptychographic nanotomography' at the 2020 MSC SMC Symposium (the meeting of the Microscopical Society of Canada) in June 2020. In March 2020, Miguel gave an (online) seminar entitled 'Synchrotron radiation techniques: applications to material science' within the HERCULES European course.

Pawel Grochulski is a Scientific Advisory Committee member of SOLARIS and a member of the IUCr Commission on Biological Macromolecules.

Thomas Tschentscher was Chair of the Virtual 2020 Hard X-ray FEL collaboration meeting, 9–10 September 2020, and Co-chair of the SRI 2021 Local Organizing Committee.

Eduardo Granado was a founding member of the LNLS Users Committee, and a member of the Organizing Committee of the 30th LNLS Annual Users Meeting, 9–12 November 2020.

Sakura Pascarelli was a member of the Scientific Advisory Committee for SRI 2021.

Asia Oceania Forum for Synchrotron Radiation

The Asia Oceania Forum for Synchrotron Radiation Research (AOFSRR) is an international network of synchrotron and XFEL light source facilities and user organizations in the Asia Oceania region. Commission consultant Richard Garrett is Secretary–Treasurer of the forum, and Commission member Youichi Murakami was AOFSRR President in 2015–2016. The Forum holds an annual week-long school for graduate students and early-career researchers, which rotates between the AOFSRR members, and an annual

workshop. In 2019 the AOFSRR announced that it would establish an Asia Oceania Synchrotron Radiation Instrumentation conference series (AO-SRI), to be held every three years between the international SRI conferences.

Owing to COVID-19 and the restrictions on international travel, all in-person AOFSRR events planned for 2020 were postponed. The 2020 AOFSRR Synchrotron School, to be hosted by the Synchrotron Light Research Institute, Thailand, is now planned for November 2021. The first AO-SRI Conference will be held in Sendai, Tohoku District, Japan, chaired by the Photon Science Innovation Center and hosted by Tohoku University International Center for SR Innovation Smart. The conference, originally planned for late 2020, has been postponed to 2022.

Pawel Grochulski, Chair

4.23. Commission on XAFS

Members and duties

In the XAFS Commission (CXAFS) we assign each member a 'portfolio' of responsibility, which aids our division of labour and hopefully productivity.

During the 24th IUCr Congress and General Assembly (August 2017) in Hyderabad, India, the following members and consultants of CXAFS were approved:

Christopher T. Chantler (Australia, initially appointed to Commission 2008), Chair 2014–2020; Valérie Briois (France, 2017), Secretary; Sofia Diaz-Moreno (UK, 2014), Secretary, website; Guiliana Aquilanti (Italy, 2014), liaison with the International Programme Committee; Dibyendu Bhattacharyya (India, 2017), coordinator of funding support including from IUCr Congress organisers and the IUCr for critical missions (IUCr Congress, Workshop, Satellite, IXAS, Q2XAFS, other); Yasuhiro Inada (Japan, 2017), working group on databases and coordinator of summary from Japan XAFS Society; Narcizo M. Souza-Neto (Brazil, 2017), IUCr dictionary of XAFS terminology; Steve M. Heald (USA, 2014), liaison with *International Tables for Crystallography* and IUCr Journals; Krystyna Lawniczak-Jablonska (Poland, 2011), coordinator for Q2XAFS workshop (Poland), IXAS liaison; Carlo Lamberti (Italy, 2017–2019, sadly deceased), IUCr Congress Workshop, liaison to *International Tables*.

Consultants: Federico Boscherini (Italy), Farideh Jalilehvand (Canada), Peter Glatzel (France), Richard Strange (UK), Hiroyuki Oyanagi (2014–2019, sadly deceased) (Japan).

Note: We have created a special section titled 'In memoriam' on the CXAFS website to recognize the contributions of both Hiroyuki and Carlo to XAFS and the community during their careers (https://www.iucr.org/resources/commissions/xafs/in-memoriam), and we have coordinated joint sessions in honour of both at the coming (now 2021) International XAS Conference to be held in Sydney. In particular, we have invited Hiroyuki's wife and son to be at the relevant session.

International Tables for Crystallography

All Editors have been working diligently towards the new volume of *International Tables for Crystallography*, Volume I, *X-ray Absorption Spectroscopy and Related Techniques*, and good progress has been made. The Editorial Office plan to post major sections online as they become ready. Some contributors have been patient with their accepted or revised manuscripts and more are likely to be accepted within the next few months. The quality of the articles is in general excellent and will make a major contribution to the literature, reference works and field. The first 10–20 chapters of *ca* 160 have been edited and typeset by the Editorial Office and are now online at https://it.iucr.org/I/, with all Editors working towards critical and missing sections and chapters. The quality of the formatting and typesetting is excellent as expected.

IXAFS conferences

CXAFS members participated in the 2020 online conference organization (Australia) and organization preceding the primary XAFS meeting 2021 (Sydney).

25th IUCr Congress in Prague

Thanks to efforts from all of the Commission and especially our liaison Guiliana and Chairs and Co-chairs, we have a new record number of microsymposia organized/co-organized by CXAFS for Prague.

One unshared microsymposium: MS60 Catalysis: Functionalized Materials Studied by XRD and XAFS. Co-chairs: V. Briois (France), A. Roodt (South Africa).

Shared microsymposia:

MS61 XAS and Crystallography Allied for Geomaterials and Environmental Problems (shared with the Commission on Inorganic and Mineral Structures). Co-chairs: F. Mosselmans (France), A. Martucci (Italy).

MS57 Advanced Methods for Analysis of XAFS and Crystallographic Data (shared with CommDat). Co-chairs: M. Girogetti (Italy), M. Milanesio (Italy).

MS59 Disordered Materials: Spectroscopic and Scattering Techniques (shared with the Commission on Neutron Scattering). Co-chairs: A. Trapananti (Italy), J. Simon (USA).

MS58 Spectroscopy Applied to Electrochemistry: Operando Studies (shared with the Commission on NMR Crystallography and Related Methods). Co-chairs: D. Bhattacharyya (India), J. Plaisier (Italy).

MS37 Matter at Extreme Conditions at SR and XFEL: Complementarity of Spectroscopy and Diffraction (shared with the Commission on High Pressure and the Commission on Synchrotron and XFEL Radiation). Co-chairs: U. Zastrau (Germany), A. Rosa (France).

MS54 X-ray Spectrometry and X-ray Diffraction in Art and Archaeology (shared with the Commission on Crystallography in Art and Cultural Heritage). Co-chairs: G. Cibin (UK), P. Bezdicka (Czech Republic).

MS138 The Mineral/Life Interface – Prebiotic Chemistry, Biomineralization, Advanced Biomimetic Materials (shared with the Commission on Crystal Growth and Characterization of Materials). Co-chairs: J. M. Garcia-Ruiz (Spain), G. Falini (Italy).

MS181 4th Generation SR and XFEL Facilities (shared with the Commission on Synchrotron and XFEL Radiation). Co-chairs: M. Thunissen (Sweden), M. Yabashi (Japan), S. Diaz-Moreno (UK).

MS52 Combining X-ray Diffraction and Spectroscopy to Characterize Materials (shared with the Commission on Powder Diffraction). Co-chairs: C. Meneghini (Italy), S. Schmid (Australia).

Furthermore, two keynote speakers proposed by CXAFS have been accepted: Federico Boscherini, 'X-ray absorption spectroscopy and materials science: recent advances' and Britt Hedman, 'The role of XAS in biology'.

IUCr XAFS Workshop

The next workshop dedicated to XAFS for crystallographers was to be organized the day before the Congress. This one-day, almost free tutorial workshop would have provided an overview of the physics and chemistry of X-ray absorption spectroscopy with a particular emphasis on its complementarity with diffraction techniques. The curriculum included introductions to beamline instrumentation, measurement methods, and methods of data processing and analysis. Details can be found at https://www.xray.cz/iucr/workshops/xafs/. However, owing to the COVID-19 pandemic this has been postponed to the next Congress.

Impact on CXAFS of the COVID-19 pandemic

Naturally efforts during this 'bonus year' have been directed towards preparing for the Congress, the handover to new Commission members and also some efforts towards the Workshop and Q2XAFS activity. Work towards other areas has been postponed in part owing to difficulties of getting together. We are confident that the incoming Commission will be effective and able to continue many of the key works of the current Commission; and that in the next triennium *International Tables for Crystallography*, Volume I will be fully published. Some Commission initiatives may work together with IXAS on Journal Club activity and additional workshops, which will help us to keep in contact more as we prepare to emerge from our COVID cocoons.

Christopher T. Chantler, Chair, **Valérie Briois** and **Sofia Diaz Moreno**, Secretaries

5. Sub-committee on the Union Calendar

The Sub-committee receives and considers requests for IUCr sponsorship and nominal financial support, and makes recommendations to the Executive Committee. Acting on the recommendations made by the Sub-committee, during 2019 and 2020 the Executive Committee approved sponsorship of various schools and meetings, mostly with financial support. Those that were held in 2020 are listed at the beginning of this Report of the Executive Committee. Those that were postponed or cancelled are listed below.

Understanding Biology Through Structure, Santa Fe, New Mexico, USA, originally scheduled for 16–20 March 2020 (cancelled).

Powder Diffraction & Rietveld Refinement School, Durham, UK, originally scheduled for 29 March – 2 April 2020 (cancelled).

RapiData 2020, Menlo Park, California, USA, originally scheduled for 30 March – 4 April 2020 (cancelled).

CCP4 Crystallographic School in South Africa: Data Collection to Structure Refinement and Beyond, Cape Town, South Africa, originally scheduled for 31 March – 8 April 2020, postponed until 2021.

55th Erice School: Structural Drug Design 2020: Biology, Chemistry and Computers, Erice, Italy, originally scheduled for 24–29 May 2020 (cancelled).

17th European Powder Diffraction Conference – EPDIC17, Šibenik, Croatia, originally scheduled for 26–30 May 2020, postponed until 2022.

7th International School on Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials (ISC2020), Granada, Spain, originally scheduled for 29 May – 6 June 2020 (postponed).

Workshop Renewable Energy and Sustainable Development 'Casamansun 2020' (7th Edition), Ziguinchor, Senegal, originally scheduled for 4–6 June 2020 (cancelled).

European Crystallographic School (ECS6), Budapest, Hungary, originally scheduled for 5–11 July 2020, postponed until 2021.

RIXS-REXS 2020: Workshop on Resonant Elastic and Inelastic X-ray Scattering 2020, Port Jefferson, USA, originally scheduled for 15–17 July 2020 (cancelled).

School on SAXS/SANS and BioSAXS/BioSANS Data Analysis, Prague, Czech Republic, originally scheduled for 19–21 August 2020 (cancelled).

Electron Crystallography School – 3D Electron Diffraction/MicroED Bridging Small Molecule and Macromolecular Crystallography, Tabor, South Bohemia, Czech Republic, originally scheduled for 19–22 August 2020, postponed until 2021.

Modern Trends in Computational Material Discovery – 18th USPEX Workshop, Isfahan, Iran, originally scheduled for 1–5 September 2020, postponed until 2022.

15th Biennial Conference on High-Resolution X-Ray Diffraction and Imaging (XTOP 2020), Minsk, Belarus, originally scheduled for 13–18 September 2020 (cancelled).

10th International Conference of the Hellenic Crystallographic Association, Athens, Greece, originally scheduled for 3–5 October 2020, postponed until 2021.

Crystallography for Space Sciences, Addis Ababa, Ethiopia, originally scheduled for 1–5 November 2020 (postponed).

Organizers of meetings wishing to seek IUCr sponsorship should submit applications at least nine months in advance of the meeting, writing to the Chair of the Sub-committee. For up-to-date contact information, application procedures and rules, see http://www.iucr.org/iucr/sponsorship/meetings.html.

Requests from satellite meetings may be submitted, and possible financial support requested, separately or through the Organizing Committee of the main meeting.

Meetings (other than satellite meetings) scheduled to be held within one month before or after an IUCr Congress will not be considered for sponsorship. For any meetings scheduled to be held between one and two months before or after a Congress, the application for sponsorship will be sent to the Chair of the Congress Programme Committee for approval, or

otherwise. For meetings (other than satellite meetings) scheduled to be held, in the respective region, within one month before or after a meeting of a Regional Associate (American Crystallographic Association, Asian Crystallographic Association, European Crystallographic Association, Latin American Crystallographic Association), the applicants for sponsorship must seek approval of the Chair of the Regional Associate Organizing Committee.

IUCr sponsorship can only be given to meetings that are international in character and open to participants from all countries. For international meetings the membership of the Programme Committee is a good indication of this. National meetings are only supported if held in developing countries.

IUCr sponsorship should only be given to meetings that include a speaker policy and statistics relating to gender balance on the conference website. The policy should be consistent with the IUCr's policy on gender balance and publicise the IUCr Conference Code of Conduct.

Active crystallographers should be involved in the organization of the conference and one or more sessions should deal with specific crystallographic topics. This does not automatically include any session on condensed matter physics, materials science or symmetry not related to crystallography. According to these criteria all meetings organized by IUCr Commissions automatically qualify.

Explicit support from the relevant IUCr Commission(s) is required for any international meeting (except for the meetings of Regional Associates) and from the Commission on Crystallographic Teaching for any international schools (except for those organized by an IUCr Commission).

The IUCr continues to support and uphold ISC's policy of non-discrimination and adheres to its decisions and procedures concerning the free circulation of scientists. Organizers of any meetings seeking IUCr sponsorship or support must assure the Sub-committee on the Union Calendar that the authorities of the country in which the meeting is to take place guarantee free entrance of *bona fide* scientists from all countries.

Travel support for young scientists is available for all meetings (including schools). This money should not be used for waiver of registration fees or for any purposes other than travel, accommodation and subsistence for the sponsored scientists. For virtual meetings, a lower level of funding will be provided and this can be used to subsidize the cost of online hosting. It is recommended that the presentations of young scientists supported by the IUCr should be in English.

Consideration should be given as to whether the proposed meeting is appropriate in subject, form and timing with respect to other related meetings.

Except in special cases, IUCr funds should not be used to sponsor more than one event per year in the same location.

Registration fees should be the same for both local and non-local participants.

Visiting Professorships. The IUCr Visiting Professorship Scheme aims to support some of the costs of having internationally recognized scientists as lecturers for short courses at workshops or schools organized in developing countries. These schools or workshops may have national or international character. Up to a maximum of three Visiting Professorships can be granted for a single event. Travel and insurance costs will be met by the IUCr, while the local organizers cover the accommodation/subsistence expenses. Visiting Professorships can be requested in conjunction with the application for IUCr funding of a meeting, or independently as a single action to obtain highly qualified international teaching support within a teaching programme of local character. Support from at least one IUCr Commission is required. Full details may be found at http://www.iucr.org/iucr/sponsorship/vp.html.

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

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

COMCIFS consists of five voting members and a broad collection of advisers and observers. The current voting members are James Hester (Chair), John Bollinger (Co-Secretary), Brian McMahon (Co-Secretary), Herbert Bernstein and John Westbrook. All business of COMCIFS in 2020 was conducted via the associated IUCr mailing lists.

Dictionary development. No new dictionaries were approved this year. Around a dozen new definitions were added to the core dictionary.

International Tables Volume G. COMCIFS members are closely involved with the preparation of the second edition of *International Tables for Crystallography* Volume G, *Definition and exchange of crystallographic data*. The bulk of the original material for the second edition, covering updated standards, has now been written and reviewed. Further information is available in the report of the Commission on *International Tables*.

Interactions with other groups. Herbert Bernstein represents COMCIFS on the NeXus International Advisory Committee (NIAC), which primarily develops raw data standards for large facilities. NeXus standards have recently been developed to allow incorporation of CIF data names into raw data files and to use CIF semantics to describe experimental axes. Both capabilities saw significant uptake in 2020. Links were also formed in 2020 with the Open Databases Integration for Materials Design (OPTIMADE) initiative, and with the crystallography domain of the European Materials and Modelling Ontology (EMMO) consortium. Both these groups now plan to rely on IUCr dictionaries to automatically populate their ontologies, which necessarily need to include descriptions of crystal structures as part of their larger goals of

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

Looking forward. As flagged in previous years, an ever-shrinking group of people is drawn upon to support CIF maintenance and development. This situation is not sustainable, particularly as the first generation of CIF experts move into retirement. This situation improved slightly in 2020, with some new observers and participants joining both COMCIFS and the core dictionary maintenance group.

J. Hester, Chair

7. Committee on Data (CommDat)

For 2020 there are the following matters to report:

The IUCr Forum for Public Input to CommDat has had various new published reports and announcements posted there. These have been extensively accessed (http://forums.iucr.org/viewforum.php?f=39&sid=54ab61563a4d2079d9a6abaf18cbc232).

CommDat had participated fully in the work of the Programme Committee for the Prague IUCr Congress and the workshop immediately preceding it (see https://www.xray.cz/ms/bul2019-2.htm and specifically CommDat's published contribution, http://www.xray.cz/ms/bul2019-2/commdat.pdf). Since the Congress was postponed to August 2021 we have responded to various queries during the year from the Local Organizing Committee about updating of Congress programme needs.

There have been several events through the year in which CommDat members took part. These included a workshop on MX raw image data formats organized by Herbert Bernstein and Andreas Forster (http://www.medsbio.org/); a session on data and data flows at the Stanford Synchrotron Radiation Laboratory and Linac Coherent Light Source I and II Users' Meeting (https://lcls.slac.stanford.edu/ssrl-lcls-users-meeting-2020); the Photon and Neutron Open Science Cloud (https://www.panosc.eu/); and the EU EXPANDS initiative (https://expands.eu/).

Two detailed reports by myself as IUCr Representative to CODATA on the CODATA activities in 2020 were circulated both to CommDat and to the IUCr Journals Managing Editor. This led to a detailed discussion on enhancing the existing efforts within IUCr Journals to record workflows, which are already quite significant, such 'that open science should apply to publications, data/metadata *and* research workflows'.

John R. Helliwell, Chair

8. *IUCr Newsletter*

The *IUCr Newsletter* continues to be an excellent vehicle for broadcasting and promoting the interests and activities of the IUCr and of its Regional Associates and Commissions. It also strives to enhance communication within the global community of crystallographers. The complete *Newsletter* archive, going back to 1993, is available at https://www.iucr.org/news/newsletter/archive.

From 2020 to 2021, four issues were published, the last two issues of Volume 28 and the first two issues of Volume 29. A President's column has appeared in all issues plus an Editorial. In Issue 2 of 2021 (to appear shortly), the new definition of what is meant by the term 'crystal' is discussed by Carol Brock. Juan Manuel Garcia-Ruiz also describes the recent findings of pristine crystals collected by early *Homo sapiens*. The recent award by English Heritage of a blue plaque to the home of Kathleen Lonsdale is discussed by Claire Murray, at the same time drawing attention to Lonsdale's hand-written tables. Istvan and Balazs Hargittai have also written an article on the great Russian crystallographer, Aleksandr Kitaigorodsky, illustrating his important contributions to molecular packing. An obituary for Sidney Abrahams, ex-Editor-in-Chief of the IUCr journals, was written by Carol Brock and Mike Glazer.

In Issue 1 of 2021, an important article on quantum crystallography (Macchi) was published. In addition, Hargittai wrote an article on the crystallographic artwork of Mamedov, comparing this with the work of Escher. In the previous two issues, the subjects covered included articles on quasicrystals (Hargittai), serial crystallography (Spence), protein folding (Helliwell), computational modelling (Catlow), the Rosalind Franklin coin, an interview with Walter Friedrich (Heaney and Kaliwoda), and the story of Jan Czochralski (Glazer). The winners of the W. H. and W. L. Bragg Prize, Jean-Phillipe Julien and James Fraser, were announced, as well as the award of the prestigious Gregori Aminoff Prize to Chapman, Hajdu and Spence.

In addition to feature articles, the usual meeting reports, results of competitions and obituaries were reported. An average of 32 items was published in each issue. The e-mail editions were circulated to 13 500 crystallographers and structural scientists worldwide, and social-media channels provided additional exposure. A modest amount of full-page and banner advertising was achieved but it is hoped this can be increased to help cover costs. Two new low-cost advertising opportunities – New products and Press releases (for company news) – were introduced in 2020.

The Editor is grateful for the help from Andrea Sharpe, Sarah Froggatt, Michele Zema, Brian McMahon and many others in Chester.

Mike Glazer, Editor

9. IUCr/Oxford University Press (OUP) Book Series Committee

The Book Series Committee members provided assessments of two new monograph book proposals, which I then brought together as Chair's reports. These two reports were first provided to the IUCr Executive Committee, which endorsed them, and then they were submitted to OUP.

The book by Sir John Meurig Thomas entitled *Architects of Structural Biology: Bragg, Perutz, Kendrew, Hodgkin*, was published in February 2020 by OUP. This book was outside of

the IUCr Book Series, being neither a research monograph nor a teaching book. Nevertheless, at the request of OUP the Committee reported in detail on both the first draft and the subsequent draft.

The second edition of the book *Polymorphism in Molecular Crystals* by Joel Bernstein was published in hardback in May 2020. Joel was a long-standing member of the IUCr OUP Book Series Committee and we mourn his passing in 2019. His obituary by Ehud Keinan and Menahem Kaftory was published in *Acta Cryst.* (2019), B**75**, 113–114.

In order to ensure consistency to IUCr nomenclature policies, and to reduce the chance of errors, we have re-affirmed to OUP the need for us to assign volunteer(s) with requisite subject expertise, ideally from our Committee, so as to review a full draft of a new text in our Book Series before publication by OUP in the IUCr's name.

John R. Helliwell, Chair

10. Gender Equity and Diversity Committee (GEDC)

The 2020 Committee comprised 12 members: five from Europe, four from Asia–Pacific and three from the Americas: Jenny Martin, Chair (IUCr Executive Committee member, Australia), Sven Lidin (IUCr President, Sweden), Natalie Alvarez (Uruguay), Ruchi Anand (India), Christine Beavers (UK), Annalisa Guerri (IUCr Calendar Committee, Italy), Genji Kurisu (Japan), Helen Maynard-Casely (Australia), Claire Murray (UK), Bernie Santarsiero (USA), Eddie Snell (USA) and Michele Zema (IUCr Executive Outreach Officer).

This 2020 report is provided in the context of the worldwide COVID-19 pandemic.

Our plans for 2020 included development of an IUCr rights and responsibilities statement, and facilitating a session at the IUCr Congress to update the IUCr vision, mission, purpose and values. Our plans were significantly disrupted by COVID. The vision, mission, purpose and values statement needs to be developed specifically for the IUCr. This is most easily done in a 2–3 hour facilitated session, which we had planned for the 2020 IUCr Congress. It is difficult to do this as a virtual group across different time zones. These plans were put on hold because of the postponement of the Congress until 2021. Members of the Committee are unlikely to attend the Congress in person in 2021, so our plans for this session will need further development in 2021.

The GEDC-approved Code of Conduct and Diversity Statement were approved by the IUCr Executive Committee and are now on the IUCr website. The Calendar application form for IUCr funding now includes a link to these statements and these are considered as part of the process for funding support from the Calendar Committee.

GEDC members continue to raise issues of discrimination and exclusion within our community. One example was addressed in 2020, when a public statement was released from a vendor about blocking software availability to Chinese universities. President Lidin contacted the person involved and the statements were removed from the website.

In September 2019, the International Organization for Standardization (ISO) Council approved the ISO Gender Action Plan 2019–2021. Priority 1 of this Action Plan is the collection of gender data on ISO members' top management, technical committees, experts and governance bodies representatives. The goal is to understand the current gender balance as well as the participation of the next generation in ISO's activities and to use this as the baseline for the effective monitoring of progress towards long-term objectives. The ISO Central Secretariat shared its Gender Action Plan – Expert survey with the IUCr, and Sven Lidin (President of the IUCr, and a member of the GEDC) completed the survey on behalf of the IUCr and the GEDC.

The International Science Council (ISC) also surveyed its international disciplinary members on their efforts to promote women and gender diversity in their organization and activities. This survey was coordinated by GenderInSITE (Gender in Science, Innovation, Technology and Engineering) on behalf of the ISC. A similar survey of women's participation in academies was conducted with the Inter-Academy Partnership (IAP) in late 2019. President of the IUCr and member of the GEDC Sven Lidin completed the survey on behalf of the IUCr and the GEDC. The results of these surveys will be analysed in a report on the status of women's participation in global science that will be shared with ISC members.

In 2020, nine ISC-affiliated scientific unions and organizations signed a Memorandum of Understanding created by the Standing Committee for Gender Equality in Science (SCGES). The GEDC recommended to the IUCr Executive Committee that the IUCr also sign this statement and join the SCGES. This decision is now with the Executive Committee for approval.

IUCr Journals signed up to the Coalition for Diversity and Inclusion in Scholarly Communications. A number of societies have revised or re-affirmed their diversity statements to encompass race and ethnicity. Andrew Allen (Editor-in-Chief of IUCr Journals) and Alex Ashcroft (IUCr Executive Secretary) expanded the IUCr statement accordingly. The GEDC approved the updated IUCr Diversity Statement, which is now with the Executive Committee for approval to take to the General Assembly in Prague. The GEDC recommended that the equity and diversity of journal Editors and Commissions, as well as IUCr-supported conferences and workshops, be reported at each General Assembly.

Michele Zema (member of the GEDC) worked with the LAAAMP Executive Committee to improve the gender balance (the IUCr are partners in LAAAMP). LAAAMP has now adopted the IUCr GEDC code of conduct. This is a good example of a positive influence spreading out from the GEDC.

The 3rd Latin American Crystallographic Association School took place virtually in November 2020, and achieved a 50/50 male/female attendee ratio from 15 countries. The development of virtual meetings in 2020 has provided an important opportunity to facilitate geographical and gender

balance at conferences, and we should aim to highlight this for future meetings.

More broadly, the impact of decisions made by the Executive Committee on IUCr equity and diversity is now routinely considered as a consequence of two Executive Committee members also being members of the GEDC. The gender balance of Editors on IUCr journals is improving, and we are optimistic that the gender balance on the IUCr Commissions can be improved at the General Assembly hosted by Prague.

J. Martin, Chair

11. The IUCr Crystallography in Africa Initiative

The OpenLabs and Schools planned for 2020 (and possibly 2021) in Ethiopia, The Congo, Gabon and Nigeria were cancelled. Restarting all OpenLabs in 2022 or at the end of 2021 is planned.

Thanks to the efforts of J. P. Ngome, Patrice Kenfack and C. Lecomte, UNESCO Yaoundé agreed to pay part of the transportation cost for diffractometers from Paris to Yaoundé, Cameroon, and the customs fees and transportation to Dschang. However, administrative constraints from Bruker postponed the installation. Patrice Kenfack, J. Guillin (Bruker France) and C. Lecomte are trying to solve the problem rapidly as UNESCO will not keep the money aside for this project indefinitely.

The funding for Openlabs and other Schools in Cote d'Ivoire in 2020 was used in December 2020 to buy two devices for stabilizing the power supply. The supply of electricity is very unstable and the variations and sudden outages damage the X-ray tubes and electronics of the diffractometers.

The Steering Committee for AfCA (Chair Professor D. Haynes, Secretary Dr P. Kenfack) formed during the PCCr2 meeting is working well: each month a remote meeting is organized. The AfCA statutes are being discussed as AfCA will be launched during PCCr3 (Nairobi, Kenya, 2022). PCCr3 will be an on-site and remote meeting as decided by the Steering Committee (which has among its duties the PCCr meetings).

It is planned to organize at least one OpenLab in November 2021.

Claude Lecomte, Chair

12. Regional Associates

12.1. American Crystallographic Association (ACA)

The American Crystallographic Association, Inc. (the ACA) is a nonprofit, scientific organization of 1189 registered members. It was founded in 1949. The objective of the ACA is to promote interactions among scientists who study the structure of matter at atomic (or near atomic) resolution. For more details please visit the regularly updated, very informative and easy to navigate ACA web page (http://www.amercrystalassn.org). During this unsettling year the Council has been very successful adopting new strategies for increasing membership and meeting attendance, increasing the diversity of the ACA and stabilizing the ACA's financial position. They even found time to stress the role of crystallography and structural science in COVID-19 therapies (https://www.amercrystalassn.org/aca-special-article-crystallography-covid-19).

The 2020 ACA Council consisted of Brian Toby (President), David Rose (Vice-President), Joseph Ferrara (Past-President), Ilia Guzei (Treasurer), Diana Tomchick (Secretary), Narasinga Rao (Chief Financial Officer, CFO) and Chelsy Chesterman as the Young Scientists Special Interest Group (YSSIG) representative to the Council (*ex officio*). Gerald Audette served as the Canadian National Committee for Crystallography (CNCC) representative and Hanna Dabkowska as the IUCr representative (*ex officio*). Lisa Keefe volunteered as the interim Chief Executive Officer (CEO), and was instrumental in promoting the position of Director of Administrative Services to the position of Executive Director, held by Kristin Stevens. This eliminated the need for a CEO. Kristina Vitale continues as the Membership Secretary. S. N Rao retired at the end of 2020 as CFO; we all hope that Dr Rao will be around for many years helping us all with experienced advice. The Finance Committee (FC) was created and it is chaired by the Treasurer. The other members of FC are Brian Toby, Narasinga Rao, Kristin Stevens, Jim Pflugrath, Jim Kaduk and Joe Ferrara.

In 2020 the Council met only once in person before COVID-19 restrictions started. Once-a-month teleconferences proved to be very successful.

After many discussions and consultations the name of American Crystallography Association was modified to ACA: Structural Science Society (ACA:SSS). A Logo Task Force was created to update the ACA:SSS logo.

Creation of the US National Division (USND) of the ACA:SSS was confirmed by the Council. Amy Sarjeant served as the first President of the USND followed by Tamir Gonen. Charlie Carter served as Secretary until January 2021 followed by Eric Reinheimer.

The 2020 (70th) Annual ACA Meeting (virtual only) was a great success. Nozomi Ando and Carla Slebodnick co-chaired this meeting. Poster Chairs were Louise Dawe and Tiffany Kinnibrugh. The meeting had the overall theme of Training the Next Generation. There were six days of sessions, four days of posters and four workshops, and 605 attendees took part in the meeting. Other meeting statistics are available at https://www.amercrystalassn.org/past-meetings.

The 2019 ACA Award Winners are Wah Chiu (Burger Award), Jacqueline Cole (Warren Award) and Julia Zaikina (Etter Award). The virtual meeting was supported by 16 sponsors (including IUCr support of USD 2000). The 2020 ACA Fellow titles were bestowed on Carol Brock, Stephen Burley, Larry Falvello, Bruce Foxman, Marvin Hackert, James Kaduk, Lisa Keefe, Amy Sarjeant, Hao Wu and Victor Young.

The new ACA:SSS Committee on Diversity is chaired by Jen Aitken and the members are Matthew Brown, Bennie Chan, Leighanne Gallington and David Rose.

It is with great sadness that I report that in May 2020 Paul Swepston, a long-time Editor of *ACA RefleXions*, passed away. Edwin D. Stevens is now the sole Editor. *ACA RefleXions* (https://www.amercrystalassn.org/aca-reflections) is an excellent magazine publishing details about the ACA:SSS activities, reports and projects as well as the results of ACA elections.

The 2021 (71st) ACA:SSS Meeting will be held virtually, 31 July – 3 August.

The 2022 (72nd) ACA:SSS Meeting is planned to be held in Portland, Oregon, 30 July – 2 August.

The ACA/AIP journal *Structural Dynamics* achieved an impact factor of 2.84 in 2020.

The ACA:SSS supported many progressive statements and actions regarding the situation of science and social activities in the USA (often acting together with the APS).

The 2020 and 2021 ACA:SSS Summer Courses in Chemical Crystallography, info@acasummercourse.net, were cancelled owing to the continuing global pandemic.

The Canadian National Committee for Crystallography (CNCC) (http://xtallography.ca/) is chaired by Tomislav Friscic, the Vice Chair is Louise Dawe, the Secretary is Michel Fodje and the Treasurer is Brian Patrick.

The 11th Canadian Chemical Crystallography Workshop (CCCW20) was held virtually from 19 to 22 May 2020.

The 13th Canadian Powder Diffraction Workshop was also held virtually from 26 to 30 October 2020.

The 2nd Canadian Materials Diffraction Workshop (CMDW2020) planned for June 2020 has been cancelled owing to COVID-19 restraints.

H. A. Dabkowska, IUCr Representative

12.2. Asian Crystallographic Association (AsCA)

AsCA continues to play a leading role in the nurturing of collective crystallographic activities in the Asia–Pacific region with successful scientific meetings being held in those years in which there is no IUCr Congress and General Assembly, although activities in 2020 were impacted by the COVID-19 pandemic.

The AsCA Executive Officers for the term 2020–2022 were elected in Singapore and are Xiao-Dong Su (President, China), Genji Kurisu (Vice-President, Japan), Siegbert Schmid (Secretary/Treasurer, Australia) and Jennifer Martin (Immediate Past President, Australia).

No AsCA meeting was planned for 2020 because of the scheduled 25th IUCr Congress and General Assembly.

At the Council meeting held at Hanoi (6 December 2016) a proposal was received from the Malaysian representative to host the 17th AsCA Conference at Sunway University, Petaling Jaya, Malaysia, during December 2021. Unfortunately, this conference had to be postponed to 2024 owing to COVID-19 travel restrictions. The next AsCA conference therefore is to be held in Korea (Republic of) in October 2022 on Jeju Island (also subject to favourable global development regarding the pandemic as well as travel funds). The AsCA Executive Committee is in conversation with the local organisers regarding establishment of the local organizing committee as well as the programme committee.

As Singapore and Bangladesh are in the process of becoming/have become full members of the IUCr, it is planned to include Cambodia and Sri Lanka in their place as members of the AsCA Regional Committee of the IUCr (along with Malaysia, Thailand and Vietnam). An application was received from the crystallographic community in the United Arab Emirates in 2020 for membership of AsCA. This was favourably considered by the Executive Committee and will be put to the AsCA Council for approval at the upcoming business meeting during the IUCr Congress in 2021.

At its 2018 meeting, the AsCA Council approved a proposal by Genji Kurisu from Japan to offer a prize to honour those who have made an outstanding contribution to AsCA over a prolonged period of time. This proposal is now being developed in more detail by Genji Kurisu to present to Councillors at the next meeting.

Siegbert Schmid, Secretary/Treasurer

12.3. European Crystallographic Association (ECA)

The ECA is a scientific association with national and individual members, and corporate affiliates. It has 13 SIGs (Special Interest Groups) and 3 GIGs (General Interest Groups). The ECA main events are the ECMs (European Crystallographic Meetings).

ECM-33 will be in Versailles, France, organized together with synchrotron Soleil. It was originally planned for 2021 but after the IUCr Congress in Prague (IUCr2020) was moved from 2020 to 2021, ECM-33 was also moved to 23–27 August 2022 (the 2021 organizers were Sylvain Ravy, Jean-Paul Itié and Andrew Thomson) and ECM-34 was moved to August 2024 in Padova, Italy. Owing to postponing IUCr2020 and not postponing IUCr2023, the ECA lost one ECM.

Online ECA Executive Committee meetings were organized to discuss changes to the statutes, with new candidates for national membership and with the bidders for holding an ECM in 2025. There are two new candidates for national membership – Romania and United Arab Emirates.

The ECA schools – the European Schools of Crystallography (ECS) – are already regular and are organized under detailed ECA guidelines. The 6th ECS in Budapest was postponed from July 2020 to July 2021 and will be purely online. The 7th ECS will be in Lisbon, Portugal, and preliminary interest for ECS8 was shown by Manfred Weiss from Berlin.

The African Crystallography Steering Committee has been established and defined six African regions. It is chaired by Delia Haynes and it is expected that it will lead to the foundation of the African Crystallographic Association (AfCA). The 3rd PanAfrican Crystallographic Conference (PCCr3), initially scheduled for January 2022 in Kenya, will now be online (e-PCCr3) but still in January 2022, with the aim of

consolidating the network of African crystallographers, followed by an in-person meeting, PCCr3, in 2023, which will serve as a platform for the launch of the African Crystallographic Association.

Schools and workshops are supported by about EUR 10 000 per year, with the exception of 2020 because most of the planned meetings were postponed.

The ECA Council decided to terminate the ECA's membership of the ISE (Initiative for Science in Europe, https://initiative-se.eu/) because the organization was not particularly active. However, this has changed since the appointment of a new secretary. Currently, the ECA is on (non-paying) observer status at the ISE. The ISE has launched a Petition for More Investment in Horizon Europe. The ECA has signed and supported this petition.

Discussion continues on how to strengthen the position of the ECA as European association, which poses some legal issues and the offers the possibility of professional management. The search for administrative support for the Executive Committee by an external service provider was suspended because the commercial offers received were judged to be too expensive. The ECA is registered in Netherlands, and permanent legal domicile and an address in the Netherlands is desirable. The ECA seeks to secure ANBI (Algemeen Nut Beogende Instelling) tax and legal status in the Netherlands. This requires changes to the ECA statutes. The work on this is underway and the new statutes will be submitted to the ECA Council.

The Executive Committee also suggested the organization a regular series of virtual ECA Lunchtime Seminars.

R. Kužel, IUCr Representative

12.4. Latin American Crystallographic Association (LACA)

The Latin American Crystallographic Association remained active despite the global health crisis due to the COVID-19 pandemic. No Regional Associate Meeting was planned for 2020 and most of the events were cancelled, but some events took place in a virtual format. Some of the activities carried out are summarized below.

The Argentinian Crystallographic Association (AACr) held the seventh edition of its very successful Crystal Growing Competition in 2020. Seventeen participating groups from different provinces in Argentina received awards in four categories. An online award session for Finalists and Special Mentions took place in November 2020. The eighth edition of the Crystal Growing Competition was launched on 7 May 2021 and will hopefully take place in person in November. Online workshops for participants and elementary and high-school teachers will be conducted during May and June. The XVI Annual Meeting of the AACr was planned for November 2020 in the city of Santa Fe, but was postponed until November 2021 at the same venue.

On a sad note, the Argentinian and Latin American Crystallographic community lost one of the most respected crystallographers in our region. Profesora Graciela Punte (Universidad Nacional de La Plata, Argentina) passed away in November 2020. Graciela Punte was a tireless advocate for the integration of Latin American crystallographers that led to the founding of LACA, and taught crystallography to and was the thesis supervisor for many young scientists who have contributed to maintaining the leadership of Argentina in crystallography.

Sirius, the new state-of-the-art Brazilian synchrotron facility, started operations of the first beamline in 2020 to allow researchers from the University of São Paulo (USP) to study proteins from the SARS-CoV-2 virus.

The Brazilian Crystallographic Association (ABCr) will celebrate its 50th anniversary in 2021 and will have its XXV Meeting (virtual format) from 18 to 22 October 2021. A very special programme is planned for the occasion.

The Mexican Crystallographic Society (SMCr) joined efforts with the Mexican Chemical Society (SMQ) to hold its X National Meeting (virtual format) from 2 to 4 December 2020. Workshops on powder diffraction, Rietveld refinement and polymorphism preceded invited lectures and oral and poster presentations. Invited lecturers included T. Blanton, J. A. Henao, M. A. Cuevas-Diarte, F. Meilleur, T. Blundell, T. Pi-Puig, J. Rodriguez-Carvajal, C. Vázquez, J. A. Kaduk and G. Rodriguez-Gattorno.

Two new Co-editors from Latin America, Professor Vojtech Jancick (UNAM, Mexico) and Dr Alexander Briceño (IVIC, Venezuela) joined the Editorial Board of *Acta Crystallographica Section E*.

Despite the difficulties, the year 2020 provided more opportunities for Latin American scientists to participate in the Annual Meeting of the American Crystallographic Association (ACA), as the ACA provided affordable rates for LACA participants to attend. The LACA community is very grateful for this opportunity and looks forward to continuing cooperation with the ACA.

LACA had planned two very important teaching events for 2020: the III and IV LACA Schools. The III LACA School on Small Molecule Crystallography was scheduled to start on 23 March 2020, at UNAM, Mexico. Just ten days before, the organizing committee (led by Dr Vojtech Jancik) made the difficult decision of postponing the school owing to the COVID-19 health emergency. In view of the uncertainties about conducting the School as an in-person event, the organizing committee decided to move the school to a virtual format. The school was re-programmed for two weeks, 23–27 November and 7–11 December 2020. The week in between the two sessions allowed attendance at the X (Virtual) Congress of the Mexican Crystallographic Society. The school had 65 participants and 12 instructors from 15 countries (11 Latin American countries were represented). Of the students 33 were female and 32 were male, while for the instructors 5 were female and 7 male, indicating that an excellent gender and geographical balance was achieved. Each day the students had a 1.5 h lecture and two practical sessions of one hour each. The sessions were recorded and made available to participants. Spanish, English and Portuguese were used in lectures and practical sessions. Homework was assigned to the students at the end of the first week and an a final evaluation was made at

the end of the second week. Lectures were delivered by F. Di Salvo (Argentina), J. A. Ellena and Hamilton Napolitano (Brazil), V. Jancik, M. de J. Rosalez Hoz, D. Martínez Otero and J. G. Alvarado Rodríguez (Mexico), S. Ward and I. Gimondi (UK), L. Suescun and N. Álvarez Failache (Uruguay), and B. Noll (USA). The Opening and Closing Ceremonies were attended by Sven Lidin (IUCr President), Hanna Dabkowska (IUCr Vice-President), Graciela Díaz de Delgado (IUCr LACA Representative) and José Reyes-Gasga (LACA President). The students provided feedback, through a questionnaire, on the development of the school and the general consensus is that it was a very successful event. Some recommendations will be shared with organizers of other virtual schools.

The IV LACA School on Crystallography will focus on Phase Identification and Microstructure Characterization of Materials using Powder Diffraction Techniques. It was planned for December 2020 but has been postponed until December 2021. It will take place at Universidad Federico Santa María (UFSM) in Valparaíso, Chile. The school is being organized by Professor Claudio Aguilar of UFSM, Chile, and by Professor José Miguel Delgado (ULA, Venezuela, LACA Vice-President). Since Chile has implemented a successful COVID-19 vaccination programme, the school is planned as an in-person event. However, the situation will be monitored continuously, and virtual access will be provided for attendants who may not be able to travel if restrictions are still in place.

With the rescheduling of the IUCr Congress, the sites and dates for the next LACA meetings are under consideration for 2022 and 2024. Costa Rica and Uruguay have been proposed as possible venues. The LACA authorities confirmed at the 2019 LACA Assembly will continue until the next General Assembly of LACA.

Graciela Díaz de Delgado, IUCr Representative

13. Representatives on Other Bodies and Scientific Associates

13.1. ICTNS (the Interdivisional Committee on Terminology, Nomenclature and Symbols, a committee of IUPAC)

The Chair of the CCN is a member of the ICTNS.

The ICTNS held virtual meetings on 5 January, 14 February and 13 March 2020. The minutes and associated documents from those meetings show they former focused primarily on procedures and on updates to the *Gold Book* for the mole, the Avogadro constant and the amount of substance. The updates were necessitated by the 2019 revision of the International System of Units (the SI).

Requests to referee papers and reports submitted to the IUPAC arrive regularly because all submissions are sent to all members of the ICTNS. Most submissions are in specialized areas unrelated to crystallography but a review was written for a manuscript recommending that Henry's Law constants be presented in a specified way in order to avoid the current ambiguity.

Carolyn P. Brock, IUCr Representative

13.2. International Science Council (ISC)

A joint General Assembly of the International Council for Science (ICSU; founded in 1931) and the International Social Science Council (ISSC; founded in 1952) was held in Taipei in October 2017. At that time it was voted to approve the merger of the two organizations to become the International Science Council (ISC). The first General Assembly meeting of the ISC was held in July 2018 in Paris to finalize the merger, work on governance issues and elect a Governing Board. The Governing Board consists of 16 members, including the President (Daya Reddy, South Africa), the President-elect (Peter Gluckman, New Zealand), as well as four further officers and ten additional ordinary members. Heide Hackmann serves as the Chief Executive Officer of the ISC, which is headquartered in Brussels.

The ISC represents 40 international scientific unions (including the IUCr) and associations, and more than 140 national and regional scientific organizations. It has the stated aim to be 'a global voice for science'.

Despite the fact that the COVID-19 pandemic has impacted in-person activities for the ISC during 2020, efforts continued to make progress on the ISC Action Plan. The ISC launched its first action plan, Advancing Science as a Global Public Good, in 2019. The Action Plan 2019–2021 (https://council.science/actionplan/) identified twelve projects to advance, all framed by the four domains of critical importance for science and society:

Domain One: The 2030 Agenda for Sustainable Development;

Domain Two: The Digital Revolution;

Domain Three: Science in Policy and Public Discourse;

Domain Four: The Evolution of Science and Science Systems.

The ISC works closely to coordinate with other organizations on efforts related to climate change, sustainability, future Earth *etc*.

Another key area of interest for the ISC is freedom for scientists to pursue knowledge and to freely exchange ideas, coupled with the responsibility of scientists to maintain scientifically defensible conclusions, along with the responsibility of scientific institutions to apply high standards of logical reasoning, and respect for evidence, replicability and accuracy. There are four fundamental scientific freedoms that the ISC seeks to uphold:

Freedom of movement;

Freedom of association;

Freedom of expression and communication;

Freedom of access to data and information.

International Years. These are organized to educate the public and celebrate important aspects of how science impacts life and the world in which we live. The ISC works to have science recognized by the United Nations via International

Year proclamations – just as the UN designated 2014 as the International Year of Crystallography (IYCr). Recent and future International Years are:

2019: International Year of the Periodic Table of Chemical Elements;

2020: International Year of Plant Health;

2020/2021: International Year of Sound;

2021/2022: International Year of Caves and Karst; and

2022: International Year of Basic Sciences for Sustainable Development.

Grants. The IUCr submitted a proposal on behalf of Andreas Roodt (ECA and INDABA) and Michele Zema (IUCr representative) to ICSU in 2015. The original ICSU award (2016–2019) provided support for several conferences for capacity building of crystallography in Africa with a goal of cementing the African Crystallographic Association. This project has evolved and expanded into LAAAMP, 'Light-sources for Africa, the Americas, Asia and Middle East Project'.

Open access. The ISC, acting as a global umbrella body for science academies, has urged the academic community to unify in support of universal open access, arguing that all publications should allow text reuse and data mining.

ISC publications. The ISC has continued to produce a large number of publications across a broad range of topics (https://council.science/publications/). In addition to the action plan mentioned above, a few that are especially noteworthy are the *Annual Report 2019* (https://council.science/annual-report-2019/) and *Open Science for the 21st Century* (https://council.science/publications/open-science-for-the-21st-century/). The ISC Annual Report for 2020 has not yet been published.

Second General Assembly of ISC. Much of the activity of the ISC since the merger has been to review and iron out details related to its organizational structure (statutes and by-laws), voting and membership dues. Committees were formed to study these issues with the goal of presenting and obtaining feedback from its membership early in 2021 in order to revise their recommendations to present to the delegates for final discussion and approval at the second General Assembly meeting of the ISC, which will be a virtual meeting held 11−15 October 2021.

M. Hackert, IUCr Representative

13.3. International Science Council Committee on Data for Science and Technology (CODATA)

CODATA is the interdisciplinary Committee on Data for Science and Technology of the International Science Council. Full details of CODATA's activities are available from its website at http://www.codata.org. Many of the activities of the year for CODATA were recorded and are available on their video channel, https://vimeo.com/user91439529/videos. The General Assembly is at https://vimeo.com/491609839.

Owing to the COVID pandemic, meetings of CODATA in 2020 were held virtually. The General Assembly not meeting in person required a CODATA Virtual General Assembly to agree a new procedure. This was held in June 2020. This meeting also included a description of the ten-year CODATA strategy of *Data Together*, namely CODATA, RDA, WDS and GOFAIR working together. (FAIR = Findability, Accessibility, Interoperability, and Reusability of data; https://www.force11.org/group/fairgroup/fairprinciples.) Secondly, CODATA had endorsed UNESCO's request to approve an Open Science Protocol, within which the FAIR implementation profiles had the goal of interdisciplinary open science to meet the UN's 17 Sustainable Development Goals (SDGs). Thirdly, there is now a framework of services for data archiving in the regions of the world: the European Open Science Cloud (EOSC), the Commons in the USA (funded by *e.g.* the National Science Foundation), the China Cloud and the African Open Science Platform. Fourthly, progress was described on the actions towards cross-domain data integration for reuse. It was reported that the next International Data Week (IDW 2021) is to be held in Seoul, Korea, 8–11 November 2021, with the CODATA General Assembly on 12 November. To assist the Data Together effort with other data organizations the IDW for 2023 was also announced, to be held in Salzburg, 23–26 October 2023, and entitled 'A Festival of Data'. Finally, the CODATA 2019 and 2020 budgets were reported to be in balance.

The CODATA 2020 Conference was jointly organized by CODATA and GoFAIR, focusing on cross-domain data integration topics with a view to helping tackle cross-disciplinary global challenges as described by the UN's sustainability development goals (https://codata.org/events/conferences/international-fair-convergence-symposium-convened-by-codata-and-go-fair-22-23-october-2020-paris-france/). The dates were shifted from October to late November/early December. The format was again virtual owing to the COVID pandemic. There were four primary themes: (i) Crisis reduction and response (learning from COVID); (ii) FAIR specifications; (iii) FAIR society; and (iv) Data stewardship (training and career opportunities). It was emphasized that open science should apply to publications, data/metadata and research workflows. I reminded delegates of the IUCr *Response to Open Data in a Big Data World* (https://www.iucr.org/news/press-releases/open-data) presented at International Data Week in 2016 in Denver, where we focused on the importance of data quality in crystallography.

John R. Helliwell, IUCr Representative

13.4. Digital Representation of Measure (DRUM) Initiative of the Committee on Data (CODATA) of the International Science Council (ISC)

[The ISC is the successor organization to the ICSU. The ISC was formed in July 2018 by the merger of the International Council for Science (ICSU) and the International Social Science Council.]

In July 2020 the Chair of the CCN was appointed as the IUCr's Ambassador to the DRUM initiative of CODATA.

The official IUCr delegate to CODATA itself was John Helliwell.

A 90-minute virtual briefing session of the 25 Ambassadors was held on 1 October 2020. It seemed that the DRUM organizers understand they cannot effectively impose standardization on international unions, which suggests that this group will not argue against use of the ångström unit.

One of the illustrations of examples of problems described in the October session included the following: 'Microstructure images are collected with a variety of electron microscopes from different vendors, unfortunately the pixel sizes and electron beam energies vary so there is no guarantee they are in the same units (pain point)'. Correspondence with John Helliwell led to his contacting Simon Hodson, CODATA Executive Director and Liaison to DRUM, for more information but there has not been any further correspondence on the matter.

Carolyn P. Brock, IUCr Ambassador to the DRUM initiative

13.5. ISC Committee on Space Research (COSPAR)

COSPAR's (http://cosparhq.cnes.fr/) main objective is to promote international collaboration in scientific research in Space, with an emphasis on the exchange of results, information and opinions. This organization is responsible for developing world standards for the Space environment and its protection.

COSPAR's highest body is the Council. The Council comprises the Committee's President, Representatives of Member National Scientific Institutions and International Scientific Unions, the Chairs of COSPAR Scientific Commissions, and the Chair of the Finance Committee. The Council meets at the Committee's biennial Scientific Assembly. Between Assemblies on a day-to-day basis COSPAR is run by the Bureau.

COSPAR President for the period 2014–2022 is Lennard A. Fisk (USA) and the Vice-Presidents are Karl-Heinz Glassmeier (Germany) and Mikhail Panasyuk (Russia). The members of the Bureau are Catherine Cesarsky (France), Masaki Fujimoto (Japan), Manuel Grande (UK), Charles Kennel (USA), Pietro Ubertini (Italy) and Chi Wang (China).

The most recent 43rd COSPAR Assembly was held in hybrid format (mainly virtual and partially in Sydney) in January 2021 just after the period of this annual report.

The 44th COSPAR Assembly will be in Athene, Greece, 16–24 July 2022 (http://www.cosparathens2022.org/).

The 45rd COSPAR Assembly will take place in Busan, Korea, in 2024.

Following the success of the Capacity Building Workshop (CBW) on Crystallography for Space Science in April 2016 in Puebla, Mexico (http://www.inaoep.mx), a similar workshop/school has been proposed for Addis Ababa, Ethiopia, in 2021 or later. Eyasu Leta is the CBW organizer and Yuki Kimura (IUCr) and Carlos Gabriel (COSPAR) will co-chair it.

The Chair of the Scientific Commission on Materials Science in Space (MSS Commission G) is M. Avila (Germany), and co-chairs are T. Könemann, (Germany), J. Porter (Spain) and T. Yano (Japan).

The official journal of COSPAR is *Advances in Space Research (ASR)*, https://www.journals.elsevier.com/advances-in-space-research, which had an impact factor of 2.177 in 2019. *ASR* includes COSPAR's information bulletin *Space Research Today*. Another COSPAR journal, *Life Sciences in Space Research*, is a quarterly peer-reviewed scientific journal covering astrobiology, origins of life, habitability, life in extreme environments, effects of spaceflight on the human body, radiation risks and other aspects of life sciences relevant in Space research.

In 2020 COSPAR organized one CBW and postponed two CBWs:

Coronal and Interplanetary Shocks: Analysis of Data from Space and Ground-based Instruments, 6–17 January 2020, Kodaikanal, India;

Data Analysis for Planetary Sciences, 20–31 July 2020, Antofagasta, Chile (postponed);

Pan-Ocean Remote Sensing Conference Tutorial, 15–19 September 2020, Johor Bahru, Malaysia (postponed).

The Panel on Capacity Building (PCB) Fellowship programme is open to young scientists who participated at one of the COSPAR CBWs, enabling them to build on skills gained at the workshop. It provides for visits of 2–6 weeks duration for the purpose of discussing ideas for a future workshop or carrying out joint research with one of the previously agreed lecturers/advisors of the corresponding workshop.

COSPAR co-organizes a limited number of meetings and colloquia each year that are of interest to its Associates. More information about these initiatives can be found at https://cosparhq.cnes.fr/events/co-sponsored-meetings.

Yuki Kimura, IUCr Representative

13.6. International Standards Organization (ISO)

The Chair of the CCN is a member of ISO. The group sends out e-mails once a week that list 25–50 reports on a mind-boggling variety of topics (*e.g.*, information technology, plastics, railway infrastructure, cheese).

There were no ISO activities in 2020 related to crystallography.

Carolyn P. Brock, IUCr Representative

13.7. International Organization for Crystal Growth (IOCG)

The activities of the IOCG slowed down owing to the pandemic.

The Executive Committee of the IOCG decided, owing to the pandemic, to move the 20th International Conference on Crystal Growth and Epitaxy to 30 July – 4 August 2023.

A. Zappettini, IUCr Representative

13.8. International Centre for Diffraction Data (ICDD)

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. Billing, IUCr Representative

13.9. Worldwide Protein Data Bank (wwPDB)

The Protein Data Bank (PDB) has been a key resource for macromolecular crystallographers for almost 50 years, and its policies and development have been strongly influenced by the crystallographic community. Now known as the Worldwide PDB (wwPDB) it now comprises five core entities, the RCSB PDB in the USA, PDBe in Europe, PDBj in Japan, BMRB (NMR database) and EMDB (Electron Microscopy Database). The latter became a core partner in 2020. The centres collaborate intimately and share the load, maintaining a single, freely accessible curated archive.

The wwPDB was formally designated a Scientific Associate of the IUCr in 2015, and the IUCr provides a representative on the wwPDB Advisory Committee (wwPDB-AC). This committee also has representatives from the NMR and cryo-EM communities, as well as regional representation, and is currently chaired by Dr Peter Rosenthal (UK).

The COVID-19 pandemic necessitated that the 2020 meeting of the wwPDB-AC should be a virtual one, held over two days (30 September – 1 October). Although informal discussions were necessarily truncated, it is clear that the day-to-day activities of the wwPDB have been little affected, and the database has continued to develop at a fast pace to meet the demands of new technologies and leading-edge science. Major items of progress with relevance to the IUCr were as follows:

(i) By the end of the year the archive comprised over 172 983 macromolecular structures, which continue to grow in both size and complexity. Of these 88% have been determined by crystallography, but the number determined by cryo-EM continues to increase rapidly (2390 in 2020 compared with 11 248 by crystallography). In contrast, the number determined by NMR remains static at under 400.

(ii) The wwPDB is proving to be a major resource in the fight against COVID-19. The first SARS-CoV-2 protein structure was deposited and released in February 2020 and since then about 15 new structures have been released every week as crucial data towards new therapies.

(iii) Current policy for structure depositions allows requests for up to 12 months delay in the release of new structures. With the urgent need for new COVID-19 therapies, however, all depositors of COVID-related structures are now asked to voluntarily release their data immediately. Encouragingly, compliance has been almost 100%.

(iv) Full validation reports have now been implemented for structures determined by both cryo-EM and NMR. These are substantially based on the analyses developed for structures determined by crystallography, but with method-specific variations. For cryo-EM structures these include EM map validation and improved map/model validation. Metrics are being evaluated for definition of concepts of 'local' resolution.

(v) The remediation of carbohydrate structures in the archive has now been completed, giving conformity with IUPAC/IUBMB conventions of stereochemistry and atom naming. This is a major step forward in making glycan structures searchable.

(vi) In response to requests from users, the wwPDB partners have agreed to make the e-mail contact addresses of lead depositors available to users. This is necessary because of the growing number of structures that are never published in the primary literature. The depositions themselves are given a DOI, and are increasingly seen as publications in their own right.

(vii) The wwPDB has agreed with an IUCr initiative aimed at ensuring proper, curated deposition of the raw data underpinning structures deposited to the PDB. It is proposed that all depositors will be directed towards curated depositories and the PDB will seek further funding to expand on this initiative.

(viii) Plans to establish a Chinese partner site (PDBc) for the wwPDB have been delayed by the COVID-19 pandemic. A necessary first step, the training of key personnel and annotators, was to have been undertaken at PDBj in Osaka, Japan. This is necessary to safeguard uniformity in the processing of new depositions, and will enable PDBc to fully share the load of increases of depositions. Arrangements have now been made to carry out this training online.

(ix) The PDB will celebrate its 50th anniversary (PDB50) in 2021. Meetings are planned to celebrate this at meetings of the ASBMB (May 2021), the ACA (July 2021), the IUCr Congress (August 2021), the ECM (October 2021) and AsCA (December 2021). Most, if not all, of these meetings are likely to be virtual.

The IUCr can be proud of the contribution made by the crystallographic community to this vital resource, and I am happy to be able to report that the relationship between the IUCr and the wwPDB is strong, and much appreciated by the wwPDB.

E. N. Baker, IUCr Representative

14. Finances

The Report and Financial Statements for 2020 are given as supporting information.

Transactions denominated in foreign currencies are translated into US dollars (USD) at the rates applying at the dates of the transactions. Monetary assets and liabilities denominated in foreign currencies at the balance-sheet date are retranslated at the rates applying at that date.

Investments are stated at market value. Changes in market value are taken through the income and expenditure account.

The balance sheet shows that the assets of the Union have increased during the year, from USD 3 875 826 to USD 4 697 664. The movement in market value of the investments was a gain of USD 79 806 in 2020 (compared with a gain of USD 170 654 in 2019).

The administrative expenses were USD 223 224 in 2020, as compared with USD 314 791 in 2019. Part of the decrease was due to the lack of travel or physical meetings because of the pandemic, while the Xero accounting software reduced the expenditure on audit and accountancy fees.

The only costs for the virtual Finance and Executive Committee meetings held in 2020 were for unrefundable expenses for travel tickets and a meeting room booking in Leuven. The subscriptions from Adhering Bodies were USD 186 089. Interest on bank accounts and investments was USD 32 166.

The journals for 2020 showed a surplus of USD 1 118 381 after journal-development costs were taken into account, as compared with a surplus of USD 1 063 103 as calculated on a similar basis for 2019.

The cost of the technical-editing office has been divided between the journals and *International Tables for Crystallography* in percentages based on the staff time spent on each publication. The technical-editing costs for the journals were USD 1 150 451, as compared with USD 1 149 447 in 2019.

Books showed a surplus of USD 13 850, as compared with a deficit of USD 10 411 in 2019. The net sales income for books was USD 112 360 in 2020, as compared with USD 118 153 in 2019.

The cost for the Union in producing the *IUCr Newsletter* in 2020 was USD 8022, compared with USD 10 240 in 2019.

USD 17 517 was provided for financial support to young scientists, to enable them to attend scientific meetings sponsored by the Union. This was much lower than in previous years due to many meetings being postponed or cancelled because of the pandemic, with the few that went ahead after March being virtual. Costs of Visiting Professorships (USD 1038) were much lower for the same reason. Outreach and education costs in 2020 (USD 144 068), which includes the value of waivers and discounts for IUCr Journals, contributed to the IUCr's good works.

An Outreach and Education Fund was established as part of the IYCr2014 legacy. In 2020 donations totalling USD 24 181 were received.