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FOUNDATIONS ADVANCES

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Report of the Executive Committee for 2018

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1. Meetings

The IUCr sponsored the following meetings held during 2018:

1st LACA School – Small Molecule Crystallography, Montevideo, Uruguay (19–25 February 2018).

Powder Diffraction and Rietveld Refinement School, Durham, UK (8–12 April 2018).

RapiData 2018, Stanford, USA (22–27 April 2018).

Casamansun 2018: Workshop on Renewable Energy and Sustainable Development, Ziguinchor, Senegal (3–5 May 2018).

6th International School on Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials (ISC2018), Granada, Spain (20–26 May 2018).

Quantum Crystallography School (Erice 2018), Erice, Sicily, Italy (1–10 June 2018).

The 4-D Workshop: Deep-Time Data-Driven Discovery and the Evolution of the Earth, Carnegie Institution for Science, Washington DC, USA (4–6 June 2018).

2nd Meeting on Porous Molecular Solids (POMOS 2018), Vietri sul Mare, Italy (6–8 June 2018).

XXV Conference of Serbian Crystallographic Society, Bajina Basta, Serbia (21–23 June 2018).

Gordon Research Conference 2018: Crystal Engineering, Newry, Maine, USA (24–29 June 2018).

50 Years of Synchrotron Radiation in the UK and its Global Impact (UKSR50), Liverpool, UK (26–29 June 2018).

Aperiodic 2018, Ames, Iowa, USA (8–13 July 2018).

Sagamore XIX 2018, Halifax, Nova Scotia, Canada (8–13 July 2018).

5th European Crystallographic School (ECS5 2018), Stellenbosch, South Africa (8–14 July 2018).

Annual Meeting of the American Crystallographic Association (ACA 2018), Toronto, Canada (20–24 July 2018).

17th International Conference on X-ray Absorption Fine Structure (XAFS17), Krakow, Poland (22–27 July 2018).

Introduction to Crystallographic Methods, Riobamba, Ecuador (27–30 July 2018).

2018 Kuo Symposium on 3D EM of Macromolecules and Cells and the 11th K. H. Kuo Summer School on Electron Microscopy and Crystallography, Hangzhou, China (25–29 August 2018).

31st European Crystallographic Meeting (ECM 2018), Oviedo, Spain (22–27 August 2018).

AIC International School 2018, Bari, Italy (29 August – 2 September 2018).

Sixth SMARTER Crystallographic Conference, Ljubljana, Slovenia (2–6 September 2018).

INDABA 2018 (Modelling of Structures and Properties), Skukuza Camp, Kruger National Park, South Africa (2–7 September 2018).

Satellite to ECM31 2018: 2nd European Symposium on Chemical Bonding, Oviedo, Spain (2–7 September 2018).

14th Biennial Conference on High-Resolution X-ray Diffraction and Imaging (XTOP 2018), Bari, Italy (3–7 September 2018).

Second European School on Crystal Growth (ESCG2) and Sixth European Conference on Crystal Growth (ECCG6), Varna, Bulgaria (13–16 and 16–20 September 2018).

Third Hot Topics in Contemporary Crystallography – HTCC2018, Bol, Croatia (23–27 September 2018).

XVII International Small Angle Scattering Conference, Traverse City, Michigan, USA (7–12 October 2018).

LACA3 Satellite Workshop: Refinement of Crystal Structures Using OLEX2, Valparaiso, Chile (8–10 October 2018).

3rd International Workshop on X-ray Crystallography in Structural Biology, Karachi, Pakistan (8–10 October 2018).

Annual Meeting of the Latin American Crystallographic Association (LACA3 2018), Valparaiso, Chile (10–12 October 2018).

International Neutrons and Food Conference – Neutrons and Food 5, Sydney, Australia (16–19 October 2018).

ICCBM17 – The 17th International Conference on the Crystallization of Biological Macromolecules, Shanghai, China (29 October – 2 November 2018).

X School of the Argentinian Association of Crystallography, Buenos Aires, Argentina (5–9 November 2018).

Macromolecular Crystallography School 2018: From Data Processing to Structure Refinement and Beyond, Sao Carlos, SP, Brazil (12–22 November 2018).

International School on Fundamental Crystallography, Bogota, Colombia (26–30 November 2018).

Annual Meeting of the Asian Crystallographic Association (AsCA 2018), Auckland, New Zealand (2–5 December 2018).

The Executive Committee met in Oviedo, Spain, in August. The Finance Committee met in Leuven, Belgium, in March and in Oviedo, Spain, in 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 Editor-in-chief, Editors and Co-editors, progress of *IUCrJ*, journals development, Special Issues, open access, and other matters concerning the IUCr journals;

review of contract with Wiley for the IUCr journals;

approval of audited accounts for the previous year;

discontinuation of virtual fund accounts;

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;

promotional activities;

establishment of Ewald and Bragg Prize Selection Committees;

establishment of a Committee on Gender Equity and Diversity;

Other items dealt with in this way were:

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

crystallography in developing regions; Crystallography in Africa;

review of activities of Commissions, formation of new Commissions;

review of activities of Regional Associates;

review of reports of IUCr Representatives on other bodies;

Items concerning the Chester office were:

staffing requirements in the IUCr office in Chester;

office premises;

risk analysis;

upgrading of office technology.

2. Publications

Volume 74 of *Acta Crystallographica*, Volume 51 of *Journal of Applied Crystallography* (*JAC*), Volume 26 of *Journal of Synchrotron Radiation* (*JSR*) and Volume 5 of *IUCrJ* 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

Publication-related statistics for the IUCr journals for recent years are shown in Table 1. All of the IUCr journals performed well during 2018. This is despite the challenges of a changing world for scientific journals, with a continuing transition to open-access publication and consequent increased competition from new fully open access journals around the world. Nevertheless, for the first time ever, the impact factor of every IUCr journal (that has one), as published in June 2018, increased over the impact factor published one year earlier. While a few of these impact factors were associated with a small number of highly cited papers and therefore may prove transient, the underlying impact factors of the journals remain healthily consistent or are increasing. This success represents a fitting culmination to my immediate predecessor, Samar Hasnain's, tenure as IUCr Journals Editor-in-chief. I succeeded Samar in the Summer of 2018, and I plan for the IUCr journals to continue to build on Samar's achievements.

During 2018, the number of submissions to all of the journals remained similar to 2017, with just under 2700 submissions in total. However, if we exclude *Acta Cryst. E* and *IUCrData* (latter included in the individual reports below for

Table 1
Statistics for IUCr journals.

	Year					
	2013	2014	2015	2016	2017	2018
No. of submissions (all)	4514	3814	3278	2231	2685	2676
without Acta E or IUCrData	2391	2336	2006	1689	1694	1880
Rejection rate (%)	23	24	25	26	31	28
without Acta E or IUCrData	30	33	32	33	36	34
No. of published papers (all)	3481	2925	2557	2065	1880	1793
without Acta E or IUCrData	1517	1589	1390	1139	1047	1139
No. of open-access papers (all)	2187	1628	1534	1240	1129	987
without Acta E or IUCrData	223	292	366	273	296	333
No. of pages (all)	12410	14408	13867	12451	11565	12473
without Acta E or IUCrData	9773	12057	10936	9181	8564	9856

the first time), where some evolution is occurring affecting a significant number of submissions, the total number of submissions to the other journals increased in 2018 from just under 1700 to nearly 1900. The average rejection rate for articles submitted continues to hover around 30%, or slightly more if *Acta Cryst. E* and *IUCrData* are excluded. Taking these points into account, the total number of published articles in all of the journals decreased slightly, compared to 2017, but the number increased slightly for all journals excluding *Acta Cryst. E* and *IUCrData*. Meanwhile, the total number of pages published increased in 2018 by nearly 8% compared to 2017 if all journals are counted, and by 15% if *Acta Cryst. E* and *IUCrData* are excluded.

As mentioned above, open access is an increasingly important aspect of scientific publication. Three of the IUCr journals are already fully open access: *Acta Cryst. E*, *IUCrData* and *IUCrJ*, while the other seven journals are hybrid. Counting all of the regular papers published in the hybrid journals, plus those in *IUCrJ*, the fraction of published papers that were open access was close to 30% in 2018, significantly higher than for most publishers of hybrid scientific journals. The proportion of open-access papers is anticipated to increase further in coming years, particularly with the development of transformative 'publish and read' arrangements.

In 2018, and continuing into 2019, the Editor-in-chief and Journals Management Board (JMB) are working to recruit new editors, increase high-quality submissions, and commission topical Special Issues of interest to readers. The appointment of new Commissioning Editors should also greatly facilitate these developments.

A. Allen, Editor-in-chief

4.1.1. IUCrJ

IUCrJ had another good year in 2018. It continued to establish itself within the wider scientific communities that use the results obtained from diffraction methods. Impressions from authors, readers, referees and commentators are very positive, and the journal published a record number of papers in the year.

The impact factor announced for *IUCrJ* in 2018 was 6.5. The journal has a rapid and efficient review process with all submissions undergoing 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). The screening is generally complete within 72 h, and many of the articles that do not meet the journal's requirement for broad scientific significance are 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.

In 2018, *IUCrJ* published six issues. They featured papers from a wide variety of areas including biology, chemistry, crystal engineering, cryoEM, materials, physics and free-electron lasers (FELs). The number of articles submitted to the journal was 138; a total of 95 papers were published with an average turnaround time of 16 weeks. Articles have been highlighted by a number of different methods, with seven articles highlighted *via* in-depth commentaries.

The Biology and Medicine section of *IUCrJ* remains strong, with a total of 28 papers published in 2018 (21 articles, and 7 commentaries/letters). These cover reports of both novel biological structures, in most cases disease-related, and of innovative methods applied to biological systems. The latter include papers on dynamic processes, in crystals or in individual proteins, and on improved methods for the derivation of structural models from weak data or from complementary approaches such as small-angle scattering. A significant emerging theme is the use of serial synchrotron crystallography or various forms of time-resolved studies (for example collecting multiple structures from a single crystal) to determine detailed chemical mechanisms for biological processes – a nice merging of chemistry and biology. In addition, many of the papers published in other sections of the journal (*e.g.* the cryoEM, neutron/synchrotron and physics/FELs sections) focus on applications to biology, making this a strong focus for the journal. One area that is not yet well represented in *IUCrJ* but which we anticipate will be very important in the future is in applications of microED (micro electron diffraction) to both chemistry and biology.

The Chemistry and Crystal Engineering section of the journal continued to make good progress in 2018. There were 37 submissions of which 33 articles were voted for review in 2018. Of these, 25 were accepted for publication, with 5 rejected and 3 still in review at the end of the year. These numbers are satisfying but one would expect around 50 submissions every year (one per week). This section continues to pull its weight in contributing to the impact factor of 6.5. At the present time, one would hope to see more submissions in frontier areas where fundamental concepts are advanced in keeping with the overall goals of *IUCrJ*. Co-editors should encourage scientists to submit papers to the journal. There is some concern about the open-access charges in some countries. 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. We are on the lookout for a Co-editor in the important charge-density area.

The cryoEM section is still at an early stage, but cryoEM submissions are picking up and growing. In addition, cryoEM publications feature strongly in the list of most-read articles in *IUCrJ*, which is a good indicator. We plan to continue to encourage both biologically oriented and method-oriented manuscripts – the latter, in particular, have potential for high citation frequency given the active interest in improving computational tools in the cryoEM field.

The other sections of the journal, covering Materials and Computation, Neutron and Synchrotron Science and Technology, and Physics and Free Electron Laser Science and Technology have published 18, 9 and 13 papers, respectively, in 2018. We would like to see more papers of broad scientific significance submitted to the journal in these areas.

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

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

4.1.2. Acta Crystallographica Section A

Acta Cryst. Section A had another successful year in 2018, publishing articles on a very wide range of topics. The journal's impact factor of 7.9 was still high, mainly owing to recent articles on *SHELXT* and *OLEX*. (The impact factor is likely to drop again when the 2018 impact factor is announced in 2019 as these two articles pass out of the calculation 'window'.)

During 2018, we published nine research papers as Advances, plus the topical review *Quasicrystals: What do we know? What do we want to know? What can we know?* by W. Steurer and a feature article *Precise implications for real-space pair distribution function modelling of effects intrinsic to modern time-of-flight neutron diffractometers* by D. Olds, C. N. Saunders, M. Peters, T. Proffen, J. Neuefeind and K. Page. Two scientific commentaries explained the wider implications of two other studies: *Rigid units revisited* by A. E. Phillips, which discussed the article *An algebraic approach to cooperative rotations in networks of interconnected rigid units* by B. Campbell, C. J. Howard, T. B. Averett, T. A. Whittle, S. Schmid, S. Machlus, C. Yost and H. T. Stokes, and *A symmetry roadmap to new perovskite multiferroics* by P. M. Woodward, which discussed the article *A group-theoretical approach to enumerating magnetoelectric and multiferroic couplings in perovskites* by M. S. Senn and N. C. Bristowe.

Three articles provoked some debate: *Comments on A new theory for X-ray diffraction*, by J. T. Fraser and J. S. Wark was published alongside a response from P. F. Fewster, and the article *The development of powder profile refinement at the Reactor Centre Netherlands at Petten* by B. van Laar and H. Schenk outlined the early days of what became known as the Rietveld method.

The number of submissions during 2018 was high (possibly as a consequence of the high impact factor) and the number of published articles was also higher than in recent years. We also saw an increase in the number of articles being published as open access.

We are grateful to Gloria Borgstahl, Pat Thiel and Alan Goldman for selecting interesting articles from the Aperiodic 2018 conference on which to base a 'virtual' Special Issue of the journal. Pat and Alan acted as Guest Editors for a collection of eight excellent articles, the first of which were published at the end of 2018.

We would also like to thank all our Co-editors for handling the unusually high number of submissions during 2018 while ensuring that the standard of articles stayed high. We are planning to appoint more Co-editors in 2019 to help ease the workload and to cover new areas, and we plan to make full use of the new Commissioning Editors when these are appointed.

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

4.1.3. Acta Crystallographica Section B

Acta Crystallographica Section B continues to publish six issues per year. Whereas in 2017 the journal achieved the highest numbers of submissions (175), published papers (134) and pages (1199) in recent years, partly because of the publication of two Special Issues, in 2018 only one Special Issue was produced, on Mineralogical Crystallography. We are very grateful to Guest Editors Sergey V. Krivovichev, Janusz Lipkowski and Stuart J. Mills for their hard work in bringing about this Special Issue. Further Special Issues on Electron Crystallography (Guest Editors Joke Hadermann and Lukas Palatinus) and Quantum Crystallography (Guest Editor Piero Macchi) are underway; others are under consideration.

We also note that the rejection rate in 2018 (43%) was somewhat higher than the long-term range for the journal of 28–40% and while we are monitoring the rate, we do not feel there is a need for immediate action. The average length of a paper has risen to 10.7 pages, resuming the trend towards longer papers. In 2018, Russia was the source of more papers than any other single country (12.9%), followed by Germany, Canada, China and Poland.

The journal's 2017 impact factor reached 6.467, but this is largely because of a very small number of highly cited Feature Articles which will still be within the citation window for 2018

but will then drop out. We wish to take full advantage of this increase in impact factor to promote the journal and attract more high-quality submissions, so that we can reduce our dependence on a very small number of articles. We will continue to pursue Invited Articles from prominent scientists such as keynote lecturers at IUCr Congresses and Regional Associate Meetings, and we look forward to working with the new-appointed Commissioning Editors. We also welcome the opportunity to highlight outstanding *Acta* B articles in *IUCrJ*.

We would like to express our appreciation to retiring Co-editor Simon Parsons for all his contributions to the journal since his appointment to the Board in 2008; in particular, we are grateful to Simon for acting as a Guest Editor for the Special Issue on Energy Materials published in 2015. New Co-editor appointments are underway and will be announced later this year. We would like to express our thanks to the Chester staff, especially the *Acta B* Managing Editor Amanda Berry, for all their support.

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

4.1.4. Acta Crystallographica Section C

The continuing influence of the 2015 *ShelxL* and *PLATON* SQUEEZE papers produced another significant increment for our 2017 impact factor (published in 2018), this time to 8.678. This is expected to suffer a large drop for the 2018 impact factor, to be published in 2019. However, the metrics available at the time of this writing seem to indicate that the new impact factor will be of the order of two times what it was before the impact of these two papers entered into the figures. An optimistic viewpoint on that possibility is that we have actually managed to leverage the effect of these two papers and perhaps of some of the Special Issues to attract papers of higher quality and greater capacity for generating citations.

During 2018 we published one Special Issue, on the topical area of polyoxometallates (POMs). The Guest Editors, Ulrich Kortz and José Ramón Galán-Mascarós, are prominent chemists and well known in the field of POMs. Probably as a result of this, and of the proactive approach of the Guest Editors, the author response was very positive, and some 23 articles appeared in the Special Issue. Three of these are reviews in nature and have unrestricted access; it is hoped that these will have an enhanced citation rate. Meanwhile, the 2017 Special Issue on NMR Crystallography is expected to perform well in its bibliometrics. We need to be more proactive in commissioning effective Special Issues and review articles to continue the upward impact-factor trend that lies beneath the spike occasioned by the *ShelxL* and *PLATON* SQUEEZE papers.

The number of submissions to Section C was 441 in 2018, reflecting the perceived desirability of publishing in this journal as a result of our impact factor. The total page count for Section C leapt from 1159 in 2017 to 1782 in 2018. The rejection rate was down from 47% to 43%. It can be expected that the number of submissions will decrease with the announcement of the 2018 impact factor. However, the broader content of most of our articles, reflected in the average page size (7.7 in 2018 compared to 4.5 in 2013), is likely to be an irreversible trend aided by the fact that our sister journal, Section E, is now entrusted with the publication of structure communications.

The composition of the Review Board and the Co-editors remained largely unchanged in 2018, and these still reflect our past remit as a structure communication journal. The positive aspect of that stability is that we continue to be a trusted source of accurate diffraction analyses while we cultivate our larger chemical subject areas. At the same time, we are expected to lose some 13 Co-editors in 2019, a change which must be addressed with an eye to the structural chemistry remit of the journal. In addition to fulfilling the need for diversity, we are seeking Co-editors who have a strong base in structural chemistry beyond, and in addition to, single-crystal structure analysis.

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

4.1.5. Acta Crystallographica Section D

There are signs that *Acta D* is recovering from the effects of the impact factor having dropped five years ago, when several highly cited methods papers disappeared over the limited horizon of the impact-factor calculation. The number of submissions and published papers is gradually recovering and the impact factor of 3.1 is good relative to the historic range of 2 to 3.

Special Issues continue to play a positive role for the journal. In particular, continued publication of contributions from the CCP-EM Spring Symposium helps to consolidate the position of *Acta D* as a home for papers covering the full range of structural biology; the papers from the 2017 CCP4-EM meeting were published in June 2018. A two-part Special Issue, published in February and March, covered contributions from the 2017 CCP4 Study Weekend on the topic From Crystal to Structure with CCP4. Two other Special Issues covered the 5th International Symposium on Diffraction Structural Biology (August) and a Neutrons in Structural Biology meeting (December). Driven in part by these Special Issues, the proportion of papers published open access has risen slightly again, from 53% in 2017 to 54% in 2018.

We are pleased to note that Elspeth Garman became a new Section Editor late in 2018. No Co-editors were appointed over the year, but we plan to recruit new Co-editors over the next period to cover the expansion into different areas of structural biology.

Publication times are up slightly from 2016, but within the range seen over previous years. It should be noted that these are driven largely by the time required for refereeing and manuscript revision, but very little by 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.

E. F. Garman and **R. J. Read**, Editors

4.1.6. Acta Crystallographica Section E

In the last year the quality of papers has continued to increase, and the range of structures is far broader. Papers are generally getting longer and many report two or more structures, 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 analysis and Hirshfeld surface analysis. 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 first ever Special Issue, on Weak Interactions in Crystals: an Integrated Approach, was published in the May 2018 issue. This was very well received and the papers in it have done well in terms of the number of citations and downloads. The Section Editors have been actively trying to commission papers that will be widely read and highly cited. The first of these, on Hirshfeld surface analysis, was published in March 2019.

The number of submissions and publications decreased slightly compared to 2017 but the journal continues to attract papers from across the world, with authors from 61 countries publishing in Section E in 2018. The top five countries were the USA (15%), India (12%), Germany (7%), Turkey (6%) and Malaysia (5%).

Many of our long-standing Co-editors have retired recently and more are due to retire at the Prague Congress. In addition, Helen Stoeckli-Evans will stand down as a Section Editor at the end of 2019. One of the main challenges for the journal in the coming year is to identify potential new Editorial Board members who can help Section E to continue to develop and prosper in the future.

As always, we are grateful to our Co-editors for the excellent work they have done and also thank the staff in Chester, particularly Gillian Holmes, Sean Conway and Mike Hoyland, for their constant help and support, and Peter Strickland for his sound advice and expert guidance.

E. Boldyreva, **C. Massera**, **H. Stoeckli-Evans** and **L. Van Meervelt**, Editors

4.1.7. Acta Crystallographica Section F

Acta Crystallographica F is a 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. As a result, the rejection rate is higher (34%) than a few years ago, but the cited half-life has increased every year since 2013. The impact factor has also increased, and hopefully will remain on an upward trend. 2018 has seen a slight increase in the number of published papers with respect to 2017, but we still need to attract more authors. The average publication time has risen to over three months (ideally it should be less than three months) and we are working to bring this time down. However, this may be related to the average length of manuscripts, which has also increased in line with the increase in manuscript quality.

In 2018, a new Section Editor was recruited (Janet Newman). Several Co-editors are now near the end of their nine-year term, so we need to recruit a few new Co-editors. Ideally, most of these will be female, to improve the gender balance of the Editorial Board, and we will also be keeping an eye on geographical balance. Some of these new Co-editors may be recruited from the Review Board, and the Review Board may also be refreshed with new additional members.

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.

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*. To achieve this, Special Issues on interesting topics are being pursued. An issue on protein/carbohydrate structures was published in August 2018 and a number of papers on cryoEM were published in January 2019. More Special Issues will hopefully follow. We have not had much success in procuring Inaugural Articles from new Co-editors, so some effort will need to be made here, and also in procuring more Topical Reviews.

Looking to the future, a new article type, Methods Communications, has been proposed and is in development. This will provide researchers with quick tips as well more detailed methods, and hopefully obtain more citations for *Acta Cryst. F*.

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

4.1.8. Journal of Applied Crystallography

The Editorial Board of *Journal of Applied Crystallography* saw a major change in 2018, with Main Editor Andrew Allen stepping up to the role of Editor-in-chief of all the IUCr journals. Andrew has served on the Editorial Board of *Journal of Applied Crystallography* in various guises since 2002, first as a Co-editor, then Deputy Editor and finally Main Editor. We thank him for the huge contribution he has made to maintaining the journal's integrity and scientific standards. Andrew has worked particularly hard to strengthen the journal's historic links with the small-angle scattering community and acted as Editor on two Special Issues related to the International Small-Angle Scattering Conferences. We will miss the immediate contact with Andrew that we have enjoyed to date, but we are pleased for Andrew and all the IUCr journals that he has accepted this new role. A successor to Andrew as Main Editor will be appointed in 2019. No additions have been made to the board of Co-editors since 2015, and a priority for the coming year will be to appoint several new Co-editors to

build on the journal's core strengths and reach out to new authors in emerging areas.

2018 marked the 50th year of publication of *Journal of Applied Crystallography*, celebrated by an editorial and a cover featuring a collage of front covers from April 1968 to the latest Special Issue. It was also marked by a virtual Special Issue on Advanced Neutron Scattering Instrumentation. This was published in June 2018 with 23 articles and Guest Editors Dimitri Argyriou and Andrew Allen, a fitting and excellent swansong to Andrew's direct association with *Journal of Applied Crystallography*. Virtual Special Issues, which collect together selected full-length research papers associated with particular conferences or solicited on a relevant and topical technical theme, continue to be popular and a search for the theme of the next Special Issue is underway.

Journal of Applied Crystallography, in common with other IUCr journals, has now been online since 2014. We should be wary of reading great significance into the publication statistics of recent years compared to earlier years, but it is notable that the numbers of submissions and of published papers were lower in 2017 and 2018 than in the four previous years. This may be due to the introduction of *IUCrJ* and to synchrotron users favouring *Journal of Synchrotron Radiation*, both of which saw an increase in submissions in 2018. The fall in submissions was also probably influenced by the fall in impact factor in 2015–2016. The average number of pages per paper continues to be higher than during the more costly paper era. The fraction of each type of article has remained fairly stable over the past six years, but we should encourage more Feature and Lead Articles. Such articles on subjects that are emerging could attract a new readership.

As befits the vision of the journal, the category Research Papers dominates. Amongst the other categories, the category Computer Programs leads by a significant margin, in part as a result of active encouragement by the Editorial Board, in part because of the increasing need for user-friendly, broadly applicable and robust data-collection and data-analysis tools for researchers without extensive training in crystallography.

Techniques, instrumentation and applications to specific materials continue to dominate in Research Papers. Some topics that stand out by their frequency are small-angle scattering, whether X-ray or neutron, nanostructures in various forms, and texture and microstructure.

The latest impact factor of 3.422, published in 2018 for 2017, is the median of recent years. As noted in earlier reports, the fluctuation in impact factor is largely due to the sporadic publication of articles on computer programs that draw high and obligatory citations. The journal may be the primary place where crystallographic computer program information is published, but the number of crystallographic programs that are widely used is naturally limited by the extent of necessary validation and popular acceptance.

The journal will continue to publish Special Issues on software and review developments in emerging new areas. Based on the impact of an earlier Special Issue on software for research with free-electron lasers, we expect interest in this area to grow, extending also into optically driven X-ray lasers and ultrafast spectroscopic and structural studies.

Overall, *Journal of Applied Crystallography* is performing well in the all-electronic era, thanks in no small part to the dedication and professionalism of our Co-editors and reviewers. The format offers a cost-effective open-access option, with free access to selected articles to attract a new readership.

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

4.1.9. Journal of Synchrotron Radiation

Two hundred and eleven papers were accepted in 2018 compared with 164 in 2017. The rejection rate decreased to 20% from 25% and publication times were the same as for 2017, *i.e.* 5.6 months. The number of pages published increased to 1894 pages from 1300 pages. The increase in page numbers in 2018 was partially due to publishing two Special Issues – papers from the PhotonDiag2017 Workshop and papers from the Q2XAFS2017 Workshop – compared with only one Special Issue published in 2017 – papers from the 9th International Workshop on X-ray Radiation Damage to Biological Crystalline Samples.

The Special Issue on the PhotonDiag2017 Workshop formed part in the January 2018 issue, like the previous one on the PhotonDiag2015 Workshop published in the January 2016 issue. The Guest Editors were E. Plönjes, M. Zangrando and D. Cocco, and the issue featured 22 Special Issue papers amounting to 150 pages. For the Q2XAFS2017 Workshop Special Issue, the Guest Editors were Sofia Diaz-Moreno and Richard W. Strange, and the issue featured 11 Special Issue papers amounting to 92 pages in the July 2018 issue.

JSR is continually looking to publish such themed issues of selected papers from workshops and 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. Three Special Issues are expected in 2019: one containing papers presented at the 10th Workshop on X-ray Radiation Damage to Biological Crystalline Samples (scheduled for the July issue), and two virtual issues, one on XFELs and one from papers presented at the PhotonDiag2018 Workshop.

The Facility Information pages continued in 2018. These provide an opportunity for facilities to communicate important news and updates to the international community of synchrotron radiation users. In 2018, facility pages were provided by the Advanced Photon Source, LAAAMP (Lightsources for Africa, the Americas, Asia and Middle East Project), MAX IV and the Paul Scherrer Institute.

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

Y. Amemiya, **M. Eriksson**, **I. Lindau** and **I. Schlichting**, Editors

4.1.10. IUCrData

During 2018 the quality of submissions to *IUCrData* has risen and the rejection rate remains comparatively modest at 17%. In particular, authors have increasingly adapted to the significantly revised and reduced format of the new journal, in comparison to that of the former Data Reports section of *Acta E*. However, a number of articles that are transferred to the journal from *Acta E* need to be extensively reformatted. There has been a considerable reduction in the number of submissions compared to the two previous years. This may reflect the fact that authors are willing to put additional work into papers to get them into other journals. The fact that the Cambridge Structural Database now assign a doi to data sets deposited with them may also have an impact. Nonetheless, the submissions clearly show that there is a genuine need to provide a means of publishing brief and simple, one-off, peer-reviewed reports on structures that might not otherwise appear in the public domain. Providing such a vehicle was a significant goal for the establishment of *IUCrData*.

The geographical spread of papers received by the journal is very wide, with contributions from 40 countries in 2018. India head the list with 18%, closely followed by the USA with 17%. It is nice to see Morocco in third place with 13%.

Over the past year we have lost several long-standing Co-editors; we thank them sincerely for their work, and wish them well in their 'retirement'. We also thanks the efficient and effective team of current Co-editors who make the journal happen on a daily basis. As always the help and advice of the great team in Chester, who are always there for us, is much appreciated.

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 series of major reference books published by the IUCr in conjunction with Wiley. Eight volumes designated A (and A1) through G are currently in print. Parts of a ninth (H, *Powder diffraction*) are already available electronically; completion is imminent. Most of the content for a tenth volume (I, *X-ray absorption spectroscopy and related techniques*) has been received and many of the articles have been accepted. The *Brief Teaching Edition* of Vol. A (*Space-group symmetry*) is also part of the series.

The series has long embraced the electronic age; volumes with extensive hyperlinks began appearing online in 2006. Printed volumes can still be purchased individually but they are now a less reliable source of revenue than are annual online subscriptions to the entire series. Market forces will require additional adjustments. Print runs will be reduced, although demand for tabulations of symmetry tables (*e.g.* Volumes A and E) seems likely to remain strong. Wiley advises the IUCr that there needs to be 10% new or revised content annually to keep the subscription model viable.

A series that is largely electronic will provide welcome flexibility. Parts 1–3 of the new Volume H (*Powder diffraction*) appeared online at the end of 2018, *i.e.* well in advance of the appearance of the full volume. Commission discussions in Hyderabad endorsed the plan of putting some articles online as they become available because authors who meet deadlines can then be rewarded with prompt publication. Shortcomings identified after a volume is finalized can be remedied quickly (see the paragraph below about Volume A).

Descriptions of activities during 2018 for the individual volumes follow.

Volume A (*Space-group symmetry*; most recent online edition is dated 2016; Editor Mois Aroyo). Following discussions with the users of the 2016 edition of Volume A, the text and the tables of reflection conditions of the chapter on space-group determination (Chapter 1.6) have been extended to include the so-called 'diffraction symbols' (known also as 'extinction symbols'). It is expected that the new material and data will be included in the online edition during 2019.

Symmetry Database server of the Online Edition of *International Tables* (updated continuously; Editor Mois Aroyo). The *Symmetry Database* provides a set of tools for studying general group–subgroup relations such as transformations, coset decomposition, Wyckoff-position splittings, graphs of maximal subgroups *etc.* During 2018 activities focused on the following:

(i) Interactive 3D visualization with *JSmol*: All the functionalities of *JSMol* are being implemented for visualizing space-group symmetry operations. For a given space group the user will be able to follow the relations between the symmetry operations and the general positions in a 3D representation of the unit cell.

(ii) A step-by-step procedure for calculating the transformation matrix for a given group–subgroup pair: This development will aid the study of symmetry relations between space groups. An initial version of the procedure to obtain the shortest path for a given group–subgroup pair is ready for comments and suggestions.

(iii) *Teaching Edition of the Symmetry Database*: The *Teaching Edition* is being developed as a resource for users of the new edition of the *Brief Teaching Edition* (see below). There will be access to the crystallographic data of a restricted number of space and point groups. Group–subgroup relations (which might require data for groups not accessible in the *Teaching Edition*) will be replaced by specific examples. A sample version of this software is available on the development platform of eFaber.

Brief Teaching Edition of Volume A (current edition is dated 2010; Editor Mois Aroyo). Almost all of the material for the considerably revised version is awaiting typesetting in Chester; completion in 2019 is anticipated. The new version is designed more specifically for people new to the field of crystallographic symmetry; the revision will also serve as an introduction to Volumes A1 and E of *International Tables*, to magnetic space groups, and to the *Symmetry Database*.

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

Volume B (*Reciprocal space*; most recent online edition is dated 2010; Editors Gervais Chapuis & Michal Dušek). An article on 3D pair distribution functions (3D-PDF) is under review. An article on electron diffraction is being prepared. Before Ted Janssen passed away in 2017 he had completed a revision of the article on modulated structures that is being moved from Volume C to Volume B.

Volume C (*Mathematical, physical and chemical tables*; online edition is dated 2006; Editor Richard Welberry). Many of the articles commissioned for a very major revision have been received; some are ready for publication. The end of March 2019 has been set as the submission deadline. It is planned to start putting articles online in September, with the goal of finishing the revision before the 2020 Congress.

Volume D (*Physical properties of crystals*; most recent online edition is dated 2013; Editor was André Authier, who has since retired). It has not yet been possible to identify a new editor for Volume D. Revision seems not, however, to be a pressing matter.

Volume E (*Subperiodic groups*; most recent online edition is dated 2010; Editor Danny Litvin). Danny Litvin has notified the Commission that he will retire after the 2020 IUCr Congress. A new Co-editor has been identified but has not yet been formally appointed. Plans for increasing the material about the applications of the subperiodic groups have been discussed informally, as has the possibility of including tables of the penetration rod groups. [These groups are the rod groups that are compatible with each of the crystallographic space groups; see U. Müller (2017), *Acta Cryst.* B**73**, 443–452.] Corresponding tables for layer groups are included in Volume E but should perhaps be relabelled in a way that would make them more accessible.

Volume F (*Crystallography of biological macromolecules*; most recent online edition is dated 2012; Editors Liang Tong, Michael Rossmann & Eddy Arnold). A clear plan has been reached for the organization of the third edition. There are 96 chapters in the second edition; 34 will be retained with no or minimal changes, and 60 will undergo more substantial modifications, mostly by the original authors. To reflect the new technological developments over the past ten years, especially in electron microscopy, 15 new chapters will be introduced; potential authors of these new chapters have been identified. Upon approval of this plan by the IUCr Executive Committee formal invitations will be sent out to authors, with a six-month time frame to submit the first version of the manuscript.

Volume G (*Definition and exchange of crystallographic data*; online edition is dated 2006; Editors Brian McMahon & James Hester). Progress during the year was limited by the need to develop and test specifications and resolve issues that arose during preparation of the chapters covering the foundational standards. The foundational chapters are now in draft form and attention during 2019 will shift towards the dictionary chapters, many of which should require only minor updates from their counterparts in the first edition.

Volume H (*Powder diffraction*; new volume; Editors Henk Schenk, Chris Gilmore & Jim Kaduk). Parts 1–3 went online in December 2018; the remaining four parts are expected to be online by April 2019. The print volume should be available in May 2019. Hardcopy of the existing chapters was shown at the July 2018 European Powder Diffraction Conference (EPDIC) in Edinburgh to good reviews.

Volume I (*X-ray Absorption Spectroscopy and Related Techniques*; new volume; Editors Chris Chantler, Federico Boscherini & Bruce Bunker). Close to 90% of the manuscripts have been received; a large percentage have moved through to acceptance. New manuscripts are being received every month or two, so that the process is converging. The quality of submission is excellent, with much significant new material not available elsewhere. It is hoped that some material will go online during 2019.

Further information about the volumes can be found 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/).

During the last year André Authier retired as Editor of Volume D (*Physical properties of crystals*), which was essentially his creation. We thank him for his important contributions to *International Tables* and for having served the IUCr in many other ways.

No annual report can be complete without acknowledgement of the contributions of the staff in the Chester office and especially of Nicola Ashcroft. She is expert in typesetting complex equations and in inserting appropriate hyperlinks. She is equally skilled in seeing how an unclear sentence can be fixed, and her natural tact encourages authors to accept her suggestions. Editors learn quickly to rely on her advice. It is also important to thank Nicola and Peter Strickland for their interactions with the publisher Wiley.

C. P. Brock, Chair

4.3. Commission on Aperiodic Crystals

In 2018, the Commission (CAC) continued to actively promote aperiodic crystallography, in organizing, supporting and promoting meetings, workshops and educational activities worldwide. In doing so, CAC continued its ongoing coordination of interaction between the various sub-communities and disciplines involved in the different aspects of research in aperiodic crystals, as well as the dissemination of research results to the greater scientific community.

Our flagship scientific event in 2018 was the 9th International Conference on Aperiodic Crystals (Aperiodic 2018), which was held on the campus of Iowa State University in Ames, Iowa, USA, during the week 8–13 July 2018. The conference, which was chaired by Patricia Thiel, Alan Goldman and Gloria Borgstahl, is the ninth in the series of triennial conferences organized under the auspices of CAC. The conference was attended by about 100 delegates from

more than 20 countries. In the six conference days, a broad range of topics, including classical modulated structures, quasicrystals and magnetic structures, symmetry aspects, mathematical aspects, tiling theory, high-pressure crystallography, diffuse scattering, lattice dynamics, physical properties, crystal growing, architecture and commercial aspects were covered. A special session was devoted to the memory of Ted Janssen, one of the pioneers of superspace theory, who had sadly passed away on 29 September 2017 at the age of 81. The programme also included the public lecture given by the Nobel Prize winner Professor Danny Shechtman on The Role of TEM in the Discovery of the Quasi-Periodic Materials on 12 July.

The Commission wishes to express its gratitude to Patricia Thiel, Alan Goldman and Gloria Borgstahl, as well as the entire team who made this event a success. For more details, see the conference website at https://register.extension.iastate.edu/aperiodic2018/.

A Commission meeting was held on 12 July during Aperiodic 2018, and the Commission enthusiastically supported the proposal to hold the next meeting in Japan. The 10th International Conference on Aperiodic Crystals will be held in 2021 at Hokkaido University campus at Sapporo, Japan, organized by Hiroyuki Takakura and Ryuji Tamura.

The Aperiodic 2018 conference was followed by the 31th European Crystallography Meeting (22–27 August 2018, Oviedo, Spain). It featured two microsymposia dedicated to modulated crystals, quasicrystals and magnetic order. Other events in 2018 that were supported by CAC included the Jana Modulation Workshop, La Jolla, CA, USA, 10–13 December 2018, which attracted 24 participants from the USA (see http://crystals.ucsd.edu/meeting4.html for details).

The Commission is looking forward to exciting events in 2019. Planned activities include the 4th International School on Aperiodic Crystals, which will be held in Portbail, France, in September 2019, and is being organized by Olivier Pérez. It follows on from the successful schools in Carqueiranne, France, in 2010, in Bayreuth, Germany, in 2013 and in Antwerp, Belgium, in 2016. This is our central educational activity, with the objective of providing an overview of aperiodic order, of the basics of the mathematical description of both modulated structures and quasicrystals, and of physical properties and chemical understanding of aperiodic crystals, as well as a working knowledge of structural analysis of aperiodic crystals. The other important meeting to take place in 2019 is the 14th International Conference on Quasicrystals (ICQ14) in Kranjska Gora, Slovenia, in May 2019, which is being organized by Janez Dolinšek. The Commission has also been actively involved in shaping the programme for the forthcoming Prague 2020 Congress, and we are hoping to contribute to an attractive and exciting programme.

O. Pérez, Chair

4.4. Commission on Biological Macromolecules

The aim of the Commission on Biological Macromolecules (CBM) is to support macromolecular crystallography worldwide through scientific exchange, training, and promotion of policies that encourage the generation and dissemination of knowledge and technologies.

The availability of diffraction data. The CBM coordinated its efforts with the IUCr Committee on Data (CommDat) and the Editors of all relevant IUCr journals to further evaluate practical aspects of the deposition of diffraction images, which constitute the primary data in a macromolecular X-ray diffraction experiment. The Executive Committee approved the White Paper entitled *Proposed mechanisms for making diffraction experiments available*. Subsequently, all relevant IUCr journals will publish an editorial with the title *Findable Accessible Interoperable Re-usable (FAIR) diffraction data are coming to protein crystallography*, which is co-authored by the Chair of CommDat, the Chair of the CBM, and the Editors of all the relevant IUCr journals. During the last year, the combined number of diffraction experiments submitted to the two most popular servers of diffraction data was close to 8000.

Standards for data to be provided to reviewers of macromolecular structures. The CBM has continued to work with the American Crystallographic Association, the Asian Crystallographic Association, the European Crystallographic Association and the Worldwide Protein Data Bank (wwPDB) to continue the development of standards for information that reviewers of macromolecular structures and the public (after PDB deposition) should receive. There is an agreement that reviewers should receive (1) the PDB validation report and (2) pictures of omit maps for any ligands and unusual structural elements. Additionally, the draft standards suggest making the data (structure factors, coordinates) available to reviewers. The CBM continued the discussion about the deposition process and modelling standards. The ultimate goal is to set the standard for deposition of models that describe the disorder within structures.

IUCr Congress. Discussion about the programme of the next IUCr Congress in Prague involved three CBM representatives (Alice Vrielink, Julie Bouckaert and Marcin Nowotny) and some members of the CBM. There were numerous conference calls to discuss the programme, and the proposal was sent to the entire CBM and appreciated by a number of CBM members.

Meetings, workshops and other outreach activities. The CBM has recommended support from the IUCr for a number of meetings and workshops that can provide teaching or play a major role in the dissemination of data in macromolecular crystallography.

W. Minor, Chair

4.5. Commission on Crystal Growth and Characterization of Materials

In 2018 the members of the Commission (CCGCM) collaborated actively but mostly *via* the Internet. However, a few members of CCGCM had the chance to meet at the 6th European Conference on Crystal Growth, in Varna, Bulgaria, on 18 September 2018. The meeting was attended by Thierry Duffar, Stepane Vessler, Elias Vlieg and Andrea Zappettini.

The meeting was also attended by Koichi Kakimoto, a consultant for CCGCM and President of the IOCG. This was a very nice chance to discuss emerging topics, such as the organization of the next International Schools on Crystal Growth, the search for interesting topics for the microsymposia of the next IUCr Congress, and the preparation of a document on the future development of crystal growth activities.

The Sixth European Conference on Crystal Growth was really successful. Before the conference, the Second European School on Crystal Growth was also held in Varna. Many commission chairs and consultants were involved in the organization of these events. I was one of the School Co-chairs. It has been decided that both the European School and Conference will take place in three years' time in Paris. We are very happy that the tradition of European Crystal Growth Conferences has been established again and with it also the tradition of European Schools on Crystal Growth.

In 2019 the IOCG Conference will be held in Keystone, Colorado, USA. Our Commission is involved at different levels in the organization of this important event, and more details are given in my report as IUCr Representative to the IOCG.

In 2018 the CCGCM supported the following schools/meetings that were important for the crystal growth community:

2019 Gordon Research Seminar on Crystal Growth and Assembly, which will take place in June 2019;

7th International School on Biological Crystallization (ISBC2019) to be organized in Granada, 26–31 May 2019;

International Summer School on Crystal Growth ISSCG17, which will take place in Colorado, USA, 21–27 July 2019; and

17th International Conference on the Crystallization of Biological Macromolecules (ICCBME17), which was held in Shanghai, China, 27–31 October 2018.

Finally, I would like to express my great honour and pleasure to be Chair of this Commission, thus hopefully contributing 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

In a year without an IUCr Congress, the main activities of the Commission in 2018 concentrated on the regional meetings of the ECA, ACA, AsCA and LACA. At these meetings, the Commission supported microsymposia involving computing and software development. Some additionally had satellite meetings involving computing and organized other events advocating crystallographic software (for example software fayres). Several software projects had their own dedicated meetings and schools. The Commission wholeheartedly supports such initiatives.

In 2018 the Commission was involved in the preparation for the 2020 Congress in Prague. Our member on the International Programme Committee is Thomas Proffen. In advance of the main Congress, the Commission plans to organize a computing school in Nove Hrady, Czech Republic. The planning for this school is ongoing.

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*, the Chair of the IUCr/OUP Book Series Committee, the Chair of the Crystallographic Teaching Commission, the Chair of the Committee for the Maintenance of the CIF Standard, and both the IUCr President and General Secretary. The total number of members and appointed consultants is about 50. While ways to reduce the size of the CCN have been considered, the importance of all members is recognized. In the case of a matter needing the vote of the whole Commission, a Working Group composed of members representing all important viewpoints would be asked to prepare a report to be circulated to the CCN in advance of the vote.

The Commission's web page invites crystallographers to bring nomenclature problems to the attention of any Commission member. No such matter arose during 2018.

The CCN is responsible for maintaining the *Online Dictionary of Crystallography* (ODC, Editor Gervais Chapuis), 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 (on the occasion of the two most recent IUCr Congresses).

The ODC has never generated much activity, even though the IUCr Commissions have been asked to provide definitions for their areas of expertise. The ODC still has only 336 definitions, with only 29 having been added in the last year At least some of the new definitions were sent to the Editor, who himself entered them into the ODC. The number of authors who created new entries or revised existing definitions remained very small.

Statistics on page views (see http://reference.iucr.org/dictionary/Special:PopularPages) show that the ODC is accessed often. The page for the term *Wigner–Seitz cell* (the 50th most viewed page at this time last year and the 57th now) has been visited more than 6000 times during the past 12 months (although many of these may be the result of robots following the embedded hyperglossary links in journal articles).

During 2018 two paragraphs about the ODC were drafted and added to the ODC home page:

Welcome to the Online Dictionary of Crystallography (the ODC) maintained by the Commission for Crystallographic Nomenclature (CCN) of the International Union of Crystallography (IUCr). The ODC functions as a virtual hyperglossary for journals published by the IUCr; when an article from one of the IUCr journals is read online the words defined in the

ODC appear as clickable links. The ODC was envisioned as a reference work that would have some aspects of a dictionary and others of an encyclopaedia.

and

The ODC is run as a wiki; the entries are created and modified by the authorized users, who are the members of the CCN and others approved by the ODC Editor. Entries in the ODC are descriptive rather than prescriptive. There is no formal review process, so if an entry in the ODC differs from a similar definition in one of the volumes of the International Tables for Crystallography the latter is the more authoritative source.

These paragraphs were designed to clarify what the ODC is and what it is not. If there is any conflict between a definition in the ODC and a definition in one of the volumes of *International Tables*, then the latter takes precedence.

An article about the ODC by Chapuis & Brock appeared in the March 2019 issue of the *IUCr Newsletter*. The goal of that article was to increase activity.

It appears that at least one other dictionary project sponsored by an International Union has encountered difficulties (see the report of the IUCr Representative on ICTNS).

C. P. Brock, Chair

4.8. Commission on Crystallographic Teaching

Members: Katherine Kantardjieff, Chair; Oluwatoyin Asojo, Vice Chair; Annalisa Guerri, Tsuyoshi Inoue, Pavel Kashkarov, Diego G. Lamas, Sol Lopez-Andres, Jarugu Narasimha Moorthy, Manfred Weiss.

Consultants: Mois Aroyo, Alexander (Sandy) Blake, Elena Boldyreva, James Britten, Saulius Grazulis, S. Krishnaswamy, Edward Michalski, Claudine Mayer, Claudia Rawn, Miriam Rossi, Nivaldo Speziali, Michele Zema, Shao-Liang Zheng.

Overview of activities. The Commission on Crystallographic Teaching (CCT) is a large and vibrant group of nine regular members and 14 member consultants. Member consultants are quite active in reviewing applications for workshops and summer schools. In each application period of 2018, the CCT reviewed 4, 3 and 5 applications, respectively. In the first period of 2019, we have recently completed review of 5 proposals. All documents are shared among the members mainly on Google Drive, while a few members and consultants continue to use e-mail. The evaluation process has been streamlined with the use of the shared drive, and standardized rubrics and an evaluation form have facilitated clarity, objectivity and transparency. The CCT strives to provide letters of evaluation that are not only supportive but informative to the applicants, the Sub-committee on the Union Calendar, and the Executive Committee. We continue to advocate for the use of a centralized electronic submission process, which will improve workflow and reduce errors. We plan to post instructions and a tip sheet for applicants, so that applications are submitted to the appropriate person in the submission cycle, and the applications received have been prepared on current forms and are complete in required content.

The CCT has been active this year to appoint a representative to the International Programme Committee (IPC) for the Prague Congress and General Assembly in 2020. We have two co-representatives to the IPC, Diego Lamas and Toyin Asojo. Because the CCT has several members who have served previously on the IPC within a certain time frame, they were ineligible to serve for the 2020 planning. Other members of the CCT have duties and responsibilities outside of their volunteer work on the CCT, and this precludes them from serving or serving full time on the IPC. Scheduling conflicts have also made travel difficult. Nevertheless, the CCT has worked together to draft proposed symposia and keynotes for the Prague Congress and General Assembly, which have been submitted to the local organizers. One of our members, Manfred Weiss, will be present for the IPC meeting in May as an observer.

Social media and web resources. Since the 2017 Congress and General Assembly in Hyderabad, the CCT has continued its efforts to reach out to the crystallographic community, the scientific community and the community at large using social media. The Commission Facebook page has been the most active (http://www.facebook.com/IuCrCommissionOnCrystallographicTeaching), and now has 1162 'likes' and 1186 followers. Our Twitter feed (@IUCrTeach) has 180 followers. Social media use is highly generationally dependent, and we are exploring the potential use of Instagram and LinkedIn for enhanced outreach. After a recent hack, and seeing little access, we have abandoned Google+. Social media posting for intentional outreach takes concerted effort, and the bandwidth of the CCT members is limited given other professional responsibilities. Account ownership should be transferred to the IUCr office before the Commission membership changes in Prague, because the accounts are currently owned and managed by the Commission Chair. This will enable the CCT to execute its plan to have members share posting responsibilities to our social media to keep our followers informed and engaged, as well as to regularly review and refresh our web resources. In addition, we hope to reactivate a quarterly newsletter with a global outlook.

Participation in and sponsorship of professional programming. As pointed out earlier in this report, and last year's report, given the current IUCr rules concerning appointments to the International Programme Committees, the CCT nominated Diego Lamas as its representative to the IPC for the Prague Congress and General Assembly in 2020. Toyin Asojo serves as our alternate. Diego has been active with the Commission over the years, and Toyin as its Vice Chair (and Chair apparent when the current Chair term ends).

Several members of the CCT would again like the IUCr to reconsider the current rule that disallows an individual who has been on an IPC to serve again for at least two Congresses. They feel that this disrupts continuity, and that prior experience is very helpful. Others who have served on an IPC have noted that things went smoothly when they served and, as someone who has served in this capacity, the current CCT

Chair would concur with this sentiment. It is further helpful if an IPC representative has previously organized sessions or microsymposia at international crystallography meetings. With the current rule in place, an individual will likely serve only once, as almost three triennia will pass before they would be eligible again. The individual will likely have served out their 6–9 years on a Commission and, after nearly a decade, will likely have moved on in their career. The IUCr may be limiting its options by excluding such people, who readily give of their time, energy and experience. The rule might be altered to state that preference would be given to those who have not served for at least one (or two) Congresses.

K. A. Kantardjieff, 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. In 2018 two CrysAC workshops were organized, in Mexico and in Chile, expanding our activities in North and South America.

Three members of the Commission (Alicja Rafalska-Lasocha, Gilberto Artioli, Petr Bezdicka) were co-organizers of the 7th Meeting X-ray and Other Techniques in Investigation of the Objects of Cultural Heritage, which was held in Krakow, 17–19 May 2018. More information is available at http://www.biurokarier.chemia.uj.edu.pl/conf/x-ray18.

Gilberto Artioli and Miguel Delgado organized the 3rd CrysAC Workshop Recent Advances in the Investigation of Ancient Mortars and Binders, which was held on 20 May 2018, before the 42nd International Symposium on Archaeometry (ISA 2018) in Mérida, Yucatán, Mexico.

Miguel Delgado also organized the 4th CrysAC Workshop CHEMFORS, which was a satellite event of the Latin American Conference of Analysis by X-ray Techniques (SARX-2018) in Pucon, Araucania, Chile (8–9 November 2018). The purpose of the workshop was to strengthen the activity that takes place in the Latin American region in the field of characterization of cultural heritage and forensic science materials. Although the theme of the workshop was centred around the use of X-ray diffraction and fluorescence techniques, applications of other techniques were presented as well. Well known international experts, especially invited, spoke about the application of various techniques in the solution of interesting problems associated with the conservation and preservation of our cultural heritage. Practical sessions were also organized for the benefit of students and young researchers. The whole programme is available at https://sarx-jfmf-2018.ufro.cl/en/chemfors-sarx-2018/.

The Commission nominated member Miguel Delgado as CrysAC representative on the International Programme Committee for the 25th IUCr Congress and General Assembly in Prague, 2020, and started preparations for the Congress.

Petr Bezdicka took part in the organization of the 7th interdisciplinary ALMA conference The Colour Theme, focused on research, technology, history and conservation/restoration of fine art, Bratislava, Slovakia, 16–18 October 2019 (https://www.alma-lab.cz/eng/news/7th-interdisciplinary-alma-conference-%E2%80%93-first-announcement).

Celerino Abad-Zapatero continued collaboration with Mr Painton Cowen to incorporate scientific content into the 'Rose Window' site (http://therosewindow.com/TheRoseWindow2/Rose-numbers.htm).

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

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

4.10. Commission on 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), M. Petrukhina (USA). Consultants: Tian Cui (China), V. L. Solozhenko (France), A. R. Oganov (USA), H. Maynard-Casely (Australia), O. Yaghi (USA), S. Qiu (China), Nan Zhang (China), Y. Sugawara (Japan). Commission website: http://uhp.iphy.ac.cn/CM/.

Our Commission was formally approved during the meeting of the General Assembly in Hyderabad (August 2017). The *ad interim* Commission was approved during the meeting of the IUCr Executive Committee in Boston (July 2012), as it covers a high-impact and deeply crystallographic topic that was not covered by other IUCr commissions.

Conferences and symposia. Changqing Jin was Chair of the International Symposium of New Emergent Materials at Extreme Conditions, held jointly with the National Conference on Crystallography of China, Tianjin, China, 25–28 September 2018 (http://uhp.iphy.ac.cn/2018iucrcm/). There were around 80 participants: all seven members of the Commission and seven of the consultants were on the International Advisory Committee.

Professor M. A. Petrukhina was a Chair of the 2nd International Fusion Conference entitled From Carbon-Rich Molecules to Carbon-Based Materials in The Bahamas, 7–10 June 2018, which had about 70 participants.

Workshops. Artem Oganov organized workshops on crystal structure prediction in Skoltech, Moscow, Russia, 17–19 September 2018 and Tianjin, China, 24–26 September 2018 (both with around 70 participants).

Plenary and keynote & invited lectures. C. Q. Jin gave a talk on 'New DMS with Independent Doping of Spin & Charges', at the International Workshop on Quantum Complex Matter (QCM 2018), 11–15 June 2018, Rome, Italy; on 'New Superconductors Tuned at High Pressures', at the 12th International Conference on Materials and Mechanism of Superconductivity and High Temperature Superconductors (M2S-2018), 19–24 August 2018, Beijing, China; and on 'The Diluted Magnetic Semiconductor with Independent Spin & Charge Doping: Materials, Properties, Approaching to Multiple Heterojunctions', at the Kavli ITS Workshop on Diluted

Magnetic Semiconductors: Challenges and Opportunities, 4–5 November 2018, Beijing, China.

Artem Oganov gave a talk 'Crystal Structure Prediction: Quo Vadis?' at the Faraday Discussion Meeting, Cambridge, 11–13 July 2018.

M. A. Petrukhina gave lectures at CURO-π^3, Oxford, UK, 5–7 September 2018; at Aromaticity-2018, Mexico, 28 November – 1 December 2018; and at the ACS meeting, New Orleans, 18–22 March 2018; and popular science talks at the University of Iceland (25 May 2018), the Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia, 13 July 2018; at the University of North Texas, 21 September 2018; and at Case Western Reserve University, 18 October 2018.

Changqing Jin, Chair

4.11. Commission on Electron Crystallography

The major goal of our Commission (the CEC) is teaching and promotion of electron crystallography science. Thus, successful organization of international workshops and schools are the major achievements of the Commission.

Europe. The 51st Course on Electron Crystallography of the International School of Crystallography, 1–10 June 2018 in Erice, Italy, was directed by Professor Lukas Palatinus (Prague, Czech Republic) (member of the CEC) and Professor Joke Hadermann (Antwerp, Belgium) (consultant of the CEC). [The CEC holds such a school in Erice every seven years, thus immediately after the completion of the school we applied for the next course on Electron Crystallography, which will be in 2025 and will be directed by Professor A. Eggeman (Manchester, UK) and Professor D. Jacob (Lille, France) (member of the CEC), who are both active members of the community.] Fifty-five PhD students and young postdocs, and 19 lecturers and workshop leaders (the vast majority of which were CEC members and consultants) participated in the 51st Electron Crystallography course, which provided lectures on the basics of electron crystallography as well as insight into the most recent developments in this field, stretching from electron diffraction to imaging for crystallographic purposes, on a wide range of materials, from proteins to inorganic materials. The participants themselves were encouraged to show their recent work during the poster sessions. Prizes were awarded during the closing ceremony for the three best posters and the Lodovico Prize, named after Lodovico Riva di Sanseverino who created the International School of Crystallography. The third place for the best poster was awarded to Stefan Noisternig, PhD student at the Faculty of Physics, University of Vienna, Austria, the second place to Paul Benjamin Klar, PhD student at the Department of Condensed Matter Physics, University of the Basque Country, Spain, and the first prize was awarded to Olga Chovnik, PhD student at the Department of Organic Chemistry, Weizmann Institute of Science, Israel. The Lodovico prize for the most active student inside and outside the lecture hall was awarded to Eu Pin Tien, PhD student at the School of Materials, University of Manchester (UK).

The two-day UK–Israel Workshop on Nano-Scale Crystallography for Bio and Materials Research, 18–19 June 2018, was held at Tel Aviv University, Israel. It was supported by the CEC, and the Chair of the CEC as well as some CEC members and consultants (from the UK and Israel) gave lectures at this meeting. The workshop was well attended (about 60 participants).

At the European Crystallography Meeting 31 (ECM31) in Oviedo, Spain (August 2018), Professor Lukas Palatinus (member of the CEC) gave a Plenary Lecture and Professor Joke Hadermann (consultant of the CEC) gave a keynote lecture, and three microsymposia on different electron crystallography related subjects were held.

China. The 2018 Kuo Symposium on 3D-EM of Macromolecules and Cells & The 11th K. H. Kuo Summer School of Electron Microscopy & Crystallography were held in Zhejiang University, which houses a newly established state-of-the-art cryoEM facility for structural studies of macromolecules and cells. Major topics of the meeting included recent developments in cryoEM sample preparation and data acquisition, advances in cryoEM image analysis and reconstruction, advances in cryoET and *in situ* structural biology, and correlative and hybrid methods for cellular structural analysis. As such it was fully supported by the CEC.

Australia. Professor Laure Bourgeois (CEC member) was part of the organizing committee of the Workshop on Scanning Transmission Electron Microscopy with Advanced Detectors, Lancefield, Australia, 4–7 September 2018. The main organizers were Professor Joanne Etheridge, Dr Scott Findlay, Dr Laura Clark and Dr Philip Nakashima. There were about 60 participants, around 40 of which were from abroad. The main topics were scanning electron diffraction, quantitative STEM and new pixelated/direct electron detectors.

L. Meshi, Chair

4.12. Commission on High Pressure

Since not all IUCr Commission on High Pressure (CHP) members attended the IUCr Congress and General Assembly in India in 2017, we scheduled an informal meeting during the Gordon Research Conference for High Pressure at Holderness, NH, USA, on 20 July 2018. Four CHP members, Haozhe Liu, Kamil Dziubek, Amy Lazicki and Yasuo Ohishi, met and briefly exchanged ideas for future workshop location selection rules, the new website *etc*.

The 2018 workshop of the IUCr Commission on High Pressure took place in Honolulu, USA, 29 July – 2 August 2018. The International Programme Committee of the workshop consisted of the members and consultants of the IUCr Commission on High Pressure. The Local Organizing Committee was chaired by Professor Przemyslaw Dera and included Dr Vitali Prakapenka, Dr Bin Chen, Dr Dongzhou Zhang and Dr Gregory Finkelstein. Owing to the strict application window for travel funding for young researchers, this workshop did not receive financial support from the IUCr. Sponsors included the US National Science Foundation, COMPRES, the University of Hawaii at Manoa, GSECARS,

HPCAT, Bruker AXS, Crystal Impact, Almax easyLab, Micro Support, Dectris, Technodiamant, Depths of The Earth and MiTeGen. The US National Science Foundation and COMPRES funded 12 young participant fellowships for students and postdocs from institutions in the USA, and the registration fees for four young scientists attending from outside the USA were funded from the proceeds of the meeting.

The main workshop was preceded a one-day data analysis training event held at the University of Hawaii at Manoa and funded by COMPRES. The software event had 45 participants, mainly graduate students and postdocs, and included six lectures and two parallel three-hours-long hands-on practical tutorial sessions.

The main workshop event was attended by 104 participants from 16 countries. The theme of the workshop was 'E3: Extreme Materials, Extreme Phenomena, Extreme Environments'. Three plenary talks were presented by Dr John Eggert (LLNL, USA), Dr Yongjae Lee (Yonsei University, South Korea) and Dr Shanti Deemyad (University of Utah, USA). The poster session featured 36 poster presentations. In addition to nine exciting scientific sessions in this workshop, there was an evening session entitled 'Women under High Pressure', which many participants expressed support for.

Five CHP members (Haozhe Liu, Kamil Dziubek, Amy Lazicki, Guoyin Shen and Andrzej Katrusiak) attended this workshop and met on 1 August 2018. They discussed future workshop on-site bidding rules, data-format issues, updating and maintenance of the new website, *etc*. The Chair of the CHP, Haozhe Liu, briefly described the history of the IUCr and the history of the CHP workshops over the last two decades at the opening and closing sessions of the workshop. The Secretary of the CHP, Kamil Dziubek, presented the Commission's effort on data format during the workshop.

CHP members communicated through e-mail in May 2018, and chose next year's workshop location as Vienna, Austria, scheduled for 13–17 August 2019. The Chair of the Local Organizing Committee will be Professor Ronald Miletich-Pawliczek from the University of Vienna, who will be one of the local hosts for the 32nd European Crystallographic Meeting (ECM), 18–23 August 2019. We expect that the back-to-back style arrangement for this 2019 workshop, right before ECM-32 and co-organized by the European Crystallographic Association (ECA) Special Interest Group SIG-11, will attract more young students and researchers to attend the workshop.

H. Liu, Chair

4.13. Commission on Inorganic and Mineral Structures

Following IUCr 2017 in Hyderabad and up to early 2018, several new members and consultants were appointed to the Commission (CIMS), while others' mandates were extended. The current list of IUCr CIMS members and consultants is as follows.

Members: P. Mercier (Chair, Canada), P. C. Burns (USA), M. Colmont (France), F. Hatert (Belgium), V. Kahlenberg (Austria), M. Nespolo (France), R. Oberti (Italy), M. Wolcyrz (Poland), A. Yoshiasa (Japan), N. Zubkova (Russia).

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), M. Welch (UK).

Members and consultants of CIMS discussed various issues via e-mail. Other forms of communication were at other occasional meetings or conferences or by using the website. The latter is kindly maintained by M. Nespolo (CIMS member) (http://www.crystallography.fr/cims/).

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

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

P. Mercier (CIMS Chair) continues to act as liaison officer of CIMS with the *IUCr Newsletter*.

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) participates in the activities of the EMU Executive Committee while serving as Commissioning Editor of the EMU *Notes in Mineralogy*, which also implies scouting for the EMU schools.

A Special Issue of *Acta Crystallographica B* on mineralogical crystallography appeared in December 2018, co-edited by J. Majzlan, Sergey Krivovichev (CIMS consultant) and J. Plášil.

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

In 2018 C. Ling (CIMS member) was President of the Society of Crystallographers in Australia and New Zealand (SCANZ) and Past Secretary of the Asia-Oceania Neutron Scattering Association (AONSA). He is Chair of Crystal-33, the 33rd meeting of SCANZ, to be held in early 2020. He is also a member of the Australian Synchrotron's User Advisory Committee and BRIGHT Advisory Committee, and a member of the Australian National Committee for Crystallography (NCCr).

P. Mercier (CIMS Chair) has been Chair of the Canadian National Committee for Crystallography since August 2015.

R. Oberti (CIMS member) is Chair of the Committee on the Participation of the CNR (Consiglio Nazionale delle Ricerche) in the IUCr, and was elected to the Socio Nazionale of the Accademia delle Scienze di Torino. She was also

Convener of the scientific session 'Puzzle Crystallography. A tribute to Prof. Fiorenzo Mazzi' at the SIMP-SGI (Italian societies of Mineralogy and Petrology and Italian Geological Society) joint meeting, Catania, 12–14 September 2018.

Frédéric Hatert (CIMS member) is our representative for the next ECM meeting, ECM32 (https://ecm2019.org/home/). Marie Colmont (CIMS member) is Chair, and Sergey V. Krivovichev (CIMS consultant) is Co-chair.

Marie Colmont (CIMS member) was a member of the scientific committee of ECM31 held in Oviedo, 22–26 August 2018 (https://ecm31.ecanews.org/en/index.php).

G. Ferraris (CIMS consultant) and R. Oberti (CIMS member) organized the meeting 'Two Hundred Years of Mixed Crystals', 22–23 May 2018, at the Accademia delle Scienze di Torino.

J. Rocha (CIMS consultant, Past Chair) was involved in the organization of SMARTER 6, taking place in Ljubljana, Slovenia, 2–6 September 2018 (https://smarter6.ki.si/index.php/committees/).

P. Mercier (CIMS) was selected to represent CIMS interests as member of the International Programme Committee for the next IUCr 2020 Congress in Prague, Czech Republic, 22–30 August 2020.

M. Nespolo (CIMS member) was Ambassador at the 22nd Meeting of the International Mineralogical Association (13–17 August, Melbourne), and main Convenor of the session on Modular Aspects of Mineral Structures (Co-convenors Isabella Pignatelli and Sergey Krivovichev, both CIMS consultants).

Sponsorship of workshops and schools. David Kingston (National Research Council Canada, Ottawa) and P. Mercier (CIMS Chair) successfully submitted a proposal to hold a workshop on Applications and Advances of Cathodoluminescence Microscopy and Spectroscopy in Mineralogy and Geosciences at the XXII Meeting of the International Mineralogical Association in Melbourne, Australia, 13–17 August 2018. However, owing to an insufficient number of registrations, the workshop did not take place.

CIMS supported the application for funding by the IUCr of the following meetings to be held in 2019:

American Crystallographic Association Annual Meeting 2019, 20–24 July 2019, Cincinnati, USA.

XIX International Meeting on Crystal Chemistry, X-ray Diffraction and Spectroscopy of Minerals, 2–5 July 2019, Apatity, Russia.

17th European Conference on Solid State Chemistry (https://ecssc17.com/), 1–4 September 2019, Université de Lille, France.

P. Mercier, Chair

4.14. Commission on Magnetic Structures

Commission members: Branton Campbell (Chair, USA), Maxim Avdeev (Australia), Maria Teresa Fernandez-Diaz (France), Ovidiu Garlea (USA), Margarida Henriques (Czech Republic), J. Manuel Perez-Mato (Spain), Juan Rodriguez-Carvajal (France), Taku Sato (Japan), Andrew Wills (UK) and Oksana Zaharko (Switzerland).

Commission consultants: Mois Aroyo (Spain), J. Campo (Spain), Danny Litvin (USA), Alexander Pirogov (Russia) and Wieslawa Sikora (Poland).

After the turnover of a large proportion of the membership of the Commission at the IUCr Congress in Hyderabad in August 2017 (see above for the present membership) in accordance with its terms of reference, the Commission has continued its activities during 2018, promoting the investigation of magnetic structures as a part of crystallographic science, developing standards, encouraging their inclusion in new software, and disseminating their use, so that the research and communication of magnetic structures can reach a level of rigour and standardization similar to that achieved for ordinary structures.

The magCIF working group actively discussed a variety of revisions to the standard magCIF dictionary that was developed in previous years. These included: (1) improvement of the descriptions of tags related to magnetic moments and incommensurate magnetic modulations; (2) addition of a tag for the magnitude of a magnetic moment; (3) 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; (4) progress on categories for magnetic reflection data from diffraction experiments; and (5) debate on the possible addition of origin-referenced modulation parameters, as an alternative to the atom-referenced ones, which are currently used in the superspace formalism.

Also within this area of development of extended CIF standards for the communication of magnetic structures, we have started to work on the so-called smCIF dictionary for the description of magnetic and other symmetry-lowered crystal structures in terms of symmetry modes (basis functions of matrix representations of the parent symmetry group). This smCIF dictionary is a much-needed addition to the magCIF standard, which will allow standardization of the communication of magnetic structures when described using the so-called representation method and, most importantly, when both representation analysis and magnetic symmetry groups are considered together, which in the most general case is the most efficient and complete approach to the description of a magnetic structure. A first draft of the smCIF dictionary, including some examples, has been proposed by the Commission Chair Branton Campbell, and has been discussed by an *ad hoc* working group of interested members and consultants of the Commission. In accordance with our terms of reference, these CIF-related activities have been done in close contact with the Chair of COMCIFS, James Hester.

Another task has been the preparation of the Erice school Magnetic Crystallography, sponsored by the IUCr and organized by the Commission, which will take place in June 2019. The organization of this school has run smoothly but has required an important amount of time and effort on the part of Branton Campbell, Maria Teresa Fernandez and J. Manuel Perez-Mato, acting as Directors of the school, and with the

fundamental collaboration of Annalisa Guerri and Paola Spadon, Executive Secretary and Treasurer of the Erice Crystallography Schools. Successive steps in the organization have been completed in 2018: design of the programme, selection and invitation of lecturers, announcement, funding raising, design of the school schedule, registration of participants, evaluation and screening of applications, *etc*. About 100 applications were received, but owing to the constraints on the size of the school only 65 participants could be selected. Many of the selected participants are young scientists from developing countries, who will receive some kind of bursary support. Seventeen presenters will deliver the lectures and practical tutorials of the school. All members of the Commission will participate, but other people responsible for some of the latest developments in methods, software and techniques will also be present. Our intention is that the school becomes a window showing the present state of the art of magnetic structure determination, and a benchmark that will encourage further developments and progress in the methods and software tools available for the analysis of magnetic structures.

The members of the Commission have also continued working on the promotion of the visibility of the research on magnetic structures in the annual meetings of the IUCr Regional Associates. Our aim is that this very specific research community is well represented within these meetings. In the last few years all the annual ECA meetings have included a specific session on magnetic structure research, and the 2018 Oviedo meeting has maintained this feature, which we hope will tend towards permanence. Commission Secretary J. M. Perez-Mato was one of the invited speakers at this session in Oviedo, and used the opportunity to promote the advantages of analysing and communicating incommensurate magnetic structures using the superspace-group formalism, which is the method used in the magCIF dictionary.

The Commission supports a variety of scientific meetings each year through formal sponsorship, and with its members and consultants participating in featured lecture presentations, workshop tutorials, organization and chairing of conference sessions, and the presentation of lecture courses. Highlights from 2018 include the following:

American Crystallographic Association Meeting, 20–24 July 2018, Toronto, Canada. Session on Theoretical and Computational Crystallography – Present and Future Opportunities at the Structural Interface of Experiment and Theory (Co-chair: Branton Campbell).

Aperiodic 2018, 9th Conference on Aperiodic Materials, Ames, Iowa, USA, 8–13 July 2018 (invited talk: M. Henriques).

Workshop at ISIS Neutron and Muon Source – Rutherford Appleton Laboratory, Didcot, Oxford, UK, 11–13 April 2018, *Jana2006* for Crystal and Magnetic Structure Determination from TOF Neutron Data (lectures and tutorials: M. Henriques).

Workshop on single-crystal neutron diffraction, The Magnetic Option of *Jana2006*, included in the IKON15 (In-Kind Contributions Meeting for Neutron Science for Instruments), Lund, Sweden, 10–14 September 2018 (lectures and tutorials: M. Henriques).

7th School on Representational Analysis and Magnetic Structures (RAMS), University of Maryland, USA, 19–22 June 2018 (organization: O. Garlea; lectures and tutorials: B. Campbell, A. Wills, O. Garlea).

Workshop on Symmetry-Mode Analysis of Magnetic and Displacive Structures, Oak Ridge National Laboratory, USA, 15–16 August 2018 (organizer: O. Garlea, lectures and tutorials: B. Campbell).

International Conference on Magnetism (ICM 2018), San Francisco, USA, 15–20 July 2018 (talk: O. Garlea).

European Crystallographic Meeting, ECM31, Oviedo, Spain, 22–27 August 2018 (invited microsymposium talk: J. M. Perez-Mato).

China Institute of Atomic Energy, Beijing, 19 December 2018 (seminar and tutorial: Max Avdeev).

XVII International Small Angle Scattering Conference (SAS2018), 7–12 October 2018, Grand Traverse City, USA (invited plenary talk: T. J. Sato).

22nd Workshop on Quasicrystals, Tohoku University, Sendai, Japan, 5–6 March 2018 (T. J. Sato).

Tutorial Workshop for Magnetic Materials, Kanda, Tokyo, Japan, 11 November 2018 (T. J. Sato).

Programme Committee for the magnetic structure section of the International Research Conference on Using Neutron Scattering on Condensed Matter NSCM, St Petersburg, Russia, 17–21 September 2018 (member: A. Pirogov).

6th International Conference on Superconductivity and Magnetism, Antalya, Turkey, 24 April – 4 May 2018 (sessions Chair: J. Campo).

International Conference on Magnetism, San Francisco, USA, 15–19 July 2018 (session Chair: J. Campo).

43rd International Conference on Coordination Chemistry (ICCC2018), Sendai, Japan, 30 July – 4 August 2018 (invited talk: J. Campo).

Manuel Perez-Mato, Secretary, on behalf of **B. J. Campbell**, Chair

4.15. Commission on Mathematical and Theoretical Crystallography

Presently the Commission is chaired by D. Pandey (India) with V. A. Blatov (Russia), D. Gratias (France), J. Hadermann (Belgium), G. McColm (USA), H. B. Napolitano (Brazil), R. Oishi-Tomiyasu (Japan), M. L. A. N. De Las Penas (Philippines), Wei Ren (People's Republic of China), L. Suescun (Uruguay) and P. Zeiner (Malaysia) as members, and M. I. Aroyo (Spain), J.-G. Eon (Brazil), E. E. Rams (Cuba), S. Hyde (Australia), D. B. Litvin (USA), K. Momma (Japan), M. Nespolo (France), D. Pradhan (India), D. Proserpio (Italy), B. Souvignier (The Netherlands) and B. Stöger (Austria) as consultants. Most of the communications among the members and consultants of the Commission (MaThCryst) took place via e-mail. These discussions were related to possible topics,

venues and funding of future schools, workshops, satellite meetings and other outreach activities.

Organization of schools/workshops: The following five workshops or schools were organized by the MaThCryst Commission, the details of each one of which are given at the Commission's and the events' home pages. Members or consultants of the Commission serving as speakers at these events are noted:

(1) Training Course on Symmetry and Group Theory – Sokendai Interdisciplinary Lecture, Tsukuba, Japan, 6–10 August 2018, with Takashi Kamiyama, Noriyuki Igarashi, Maki Okube and Yoshimi Takahashi as Programme Committee members and Massimo Nespolo as the sole speaker. There were 44 participants, all from Japan (http://www.crystallography.fr/mathcryst/TrainingCourseJapan.php).

(2) International School on Topology and Group Theory, San Sebastian, Spain, 23–26 August 2018, with Dario Bercioux, M. Reyes Calvo, Jérôme Cayssol, Adolfo Grushin and Maia G. Vergniory as Organizing Committee members. The speakers were Juan L. Mañes, Mois. I. Aroyo, Jennifer Cano and Barry Bradlyn. There were 42 participants from 11 different countries including 15 from Spain.

(3) International School on Fundamental Crystallography (Sixth MaThCryst School in Latin America), Bogotá, Colombia, 26 November – 1 December 2018. This was a workshop on the Applications of Group Theory in the Study of Phase Transitions. This event was organized by Mario Alberto P, Andreas Reiber, Edgar Vargas, Wolfram Baumann and Elizabeth Jimenez with Mois I. Aroyo, Massimo Nespolo, Leopoldo Suescun, Arbelio Penton-Madrigal and Mike Glazer as speakers. There were 39 participants of which 14 were from abroad (eight countries). The event was financially supported by the IUCr including a Visiting Professorship to two speakers (http://www.crystallography.fr/mathcryst/bogota2018.php).

(4) 1st Latin American Crystallographic Association School on Small Molecule Crystallography, Montevideo, Uruguay, February 2018, with Leopoldo Suescun, Natalia Alvarez and Guzman Peinado as organizers.

(5) A Hands-On Workshop on Density Functional Theory First-Principles Simulations in Materials Science, Baoshan Campus, Shanghai University, 17–22 November 2018, with Wei Ren, Alessandro Stroppa, Claudia Draxl and Pasquale Pavone as organizers. The speakers were Hong Guo, Jiawang Hong, Miao Liu, Hong Jiang, Andris Gulans, Pasquale Pavone, Fabio Caruso, Lucia Reining, Matthias Scheffler, Weitao Yang, Claudia Draxl, Maria Troppenz, Christian Vorwerk, Sven Lubeck and Alessandro Stroppa. There were 100 participants from the home country and 15 from abroad. This event was financially supported by the IUCr.

Satellite event: A satellite meeting to the European Crystallographic Meeting ECM31 on Crystallography Online: Workshop on the Use and Applications of the Structural Tools of the Bilbao Crystallographic Server was organized by Mois I. Aroyo, J. Manuel Perez-Mato and Gemma de la Flor in Oviedo, Spain, 20–21 August 2018. There were 16 participants from ten different countries, including four from Spain.

D. Pandey, Chair

4.16. Commission on Neutron Scattering

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

The construction of the European Spallation Neutron Source (ESS) in Sweden is progressing. The launch of the first beam has been changed to 2022, but the user programme is scheduled to start at the end of 2023 as planned. The Chinese Spallation Neutron Source (CSNS) started operation in August 2018 with three instruments (a powder diffractometer, refractometer and SANS). The current beam power is 50 kW, and the user programme has also been started. The Spallation Neutron Source (SNS) in the USA continues operation. J-PARC MLF in Japan is also in operation with 500 kW beam power, and the beam power will be upgraded in 2019. Several new neutron scattering instruments were brought into user programmes at neutron scattering facilities across the world. In addition, plans for new compact accelerator-driven neutron sources are being developed in order to preserve the possibilities for both teaching neutron scattering methods and to use them scientifically, as the Laboratoire Léon Brillouin (LLB) at the Orphée reactor in Saclay (France) and the HZB reactor in Berlin (Germany) will be shut down at the end of 2019.

Our Commission members were also involved in organizing several meetings, not only for neutron but also for quantum beam (synchrotron, neutron and ion radiation *etc*.) joint use, that took place in 2018, including various annual meetings of regional crystallographic associations.

The Australian Neutron Beam Users Group (ANBUG) and Australian Institute for Nuclear Science and Engineering (AINSE) 2018 Neutron Scattering Symposium was held at Lucas Heights, 19–24 November 2018.

The 31st European Crystallographic Meeting, ECM31, of the European Crystallographic Association took place in Oviedo, 22–27 August 2018. The satellite meetings included Neutron Macromolecular Crystallography, 21–22 August 2018. The IXth International Meeting of the Spanish Neutron Techniques Society, Sociedad Española de Técnicas Neutrónicas (SETN), was held in Santander, 17–20 June 2018 (this was the ninth of a series of biannual meetings).

Not only large facilities but also compact neutron sources are being established and constructed in various countries. The 7th International Meeting of the Union for Compact Accelerator-Driven Neutron Sources was held at Bariloche, Argentina. In Europe, the 4th Workshop on a High Brilliance Neutron Source 2018 took place near Cologne in Germany,

focusing on the development of small accelerator-driven neutron sources (non-fission) for educational purposes and dedicated applications, and both Germany and France are working on new concepts to realise these kinds of small sources.

Several neutron schools at many facilities were supported by Commission members. In the Asia–Oceania region, the 3rd Neutron and Muon School was held at J-PARC in Japan with 35 students from seven countries. The 10th Australia–Oceania Neutron Scattering Association Neutron School was held at the Australian Centre for Neutron Scattering, 11–16 November. In Germany, apart from the annual laboratory courses at HZB and JCNS, a satellite workshop was held along with the German conference on large-scale facilities for synchrotron, neutron and ion scattering to present the benefit from combining synchrotron and neutron methods for new scientific insights, *e.g.* on energy-related materials.

Commission members were involved in planning activities for several important neutron conferences and schools in 2019. For the European Crystallographic Meeting (ECM) in Vienna in August 2019 a four-day satellite workshop has been organized by the German and Swiss societies for crystallography to give newcomers to neutron scattering and imaging an overview of the state-of-the-art methods and topics in this field. The Joint French–Swedish School on X-ray and Neutron Techniques for the Study of Functional Materials for Energy will be held 13–17 May 2019 in Lund. In the Asia–Oceania region, the 11th AONSA Neutron School will be held 19–23 August 2019, near KAERI in Daejeon, Korea.

T. Ishigaki, Chair

4.17. Commission on NMR Crystallography & Related Methods

In this reporting period, our Commission is in the middle of its second triennium. The bulk of the Commission's activities continues to involve work with regional crystallographic associations and helping to organize themed sessions on NMR crystallography at their annual meetings.

Connections between the Commission and the American Crystallographic Association (ACA) are the strongest. The ACA has been very receptive to the Commission's activities. Themed half-day sessions on NMR crystallography have become regular features at the annual meetings of the ACA. The 2018 annual meeting of the ACA in Toronto, Canada (20–24 July 2018) featured a half-day session on NMR crystallography, co-chaired by Tomislav Friscic and Manish Mehta. Six speakers were part of a compelling programme representative of the broad cross section of the NMR crystallography community. They were David Bryce (University of Ottawa, Canada), Paul Hodgkinson (Durham University, UK), Robert Schurko (University of Windsor, Canada), Phillip Grandinetti (The Ohio State University, USA), Yining Huang (University of Western Ontario, Canada) and Darren Brouwer (Redeemer University, Canada). The session enjoyed a strong attendance and delivered on the high expectations set by the previous year's session. The participants felt clear momentum coming out of the meeting, as well as a certain relevance to the larger crystallography community. At the Toronto meeting, plans were made for a similar session at the 2019 meeting of the ACA in Cincinnati, USA. It was also decided that there would be no session on NMR crystallography at the 2020 ACA meeting, which is in the year of the IUCr Congress in Prague. This collaboration between our Commission and the ACA may serve as a model for connections with other regional crystallographic associations.

The Commission has an official meeting, the SMARTER Crystallography meeting, as a biannual event. The audience of the meeting is medium-sized, between 70–110 people, and it aims to be similar to a Gordon Conference. The meeting was held in Ljubljana, 2–6 September 2018. This was the 6th event after 2007 in Aveiro, 2011 in Aveiro, 2012 in Versailles, 2014 in Durham and 2016 in Bayreuth. At Ljubljana there were 80 participants. The programme follows a regular scheme of organization with the goal of leaving enough time for discussions between people from different disciplinary fields: solid-state crystallography, diffraction crystallography, topological crystallography and crystal modelling. The invited speakers are of a high scientific level and none refused the invitation to participate. One speaker gave a general scientific talk that did not belong to one of the set of strict sub-disciplines of the SMARTER meeting. The mix of disciplines still has a large fraction of NMR spectroscopists, but many young attendees are now practicing two or three disciplines (such as NMR–diffraction–modelling) and this meeting is an ideal place for presenting such research.

The NMR crystallography community is still small, but its presence in international, regional and local meetings dealing with crystallography is slowly increasing and consistently merging to a more general multimodal crystallography approach, justifying the 'Smarter Crystallography' meeting name.

F. Taulelle, Chair

4.18. Commission on Powder Diffraction

Since its formal appointment at the Hyderabad meeting, the current Commission (CPD) nominated Professor Brendan Kennedy as its representative on the International Programme Committee (IPC) for the IUCr Prague Congress. Professor Kennedy's membership has subsequently been confirmed and members of the Commission have been asked to consider possible microsymposia and plenary speakers to suggest to the IPC. This needs to be done well in advance of the meeting of the IPC, which took place in Prague in February 2019.

The CPD supported a number of meetings; however, the most significant, and which included CPD members in its organization, was the 2018 Edition of the Durham Powder Diffraction and Rietveld Refinement School (8–12 April 2018). During this, the twitter handle @iucr_cpd was also created to facilitate the distribution of powder diffraction information. Then, as always, the primary conference for powder diffractionists was the 16th European Powder

Diffraction Conference (EPDIC) that took place in Edinburgh (1–4 July 2018). Although most of the business of the CPD is conducted via e-mail communications, the EPDIC meeting in Edinburgh allowed a number of the members to meet in person and discuss CPD activities, plans and projects. The next EPDIC meeting is scheduled for 26–30 May 2020 in Sibenik, Croatia.

Ongoing CPD projects include Volume H of *International Tables*, which was finally published following the Edinburgh meeting. This will hopefully facilitate the development of derivative work, including a Recommended Practices and Guidelines publication. 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.

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. It is hoped that the Recommended Practices and Guidelines mentioned above as well as the call and subsequent results from the Quantitative Phase Analysis Round Robin will all be published in the IUCr journals.

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

The Commission also supported a number of meetings with a substantive powder diffraction component in their programmes in their applications for support from the IUCr.

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, Chair

4.19. Commission on Quantum Crystallography (formerly known as the Commission on Charge, Spin and Momentum Densities)

In 2017, the former Commission on Charge, Spin and Momentum Densities officially became the Commission on Quantum Crystallography to gain better visibility and acknowledge a broader research topic range. The purpose was also to clarify how the community combines quantum-mechanical objects (such as wave functions, density matrices, charge and spin densities in position and momentum representations) and techniques to gain a better understanding of crystalline material properties.

As briefly reported below, the Commission members have been extremely active during the past year promoting quantum crystallography (QCr) in journals, organizing (and participating in) meetings, collaborating and planning future conferences.

A project 'Establishing Quantum Crystallography' led by P. Macchi (University of Milan) has been particularly active. In addition to the usual articles reporting on research works which fall into the QCr category, several review papers describing the purpose of QCr have been published: *What is Quantum Crystallography?*, an interview with A. Genoni and S. Grabowsky in *ChemViews Magazine* (2018, Wiley); *Quantum crystallography: current developments and future perspectives*, A. Genoni, L. Bu-Bèinský, N. Claiser, J. Contreras-García, B. Dittrich, P. M. Dominiak, E. Espinosa, C. Gatti, P. Giannozzi, J.-M. Gillet, D. Jayatilaka, P. Macchi, A. Ø. Madsen, L. Massa, C. F. Matta, K. M. Merz, P. N. H. Nakashima, H. Ott, U. Ryde, K. Schwarz, M. Sierka & S. Grabowsky (2018), *Chem. Eur. J.* **24**, 10881; *Quantum crystallography: a perspective*, L. Massa & C. F. Matta (2018), *J. Comput. Chem.* **39**(17), 1021–1028; *Exploiting the full quantum crystallography*, L. Massa & C. F. Matta (2018), *Can. J. Chem.* **96**(7), 599–605; *The roots of quantum crystallography*, P. Macchi, (2018), *Acta Cryst.* **74**, e4; and *Early days of quantum crystallography: a personal account*, V. Tsirelson (2018), *J. Comput. Chem.* **39**(17), 1029–1037. It is also worth mentioning that several books, at a variety of readership levels, are in preparation, including *Quantum Crystallography* by P. Macchi, to be published by de Gruyter. Furthermore, P. Macchi has initiated a new Wikipedia page to explain and promote quantum crystallography to a wider audience.

Following its 7th meeting, it was decided that the European Charge Density Meeting series would become the International Charge Density Meeting (ICDM) series. The first of these was held 21–26 July 2019 in Göttingen and was organized by D. Stalke (University of Göttingen). Shortly before this, a satellite workshop in Bremen, chaired by S. Grabowsky (University of Bern) explained Tools for Chemical Bonding. The next ICDM will be organized by J. Overgaard (Aarhus University) and colleagues in 2022 in Denmark.

The 2018 European Crystallography Meeting in Oviedo was the occasion to explain QCr for the first time to the crystallography community. It was the topic of one keynote and one microsymposium.

The 2019 European Crystallography Meeting in Vienna hosted a microsymposium on Modern Quantum Crystallography, but members of the community were also invited to unveil their latest results in several other microsymposia. The P. Coppens Quantum Crystallography poster prize (sponsored by Rigaku Oxford Diffraction) was awarded to V. Vedran (University of Lorraine) and a plenary lecture on QCr Studies of Advanced Materials was given by B. Iversen (Aarhus University).

Following the extremely successful 1st Erice School on QCr co-organized by P. Macchi and D. Jayatilaka (University of

Western Australia) in June 2018, it was decided that the next school will be held in June 2025 and organized by P. Dominiak (University of Warsaw) and J. Contreras-Garcia.

After the 2017 CECAM meeting in Nancy (chaired by A. Genoni, University of Lorraine, and S. Grabowsky, University of Bern), a CECAM workshop on QCr is planned to take place in Milan (hosted by P. Macchi) in 2020.

In 2018, the Sagamore Meeting on Quantum Crystallography, one of the historical highlights of the community, was organized in Halifax by C. Matta (Mount St Vincent University). On this occasion, the community inaugurated two prestigious prizes. Paul L. A. Popelier (University of Manchester) was awarded the Richard Bader International Prize for Excellence in Electron Density Research for 'his exceptional contributions in the development of pure and applied Quantum Chemical Topology (QCT)'. Eduard Matito i Gras (University of Girona) received the Miguel Blanco International Prize for Early Career Work in Charge Density 'for his original and outstanding contributions in the development of new quantum mechanical methods and of new descriptors of chemical behaviour based on the electron and electron pair density distributions'. The next Sagamore Meeting on Quantum Crystallography will be organized by in 2021 by P. Munshi (IIS Bangalore) in India.

Thanks to the strong involvement of K. Wozniak (University of Warsaw), our community will be very well represented during the next IUCr meeting in Prague where quantum crystallography will be the topic of three keynotes, three QCr-specific microsymposia and three other microsymposia shared with other commissions.

J.-M. Gillet, Chair

4.20. Commission on Small-Angle Scattering

Commission members: U-Ser Jeng (Chair), David Babonneau, Kristina Djinovic Carugo, Elliot Gilbert, Duncan McGillivray, Jan Ilavsky, Eleonora Shtykova and Masaaki Sugiyama. Consultants: Andrew Allen, Javier Pérez, Daniel Clemens, Pete Jemian, Jill Trewhella, Dmitri Svergun and Iris Torriani.

For 2018, the business of the SAS Commission (CSAS) was conducted principally via e-mail and during personal meetings at national and international conferences. There was good engagement from many of the CSAS members and consultants. What follows is a summary of highlights of activities for calendar year 2018.

Commission activities, meetings and communication.

Elliot Gilbert organized and chaired the fifth international Neutrons and Food 5 conference in Sydney (16–19 October 2018), which was a satellite meeting to SAS2018. He also served on the International Advisory Committee for SAS2018 and the Scientific Committee of the 11th World Conference on Neutron Radiography (2–7 September 2018) in Sydney.

Jan Ilavsky, Pete Jemian and Randall Winans participated in the SAS2018 conference.

The XVII International Small Angle Scattering Conference – SAS2018 was held in Traverse City, Michigan, USA, 7–12 October 2018. The conference had over 400 attendees with 75% being from international institutions. A number of awards were presented with the highlight being the International Union of Crystallography Guinier Prize, honouring the great scientist and 'father' of small-angle scattering, Professor André Guinier. The 2018 Guinier Prize was awarded to Dr Dmitri Svergun from the European Molecular Biology Laboratory (EMBL), Hamburg, Germany. The Otto Kratky Prize, sponsored by Anton Paar, is awarded to an outstanding young scientist working in SAXS and was awarded to Andreas Haahr Larsen of the University of Copenhagen, Denmark.

The minutes of the Open Commission Meeting at the SAS2018 conference are available at the IUCr cSAS website (https://drive.google.com/open?id=1ufrD2knTPXxG_Ga6Pud0_EaqApKvfZ5E). Jan Ilavsky, Peter Jemian, Andrew Allen, Jill Trewhella, Dmitry Svergun, U-Ser Jeng, Elliot Gilbert, Duncan McGillivray, Kristina Djinovic Carugo, Masaaki Sugiyama, Andrew Allen, Javier Pérez and Peter Jemian were present, along with about 120 participants from the conference attendees.

Andrew Allen was selected as CSAS representative on the International Programme Committee (IPC) for the IUCr 2020 Congress to be held in Prague, Czech Republic, August 2020. He will attend the IPC Workshop and Planning Meeting in May 2019, also in Prague, both as CSAS representative and as Editor-in-chief of IUCr Journals. His role as CSAS representative will be to negotiate SAS-related microsymposia and keynote speakers as part of the overall IUCr Congress programme.

U-Ser Jeng wrote supporting letters for the To.Sca.Lake 2.0 Workshop Total Scattering for Nanotechnology on Lake Como, Italy, in May 2019, and the SAS2018 conference (October 2018) and the satellite meeting Neutrons and Food 5 conference in Sydney (October 2018). He served as the coordinator of the Guinier Prize between the IUCr and the SAS2018 conference Chairs and also chaired the Open Meeting of the Commission at the SAS2018 conference. He also worked with A. Allen and all cSAS members and consultants for proposing a SAS microsymposium package for the IUCr2020 Congress.

The IUCr cSAS website has been updated. There were communications (together with Jill Trewhella, Dmitri Svergun and Andrew J. Allen) with the IUCr Executive Secretary Alex Ashcroft on continuing the Guinier Prize in the future (https://www.iucr.org/resources/commissions/small-angle-scattering/guinier-prize), two SAS-related reviews from microsymposia at the IUCr2020 Congress, and possible proceedings of the SAS2021 conference.

U-Ser Jeng, Jan Ilavsky and Pete Jemian attended a closed meeting with the SAS2021 conference Chair Dr Florian Edouard P. Meneau about the Guinier Prize and a possible proceedings of the SAS2021 conference.

Educational activities.

Jan Ilavsky organized satellite workshops with support from the APS SAXS group in the series of Beyond Rg courses: a Beyond Rg Materials course was held during the weekend before SAS2018 (6–7 October 2018), attended by 17 students

and five lecturers; for the Beyond Rg BioSAXS course (13–14 October 2018) there were ten participants and nine lecturers (including Dmitri Svergun and others). SAS 2018 had more educational events organized by the SAS community, including the sasView Users Meeting (82 participants registered), BioSAS: Advanced Applications (28 registered) and How to Write Proposals for Large Facilities (12 registered). Jan Ilavsky also organized the Irena and Nika course at APS in May 2018 (14 students attended) and was the SAS theory lecturer at the Small Angle Scattering Training School, 4–5 June 2018. This course was organized by Diamond SAXS beamlines for their SAXS users, aiming to provide users of the I22 and B21 beamlines with a rounded knowledge of SAXS as an analytical technique.

Dmitri Svergun presented the following lectures: 'Synchrotron small-angle X-ray scattering for medically relevant macromolecular targets' at the EMBL Corporate Partnership meeting (22 February 2018, Heidelberg, Germany); 'Small angle X-ray scattering from solutions of biological macromolecules and complexes' at the FEBS practical course on integrated approaches to biomolecular interactions (7–11 May 2018, Sevilla, Spain); 'Small-angle X-ray scattering on macromolecular solutions: progress and perspectives' at EMBL-Heidelberg (25 May 2018, Heidelberg, Germany); 'Synchrotron X-ray scattering from biomacromolecular solutions – new developments and results' at the Synchrotron Radiation Instrumentation conference (13 June 2018, Taipei, Taiwan); and 'Something you never wanted to know about SAXS', a course for PhD students, EMBL-Heidelberg (27 November 2018, Heidelberg, Germany).

Eleonora Shtykova continues to run weekly seminars on processing and interpretation of small-angle X-ray scattering data at the Federal Scientific Research Centre 'Crystallography and Photonics' of the Russian Academy of Sciences for students, graduate students and employees from Moscow educational and research institutions, and also continues to give lectures and conduct training courses for students of the physical and biological faculties of the Moscow State University on the application of small-angle scattering in the study of biological objects and modern nanomaterials. She also organized and conducted a practical SAXS workshop for PhD students from Romania at the Conference on Neutron Scattering in Condensed Matter NSCM-2018, 17–21 September 2018, St Petersburg, Russia.

Andrew Allen was pleased to represent the IUCr in assisting in the presentation of three poster prizes at the SAS 2018 Conference in Traverse City, MI, USA. Each prize consisted of a free open access voucher for the winning poster author to publish any accepted paper submitted to the *Journal of Applied Crystallography* (*JAC*).

Masaaki Sugiyama helped to organized the meeting series Neutron Structural Biology Workshop (Japan) on 21 September 2018 and 29 March 2019.

U-Ser Jeng organized a SAXS workshop and practical on soft matter for people working in the arts, and gave an invited talk at the NSRRC USER Meeting on Tracing the Structural Evolution During Spin-coating of Polymer/Fullerene Thin Films (6 September 2018, Hsinchu, Taiwan). He also offered a course in the Department of Chemical Engineering of National Tsing-Hua University Taiwan (February–June 2018) and delivered several seminar talks on the applications of synchrotron SAXS in domestic universities.

Community-building activities.

Approximately 40% of the content at the fifth international Neutrons and Food 5 conference in Sydney, chaired and organized by Elliot Gilbert, highlighted the application of small-angle scattering methods to investigate a diverse array of food materials. This is a relatively new but developing community.

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

Dmitri Svergun continued to act as a Management Committee member and work-package responsible for a pan-European access grant iNEXT, and took part in the annual user meeting (19–21 March 2018, Grenoble, France).

Jill Trewhella continued her community-building work with the biomolecular structure community as a co-organizer of Working Towards Federating Structural Models and Data, a satellite meeting at the Biophysical Society Annual Meeting to be held in Baltimore, 1 March 2019. The meeting is supported by the US National Science Foundation (NSF) and sponsored by the world-wide Protein Data Bank (wwPDB). The workshop is to focus on an initiative to create an interoperating network of structural biology model and data repositories to enable the archiving of integrative structural models and associated experimental data. As a leader in the development of a data archive (the Small-Angle Scattering Biological Data Bank, SASBDB) that has the capability to interoperate with model and data archives including the Protein Data Bank, Dmitri Svergun is an invited participant and speaker. Jill continues as a Co-editor (biology and medicine) for *IUCrJ*, as an Editorial Board member for *Biophysical Journal* and as an International Advisory Board member for *Protein Science*.

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

Eleonora Shtykova continues to serve as the organizer, coordinator and designer of the Russian website on small-angle scattering. An English-language version of the site is now also available. The site can be found at: https://www.saxs.space/. The site is regularly updated. She also regularly organizes visits for research groups (10–12 people) from educational and research institutions in Moscow to the BioSAXS group in Hamburg (group leader Dmitri Svergun) and to carry out joint structural studies of biological objects and novel nanomaterials using small-angle X-ray scattering.

Andrew Allen continued as a Main Editor of the *Journal of Applied Crystallography* during the first part of 2018. However, on being appointed as the new Editor-in-chief of IUCr Journals in August 2018, he stepped down from this role (and Karena Chapman of Stony Brook University, NY, USA, has now replaced him as one of the *JAC* Main Editors).

Elliot Gilbert continues as a Co-editor for the *Journal of Applied Crystallography*.

Masaaki Sugiyama has started to organize a community 'Neutron Structural Biology for Next Generation' in Japan.

U-Ser Jeng coordinated the three institutes National Synchrotron Radiation Research Center, EMBL (Dmitri Svergun's group) and Grid Computing at Academia Sinica of Taiwan, for establishing jointly a BioSAXS data analysis platform dedicated for the BioSAS community in Taiwan.

Consultant activities.

Jan Ilavsky serves as Chair of the beamtime proposal review committee for ORNL SANS instruments.

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

Dmitri Svergun continued to serve on the Scientific Advisory Committee of the National Synchrotron Radiation Research Center, Taiwan.

U-Ser Jeng continues to serve as a board member of the Advisory Committee on Biophysics and Soft Matter of the Physics Discipline of the Ministry of Science and Technology, Taiwan.

Organizational activities.

Dmitri Svergun was the main organizer of the EMBO-supported Practical Course on Solution Scattering from Biological Macromolecules (19—26 November 2018). This was the ninth EMBO Practical Course on solution SAXS in Hamburg, and it continued the traditions set in the previous years. There were 126 applicants, close to the average number for the previous courses. Of those, 26 attendants were selected. They were from 20 countries: from 18 institutions of 18 countries and also two students from industry.

Eleonora Shtykova continues to serve as an expert of the Russian Academy of Sciences (identification number RAS 2016-01-5438-3259) to evaluate SAS-oriented projects and participates as a consultant in development of a high-brilliance biological SAXS/WAXS beamline at the Russian SSRS-4 facility.

David Babonneau continues to serve as Co-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.

Andrew Allen continues to provide informal input for drafts for ISO standards on the use of small-angle scattering, specifically SAXS for particle characterization.

Masaaki Sugiyama serves as Chair of the Beamtime Proposal Review Committee for J-PARC MLF and also serves as a member of the Neutron Advisory Committee for J-PARC MLF.

Technical activities.

Elliot Gilbert is beamline scientist for the QUOKKA SANS instrument at the OPAL facility in Australia and corresponding author for the recent instrument paper celebrating the first one hundred SANS publications [*J. Appl. Cryst.* (2018), **51**, 294–314].

Jan Ilavsky maintained and released three updates to the software packages *Irena* and *Nika* used widely by the materials science SAS community for data reduction and analysis.

The article *2017 publication guidelines for structural modelling of small-angle scattering data from biomolecules in solution: an update* by Jill Trewhella *et al.* continues to top the list of most-read papers in *Acta Crystallographica* Section D with over 7000 downloads and increasing uptake of the recommended table and data deposition in the community.

Jill Trewhella, in her capacity as Chair of the world-wide Protein Data Bank Small-Angle Scattering validation task force (SASvtf) that involves the CSAS members and consultants including Javier Pérez, Dmitri Svergun and 19 others, is coordinating an 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.

Dmitri 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 900 data sets and 1400 models. The *ATSAS* program package developed by the group is presently at version number 2.8.4.

Andrew Allen continues to provide technical support to users of the SAXS Intensity Standard NIST SRM, and continues to encourage development of a SAXD q-Calibration Standard NIST Standard Reference Material.

U-Ser Jeng has been leading the construction of a dedicated BioSAXS beamline at the 3 GeV Taiwan Photon Source of NSRRC since 2016, which is expected to be operational in 2020.

U-Ser Jeng, Chair

4.21. Commission on Structural Chemistry

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

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

In 2018, the CSC has lent support to the following conferences and schools, which draw on crystallographers in the structural chemistry sphere:

British Crystallographic Association School, UK, April 2019.

2nd Pan-African Crystallography Conference, Ghana, January 2019.

American Crystallographic Association Annual Meeting, USA, July 2019.

Zurich Crystallography School, Switzerland, June 2019.

Not all applications were supported, as the CSC members interrogated the degree to which structural chemistry was represented as a science, rather than simply a tool, at each conference. Aspects such as support for students or early-career researchers were taken into account. The diversity (gender, geographical distribution) of speakers was also identified as an important criterion for consideration of future applications for support.

We highlight here two very successful meetings in the fields represented by the CSC:

The 5th Gordon Research Conference on Crystal Engineering was held in Newry, USA. Chaired by Len MacGillivray (a consultant on the CSC), the meeting was fully subscribed and feedback from participants was very positive.

The 5th European Crystallography School was held in Stellenbosch, South Africa, July 2018. The organizing committee was ably chaired by Catharine Esterhuysen. Two members of the CSC (Alison Edwards and Susan Bourne) were among the lecturers at the school, which was held with support from both the CSC and the Commission on Crystallographic Teaching. Participants were drawn from nearly 20 African countries, and expressed appreciation for the school.

As the Commission representing many of the chemical crystallographers who contribute to the Cambridge Structural Database, the CSC is eagerly awaiting the deposition of the millionth structure in the CSD, which is anticipated in 2019.

Finally, the CSC has been active in providing suggestions to the International Programme Committee (IPC) for the IUCr Congress 2020 in Prague, Czech Republic. The CSC members on the IPC are Marijana Dakovic, Masaki Kawano and Catharine Esterhuysen. They have compiled an extensive list of suggested microsymposia and keynote speakers, in collaboration with several other commissions, and will present these at the upcoming IPC meeting. We look forward to a successful IUCr Congress in Prague, which we anticipate will include a strong chemical crystallography programme.

Susan Bourne, Chair

4.22. Commission on Synchrotron and XFEL Radiation

The mission of the Commission (CSXR) 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 for 2017–2020 (with year appointed) are: P. Grochulski (Canada) (2008), Chair; M. A. Garcia-Aranda (Spain) (2011); Y. Murakami (KEK, Japan) (2011); S. Pascarelli (France) (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), Past Chair; D. Fritz (USA); S.-I. Adachi (Japan); M. Suchomel (USA); M. K. Sanyal (India); N. Zatsepin (USA); and L. Keefe (USA).

Synchrotron radiation and free-electron laser facilities. Following the beginning of operations of the first '4th generation' storage ring, MAX IV in Sweden, many synchrotron facilities have been planning to upgrade or build new rings. For example, the ESRF is undertaking upgrade activities to be implemented in 2020. The APS upgrade was approved in December of 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 4th generation Brazilian facility, was erected in 2018. 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).

In 2018 the start-up of a couple of hard X-ray FEL facilities enabled the start of a broadened user activity. At the newly operational PAL-XFEL (Pohang, Korea), European XFEL and SwissFEL facilities user experiments were scheduled using hard X-rays. In the soft X-ray range the European XFEL started its user programme at the end of 2018. In addition, a very active user programme was performed at LCLS, both for hard and soft X-rays, before the facility shut down for the upgrade to LCLS-II. Experiments were performed over a wide range of applications, reaching from fundamental physics problems, materials and geosciences, over femtosecond chemistry with its associate electronics and nuclear dynamics, to structural biology. A new trend in the source development was the ability to generate sub-femtosecond duration X-ray pulses. First experiments have been performed using this capability. Another exciting new field is the use of non-linear X-ray techniques where several experiments were performed at various facilities using soft and hard X-rays. In summer 2018 the construction of a new hard X-ray FEL facility started in Shanghai, located near the SSRF light source and soft X-ray FEL.

Supported meetings, schools and workshops. The Commission provided letters of support and endorsement for the following meetings in 2018:

The Croatian Association of Crystallographers third edition of the workshop Hot Topics in Contemporary Crystallography (HTCC2018), 23–27 September 2018 in Bol, Croatia.

RapiData 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 April 2018.

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

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

Miguel A. G. Aranda gave two invited talks at the 10th Iranian Light Source Facility Users meeting, in Qazvin, Iran, in May 2018, the first on The ALBA Synchrotron and Highlights and the second on How to Write Good Synchrotron Beamtime Proposals, and an invited talk at the XXVII International Materials Research Congress, Cancun, Mexico (August 2018) on Cement Hydration Products Characterized by Combined PDF and Rietveld Analyses. He was Chair of the ESRF Council from 2018 to 2019, the Spanish observer at the European XFEL Council and a member of the Strategic Group-1 of LEAPS.

S. Ramaswamy gave two talks at the Biophysics and Structural Biology at Synchrotrons workshop, 17–24 January 2019, Cape Town, South Africa.

Richard Garrett co-organized a one-day workshop Advanced Light Sources in the AOFSRR Countries held by the Asia–Oceania Forum for Synchrotron Radiation Research as a satellite to SRI2018 and was invited to lecture at the 2nd Asia–Oceania Forum for Synchrotron Radiation Research (AOFSRR) School, 9–15 September 2018.

Pawel Grochulski co-organized and lectured at 8th Annual CLS Mx Data Collection School, Saskatoon, 4–8 June 2018.

Eduardo Granado was part of the organizing committee of the Brazilian Synchrotron (LNLS) Users Meeting. Since October 2018 he has been President of the Brazilian Crystallographic Association (ABCr) and a member of the Advisory Committee of the Latin American Crystallographic Association (LACA).

Sakura Pascarelli was a Vice Chair of the Gordon Conference on Research on High Pressure, Holderness, NH, USA, July 2018, and gave a Plenary Lecture at the 17th International Conference on X-ray Absorption Fine Structure XAFS 2018, Krakow, Poland, July 2018. She has also undertaken preparation work within the International Programme Committee (IPC) for the IUCr meeting in Prague.

Janet Smith is Scientific Director of the GM/CA@APS macromolecular crystallography facility at the Advanced Photon Source, Argonne National Laboratory, USA, and is on the Science Advisory Committees of the Advanced Light Source, Lawrence Berkeley National Laboratory, USA, and the National Synchrotron Light Source II, Brookhaven National Laboratory, USA. She is on the Editorial Board of *IUCrJ* and has given invited talks on Future Perspectives: Micro/Nano Beams, Serial Crystallography and Impact on Structural Biology at the CCP4 Study Weekend at the University of Nottingham, UK, 12 January 2018 and on Biology-Focused Macromolecular Crystallography: PETRA IV Possibilities at the Workshop on Biology at PETRA IV, EMBL/DESY, 12–13 February 2018, Hamburg, Germany.

Milan Sanyal delivered invited talks on Diffraction Imaging of Non-f.c.c. Gold in Bipyramid Shaped Microcrystals at the 8th Workshop on X-ray Nano-imaging of Biological and Chemical systems at PETRA-III held in DESY as a Satellite Workshop – Photon Sciences (25–26 January 2018); Ordering of Functional Materials over Water Surface at the India–UK collaboration meeting on neutron scattering held in the Chemistry Department at Oxford University (19 April 2018); and Formation and Ordering of Nanocrystals at a Liquid–Liquid Interface at the 15th International Conference on Surface X-ray and Neutron Scattering (SXNS-15) held at the Pohang Accelerator Laboratory, South Korea (15–19 July 2018). He also organized the Winter School on Synchrotron Techniques in Materials Science, 25–31 October 2018, at the S. N. Bose National Centre for Basics Science, Kolkata, India. Around 20 scientists from India and Germany, including scientists from the INDUS synchrotron, RRCAT, delivered talks on various topics. This school was attended by 90 PhD students coming from all over India, including several students from well known IITs and IISERs. He was also involved in three projects that provide preferred access to Indian scientists to internationally known facilities (The Photon Factory Synchrotron, KEK, Japan, and PETRA-III, DESY, Germany, for synchrotron X-ray experiments and the Rutherford Appleton Laboratory, UK, for neutron experiments) for carrying out diffraction and scattering experiments. These facilities are being used by large number of Indian institutes to carry out advanced materials research.

Maciej Kozak was a member of the Organizing Committee of the 17th International Conference on X-ray Absorption Fine Structure XAFS 2018, Krakow, Poland, July 2018, and now is a managing Guest Editor of the XAFS 2018 Special Issue on Radiation Physics and Chemistry (Elsevier). In 2018 he delivered invited talks at BIOCongress 2018 and the Second Polish–Korean Conference on Protein Folding: Theoretical and Experimental Approaches. Since 2017 he has been Vice President of the Polish Synchrotron Radiation Society and from December 2018 has been Project Leader at the SOLCaRYS beamline at the National Synchrotron Radiation Centre SOLARIS, Jagiellonian University, Kraków (Poland).

Thomas Tschentscher supported the HERCULES European Training School for use of large-scale facilities by providing an invited talk in Grenoble and organizing practicals for 16 school participants at the European XFEL and DESY during March 2018, and conducted several science, technology and industrial liaison workshops within the framework of the Horizon 2020 project EUCALL, a final highlight of which was the presentation of EUCALL results in Brussels on 6 September 2018. This project will be continued as a network activity. He represented the FEL community in a working group of the LEAPS initiative, which aims to group the European SR and FEL facilities as a defined community, and in the ATTRACT project, which is aimed at new developments for imaging technologies. He also gave invited talks at the Stuttgarter Lasertage (Stuttgart, Germany), Karlsruhe Institute for Technology (Germany), the ECM (Oviedo, Spain), SLAC (USA) and University Rostock (Germany). Furthermore, he served on the programme and scientific

committees of PhotonDiag-2018 (DESY, Germany), PNP-18 (St Malo, France) and RPDHM (DESY, Germany), and co-organized the HP4 international workshop (DLR, Berlin, Germany).

Asia–Oceania Forum for Synchrotron Radiation Research. A one-day workshop Advanced Light Sources in the AOFSRR Countries was held by the Asia Oceania Forum for Synchrotron Radiation Research as a satellite to SRI2018 at the Taipei International Convention Center, 10 June 2018. The programme featured speakers from new and planned storage-ring light sources in the region, and from all three XFEL facilities/projects. There were just under 80 registered participants. The 2nd Asia Oceania Forum for Synchrotron Radiation Research (AOFSRR) School was held 9–15 September 2018, hosted by Pohang Accelerator Laboratory (PAL) at Pohang in South Korea. This school is aimed at science and engineering graduate students, postdoctoral fellows, and early-career researchers from across the Asia–Oceania region who are interested in pursuing a career in synchrotron-radiation-related fields. Forty-eight students from ten countries attended the school, which included both lectures and practical sessions on PLS beamlines.

More than 850 participants from 25 countries came to Taipei for the 13th International Conference on Synchrotron Radiation Instrumentation (SRI 2018, June 10–15 2018).

Pawel Grochulski, Chair

4.23. Commission on XAFS

The members of the Commission on XAFS (CXAFS) and their roles in 2018 were as follows. Chair: Christopher T. Chantler (Australia); Secretaries: Valérie Briois (France) and Sofia Diaz Moreno (UK); liaison with the International Programme Committee: Giuliana Aquilanti (Italy); responsibility for the website: Sofia Diaz Moreno (UK); IXAS liaison: Krystyna Lawniczack-Jablonska (Poland); liaison with *International Tables for Crystallography* and the IUCr journals: Steven M. Heald (USA); IUCr dictionary of XAFS terminology: Narcizo M. Souza Neto (Brazil); coordinator for new editions of the Q2XAFS Workshop: Krystyna Lawniczack-Jablonska (Poland); coordinator for IUCr Congress Workshop and liaison to *International Tables for Crystallography*: Carlo Lamberti (Italy); coordinator of funding support for Congress and Workshop: Dibyendu Bhattacharyya (India); working group on databases and coordinator of summary from Japan XAFS society: Yasushiro Inada (Japan); consultants: Federico Boscherini (Italy), Pieter Glatzel (France), Richard Strange (UK), Hiroyuki Oyanagi (Japan) and Farideh Jalilehvand (Canada).

The activities of CXAFS in 2018 concentrated on active participation in the international XAFS conference and preparation for the 25th IUCr Congress in Prague (Czech Republic).

XAFS 2018. Two events were co-organized for this conference, which was held in Krakow (Poland), 22–27 July 2018. A one-day workshop on Advances in XAFS Experimental Techniques with a special emphasis on the advent of 4th generation light sources was co-organized by Hiroyuki Oyanagi (IXAS) and Steve Heald (CXAFS). A CXAFS/IXAS joint session, chaired by Chris Chantler, in the regular programme of the conference was also organized with four lectures, given by Farideh Jalilehvand, Peter Krüger, Hidekazu Ikeno and Ryan Trevorah, covering reactivity of antitumoral Rh complexes, new developments within the ligand field multiplet theory for *L*-edge absorption, RIXS and RIXS-XMCD spectra calculations and a robust self-absorption correction method for fluorescence data.

During the conference, a meeting of CXAFS was held with the participation of nine of the ten members, three of the five consultants and two invited visitors (Matt Newville, future Chair of the Q2XAFS Workshop, and Wojtek Kwiatek, Chair of XAFS 2018). The main topic discussed during this meeting was the preparations for the next IUCr Congress, which will be held in Prague, 22–30 August 2020. The detailed programme of the microsymposia and keynote nominations proposed by CXAFS will be submitted to the International Programme Committee (IPC) by 15 March 2019 and presented by our IPC member Giuliana Aquilanti during the IPC meeting connected with the workshop Current Trends and Future of Crystallography that will be held in May 2019 in Prague. We also discussed the workshop and the next Q2XAFS meetings. Chris also encouraged the IXAS to remember fallen colleagues including Ed Stern, Mark Ridgeway and others in celebration of their science, areas of research and achievements. Chris attended the IXAS Executive meeting as the IUCr Observer, a relation which we have been encouraging for mutual assistance.

International Tables for Crystallography Volume I. X-ray absorption spectroscopy and related techniques. Federico Boscherini, Bruce Bunker and Chris Chantler have been working very hard and energetically on this new volume of *International Tables*. Most of the chapters have been received and reviewed. Authors who have submitted chapters at the very beginning of the process might be asked to update their reference lists prior to publication. Good and authoritative chapters are still being received, and every one is being fully refereed, and usually revised.

Conference support and proposals. The Commission has priorities for the meetings, workshops *etc.* that it would like to receive funding support from the IUCr. These were the workshop that will be held at the forthcoming IUCr Congress, and the workshop and Q2XAFS satellite meeting which is proposed to be held in Chicago. The next International XAS Conference which will be held in 2021 in Australia.

IXAFS Newsletter. IXAS encourages CXAFS to contribute to the IXAFS newsletter with anything about meetings, joint activities, Commission activities, Q2XAFS or other important and interesting topics.

IUCr journals. The IUCr has sent a new directive in which each Commission should publish in the IUCr journals at least once every three years. CXAFS has published a Special Issue with ten articles related to the Diamond Q2XAFS satellite meeting of the 24th IUCr Congress in Hyderabad (India) in the *Journal of Synchrotron Radiation* (Volume 25, Part 4).

Additionally, Sofia Diaz-Moreno and Richard Strange prepared a summary of the Q2XAFS meeting and outcomes.

C. T. Chantler, Chair, **V. 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 2018 the Executive Committee approved sponsorship of various schools and meetings, mostly with financial support. Those held in 2018 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 2019 and 2020, but approved in 2018, are listed below.

5th Conference of the Bangladesh Crystallographic Association, Dhaka, Bangladesh (25–26 January 2019)

2nd PAN African Meeting on Crystallography, Accra, Ghana (28 January – 2 February 2019)

5th School on Crystal Structure Determination from Diffraction Data. Application on Powder Samples, Hammamet, Tunisia (22–24 March 2019)

XVII Intensive Teaching School in X-ray Structure Analysis, Durham, UK (6–14 April 2019)

RapiData 2019, Stanford, USA (5–10 May 2019)

7th International School on Biological Crystallization, Granada, Spain (26–31 May 2019)

To.Sc.Lake 3.0 Total Scattering for Nanotechnology on the Como Lake, Como, Italy (27–31 May 2019)

Erice – 2019 Magnetic Crystallography Course of the International School of Crystallography, Erice, Italy (31 May – 9 June 2019)

14th International Symposium on Macrocyclic and Supramolecular Chemistry (ISMSC 2019), Lecce, Italy (2–6 June 2019)

Summer School on Mathematical Crystallography, Nancy, France (3–7 June 2019)

24th International Conference on the Chemistry of the Organic Solid State (ICCOSS XXIV), New York City, New York, USA (16–21 June 2019)

Zurich School of Crystallography 2019 – Bring Your Own Crystals (8th School), Zurich, Switzerland (16–27 June 2019)

International School on Advanced Porous Materials, Como, Italy (17–21 June 2019)

2019 Gordon Research Seminar – Crystal Growth and Assembly, Biddeford, Maine, USA (22–23 June 2019)

IXS2019 The 11th International Conference on Inelastic X-ray Scattering, Stony Brook, New York, USA (23–28 June 2019)

Shanghai International School on Crystallographic Groups and Representations, and their Applications in Magnetic Structure Descriptions and Topological Insulator Studies, Shanghai, China (30 June – 7 July 2019)

XIX International Meeting on Crystal Chemistry, X-ray Diffraction and Spectroscopy of Minerals, Apatity, Russia (2–5 July 2019)

Annual Meeting of the American Crystallographic Association (ACA 2019), Covington, Kentucky, USA (20–24 July 2019)

The 17th International Summer School on Crystal Growth, Granby, Colorado, USA (21–26 July 2019)

Satellite Meeting of the 32nd European Crystallographic Meeting – High Pressure Crystallography Workshop, Vienna, Austria (13–17 August 2019)

Satellite Meeting of the 32nd European Crystallographic Meeting – Mathematical and Theoretical Crystallographic Workshop, Vienna, Austria (16–18 August 2019)

32nd European Crystallographic Meeting (ECM 32 Vienna), Vienna, Austria (18–23 August 2019)

Fourth International School on Aperiodic Crystals, Cabourg, France (9–13 September 2019)

Biophysical Approaches to Macromolecules and Cells: Integrated Tools for Life Sciences and Medicine, Nairobi, Kenya (moved to Arusha, Tanzania) (9–20 September 2019)

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.

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 ICSU'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.

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. The committee consists of five voting members and a broad collection of advisers and observers. The current voting members are James Hester (Chair), Brian McMahon, Herbert Bernstein, John Westbrook and John Bollinger.

New dictionaries. A dictionary defining datanames for topological descriptions (TopoCIF) was submitted by Vladislav Blatov and Davide Proserpio and approved by COMCIFS in June after consultation with the topological community. A symmetry-mode dictionary is currently being discussed by a specialist group.

Legacy dictionaries. Almost all legacy IUCr dictionaries have been rewritten to use an updated dictionary definition language (DDLm). The modulated structure dictionary and electron density dictionary have not yet moved to DDLm.

International Tables for Crystallography Volume G. COMCIFS members are closely involved with the preparation of the second edition of *International Tables* Volume G (*Definition and exchange of crystallographic data*). This work has led to clarification of some of the foundational standards. Further information is available in the report on *International Tables* in Section 4.2.

Macromolecular standards. The wwPDB is responsible for a large and rapidly expanding collection of CIF definitions that encompass concepts and techniques used in the macromolecular community. The wwPDB continues to develop powerful tools for easy deposition of, and access to, data in mmCIF/PDBx form, and continues to encourage an active community of users.

Interactions with other standards groups. Herbert Bernstein represents COMCIFS on the NeXus International Advisory Committee (NIAC). In 2018 NIAC approved continuation of work on tools and standards that would allow wwPDB datanames to be stored and retrieved from NeXus files. COMCIFS is also closely involved with the IUCr Committee on Data (CommDat).

Looking forward. As flagged last year, 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 did not improve in 2018.

J. Hester, Chair

7. Committee on Data

For 2018 the Committee (CommDat) had the following matters to report.

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

The CommDat Chair was approved by CommDat to be its representative on the International Programme Committee for the Prague IUCr Congress in a procedure led by committee member Dr Loes Kroon-Batenburg.

The top recommendation from the final report of the IUCr Diffraction Data Deposition Working Group (DDDWG) (that raw diffraction data should be published with a doi cited in any future submitted article for publication) has led to the following initiatives. Firstly, Amy Sarjeant and Simon Coles, who are members of CommDat, on behalf of the Commission on Structural Chemistry, announced a questionnaire in the *IUCr Newsletter* in December 2018 to survey views in the chemical crystallography community about the utility of preserving its diffraction images. The deadline for answers to the questionnaire, which is available at https://docs.google.com/forms/d/e/1FAIpQLSdD-jIhcVIai1YcL8R-g35SMCtlTqcZl3aOANAOcfrQmOrTUw/viewform, is March 2019. An article by Miguel Aranda on raw powder diffraction data and its archiving mechanisms has been published in the *Journal of Applied Crystallography* (see http://forums.iucr.org/viewtopic.php?f=39&t=407).

CommDat is seeking to ensure that raw diffraction data across all the IUCr's Commissions should be 'FAIR' *i.e.* findable, accessible, interoperable and reusable. A checkcif service for raw data to automate the reusability of raw

diffraction data is under development. Collaboration with COMCIFS is progressing towards this goal.

The Chair, as IUCr Representative to CODATA, attended International Data Week in November 2018 held in Gaborone, Botswana. His report on this and on the CODATA General Assembly can be found at http://forums.iucr.org/viewtopic.php?f=39&t=409.

CommDat member Brian McMahon presented a talk at AsCA 2018 entitled The Element of Trust: Validating and Valuing Crystallographic Data within a microsymposium entitled Database Developments, Validation and Data Mining organized by CommDat member Amy Sarjeant along with Genji Kurisu. The weblink to the slides and abstracts is available at http://forums.iucr.org/viewtopic.php?f=39&t=411. A summary of this session written by Amy Sarjeant will appear in the *IUCr Newsletter*.

John R. Helliwell, Chair

8. *IUCr Newsletter*

Having transferred the operations of the *IUCr Newsletter* to Chester, Mike Glazer was appointed General Editor to oversee the organization of a completely online newsletter to replace the hitherto hard copies. Moving to an online format opened up many new possibilities, especially regarding distribution and in the use of attractive images, both static and dynamic. Work on this had already begun at Chester by Brian McMahon together with Andrea Sharpe, Michele Zema and Peter Strickland. After a meeting at Chester, I suggested a number of small changes which were then incorporated. One of the first tasks then was to set up an international Editorial Board. These are now Ted Baker (Australia), Delia Haynes (South Africa), Abel Moreno (Mexico), Amy Serjeant (USA and Canada) and Serena C. Tarantino (Italy).

In the second half of 2018 two online issues of Volume 26 were published as the first of the new series of the online newsletters. Since starting as Editor, I have been gradually remoulding the way items are reported to include dynamic images and also articles that I hope would be of general interest. In that vein, Issue 1 had more that 30 separate items, including the usual meetings reports and journal news. The spread of articles was truly international. I also wrote an article on the use of Beevers–Lipson strips for which I have received a number of interesting e-mails. There were three advertisements from commercial companies. This issue included an item from the President Sven Lidin.

In Issue 2 there were around 40 separate items, including four advertisements. We began to see the use of moving images as a means to attract attention, including one of the commercial advertisements using a rotating crystal structure. In addition to my editorial I also supplied an article on certain aspects of the structure and use of quartz crystals. This too attracted some attention and has resulted in an extensive e-mail discussion with someone working on quartz. There was also a thought-provoking item to do with an article written by Juan Manuel Garcia-Ruiz suggesting that crystals were the first objects to be valued by primitive hominids. Another unusual article explained some latest ideas about prime numbers and their relationship to crystallography. Three interesting outreach articles appeared, one on a crystal-growth competition in Wisconsin, one on a science festival in Genoa and one on an experiment to involve school children in solving a structure using synchrotron radiation at the Diamond Light Source. An article also appeared on crystallography in Africa including an interview with Thierry d'Almeida from the Commissariat à l'Energie Atomique et aux Energies Alternatives in France, to discuss developments in Benin and neighbouring countries.

Each issue was sent electronically to more than 13 000 crystallographers and structural scientists worldwide. So far, feedback has been entirely positive.

I wish to thank Andrea Sharpe (Managing Editor), Peter Strickland, Brian McMahon, Michele Zema and the Executive Secretary, Alex Ashcroft, for their enthusiasm and help in this new venture.

Mike Glazer, General Editor

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

A visit was made to OUP in April 2018 by the IUCr Executive Secretary, the IUCr Executive Managing Editor and myself as Chair of the Book Series Committee. The meeting there discussed current book titles under contract with authors within the book series. Following the meeting, OUP confirmed that an increase of revenues to IUCr from sales of the book series would be made.

At the BCA 2018 Conference in March 2018 a poster about the book series was presented by myself as Chair. This helped facilitate community consultation, especially towards new book topics and our next book authors. This consultation was extended further via an oral presentation by myself as Chair at the ECM31 in Oviedo, Spain, in the Education General Interest Group microsymposium.

During the year, IUCr staff in Chester have very nicely restyled the books section of the IUCr website (https://www.iucr.org/publications/iucr-oup).

The Book Series Committee members individually provided two book-proposal assessments, which I brought together as reports. These two reports were first provided to the IUCr Executive Committee, which endorsed them, and then they were submitted to OUP.

John R. Helliwell, Chair

10. Gender Equity and Diversity Committee

The establishment of this committee (GEDC) was approved in 2018 at the IUCr Executive Committee meeting in Oviedo. The terms of reference for the GEDC were approved by the IUCr Executive Committee on 20 November 2018.

The Terms of Reference are as follows.

Scope. The Gender Equity and Diversity Committee (GEDC) provides advice to the IUCr Executive Committee regarding equity in crystallography.

Objectives:

Provide advice to the IUCr Executive Committee on new policy initiatives (*e.g.* speaker policy, code of conduct, demographics) that will support gender equity development and setting of gender equity goals, strategies and targets linked to IUCr strategic, operational and planning processes.

Evaluate progress towards achieving gender equity and diversity within our community and developing strategies and targets and evidencing best practice.

Provide feedback to the IUCr Executive Committee on possible equity implications of proposed IUCr policies and plans referred to the GEDC.

Ensure that IUCr-sponsored events are welcoming and accessible to all those who wish to attend. Ensure there is a clear code of conduct communicated to all that attend such events. Develop a protocol for addressing breaches and work with the IUCr to implement this appropriately.

Advocate for gender equity and diversity within the crystallography community and beyond.

Identify any impediments to progressing gender equity and diversity and work with the IUCr on strategies to overcome them.

Where appropriate, consult with and advise other IUCr committees and officers on gender equity and diversity matters.

Provide a forum for discussion of gender equity and diversity issues within the IUCr, and contribute to the communication and reinforcement of shared values around gender equity and diversity to support a culture of inclusiveness within the IUCr.

Membership. Membership will be no more than ten and will include two IUCr Executive Committee members. Members should reflect the diversity of the crystallography community including age, gender and geography.

Committee members will demonstrate:

Knowledge and understanding of the needs and issues relevant to gender equity and diversity.

The capacity to contribute to the strategic development of gender equity and diversity initiatives for the IUCr.

Terms of Appointment. Appointments will be three years initially with the possibility of a second term. The Committee will conduct its business electronically, or where possible in person at crystallography meetings.

J. L. Martin, Chair

11. Regional Associates and Scientific Associates

11.1. American Crystallographic Association (ACA)

The American Crystallographic Association, Inc. (ACA) is a nonprofit, scientific organization of under 1000 registered members. The ACA was founded in 1949 through a merger of the American Society for X-Ray and Electron Diffraction (ASXRED) and the Crystallographic Society of America (CSA). 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 visit the recently updated (October 2018), very informative and easy to navigate ACA webpage at http://www.amercrystalassn.org.

The 2018 ACA Council consisted of Lisa Keefe (President), Joseph Ferrara (Vice President), Amy Sarjeant (Past President), Sue Byram (Treasurer), Diana Tomchick (Secretary) and George Lountos as the Young Scientists Special Interest Group (YSSIG) representative to the Council (*ex officio*). Tomislav Friscic served as the Canadian National Committee for Crystallography (CNCC) representative and Hanna Dabkowska as the IUCr representative (*ex officio*). Bill Duax is the Chief Executive Officer (CEO), S. N. Rao the Chief Financial Officer (CFO), Kristin Stevens the Director of Administrative Services and Kristina Vitale the Membership Secretary. In 2018 the Council met three times in person and – additionally – once-a-month teleconferences have recently been introduced.

The 2018 (68th) Annual Meeting was held 20–24 July in Toronto, Canada. Gerald Audette and Tiffany Kinnibrugh co-chaired this meeting. The Special Plenary Lecture was delivered by John Polanyi, 1986 Nobel Laureate in Chemistry. There were 663 attendees (29% were female). Meeting statistics are available at https://www.amercrystalassn.org/past-meetings. The 2018 ACA Award Winners are Simon Billinge (Warren Award), Frank Hawthorne (Buerger Award) and Jason McLellan (M. C. Etter Early Career Award). The poster session was named after Judy Flippen-Anderson, the 1991 ACA President and activist who passed away on 21 March 2018. Memories about Judy were collected in articles in *ACA RefleXions* (Spring 2018 issue). The Toronto meeting was supported by some 25 sponsors, including the IUCr (travel award for young scientists). The 2017 ACA Fellows – a title that recognizes a high level of excellence in scientific research, teaching, and professional duties, as well as service, leadership, and personal engagement in the ACA – were Andrew Allen, James Britten, Majed Chergui, Wladek Minor, Thomas Proffen, Janet Smith and Robert Von Dreele.

More details about the ACA activities, reports and projects can be found in the excellent ACA publication *ACA RefleXions* at https://www.amercrystalassn.org/reflexions-archive (Editors Paul Swepston and Edwin D. Stevens).

The 2019 (69th) Annual ACA Meeting will be held in Covington, KY, 20–24 July 2019. Programme Chairs are Stephan Ginell and Vivien Yee, and the Poster Chairs are Louise Dawe and David Rose.

The 2020 (70th) Annual ACA Meeting will be held in San Diego, California, 2–6 August 2020. The ACA Council works very hard to work out the balanced budget for these meetings, as the ACA's main income is from the annual meetings and from the members' dues.

Structural Dynamics, an ACA/AIP journal, achieved an impact factor of 3.969 in 2018 (https://www.amercrystalassn.org/structural-dynamics).

The results of ACA 2018 election are as follows: Brian Toby was elected as President, Ilia Guzei will assume the duties of the Treasurer, Diana Tomchick will continue as the Council Secretary, David Rose is a new Canadian Representative, Krystle McLaughlin will chair the Communications Committee, Peter Wood the Education Committee and Paul Sanchagrin the Data, Standards & Computing Committee.

The ACA History Portal, which is excellently run by Virginia Pett, was financially supported, so was the African Crystallography initiative.

The ACA also supports many statements and actions regarding the situation of science and social activities in USA, acting together with the APS.

The 2019 ACA Summer Course for Chemical Crystallography, info@acasummercourse.net, will be held at Northwestern University, 23–30 June.

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

H. A. Dabkowska, IUCr Representative

11.2. 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.

AsCA Executive officers. The office bearers for the term 2016–2019 were elected in Hanoi and are Jennifer Martin (President, Australia), Xiao-Dong Su (Vice President, China), Edward R. T. Tiekink (Secretary/Treasurer, Malaysia) and Pinak Chakrabarti (Immediate Past President, India). Elections for President, Vice President and Secretary/Treasurer will be held during the next Council meeting (December 2019) in Singapore.

AsCA scientific meeting 2018. The 15th Conference of AsCA (AsCA 2018) was held at The University of Auckland, Auckland, New Zealand (2–5 December 2018). Professors Chris Squire and Kurt Krause were Co-chairs of the Local Organizing Committee and Professor Ted Baker and Sally Brooker were Co-chairs of the International Programme Committee. The conference attracted a total of 477 registrants from 28 countries: Australia 106, Austria 1, Belgium 1, Canada 3, China 47, Croatia 1, Czech Republic 1, France 3, Germany 7, Hong Kong 8, Hungary 2, India 19, Japan 86, Malaysia 4, New Zealand 86, Pakistan 1, Poland 1, Singapore 7, South Korea 34, Spain 1, Sri Lanka 1, Sweden 2, Taiwan 29, Thailand 1, UK 18, UAE 1, USA 20, Vietnam 1. The female-to-male ratio for the attendees was 31:69 (51 undisclosed). Other statistics were: Organizing Committee: 3 female, 7 male; International Programme Committee: 6 female, 8 male; plenary speakers [David Eisenberg (USA), Susan Lea (UK), Cameron Kepert (Australia) and Amy Rosenzweig (USA)] and keynote lecturers [Yanli Wang (China), Hiroshi Kitagawa (Japan), Richard Neutze (Sweden), Catherine Day (New Zealand), Deanna D'Alessandro (Australia) and Ayana Sato-Tomita (Japan)]: 6 female, 4 male; speakers in microsymposia (total 107): 33 female, 74 male; microsymposia Chairs (total 38): 18 female, 20 male; Chairs of plenary and keynote lectures: 4 female, 6 male.

Planning for future meetings. At the AsCA Council meeting held in Auckland (5 December 2018), the 16th AsCA Conference (AsCA 2019) was confirmed to be held in Singapore, and Professor JJ Vittal would be the Local Chair. Professor Edward Tiekink is the Programme Chair.

At the Council meeting a progress report was received from Irene Ling, the Malaysian representative of the Malaysian Crystallographic Association, who are hosting the 17th AsCA Conference in December 2021. A Local Organizing Committee is being formed and a Conference Organizer will be appointed soon (noting that there will be no AsCA meeting in 2020 owing to the IUCr Congress that year). Proposals for the 2022 conference will be presented to the AsCA Council at the December 2019 meeting in Singapore.

AsCA Prize for exemplary contributions to AsCA. 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.

J. L. Martin, IUCr Representative

11.3. European Crystallographic Association (ECA)

The ECA is a scientific association among national members and individual members and corporate affiliates. It has 13 SIGs (Special Interest Groups) and 3 GIGs (General Interest Groups). The ECA main event – the ECM (European Crystallographic Meeting) – was held in Oviedo, Spain, 22–27 August, with a few satellite meetings preceding the conference. The conference Chair was Santiago Garcia Granda.

The main ECA prize, the Max Perutz Prize, was awarded to Sine Larsen (a former IUCr president) in recognition of her multi-faceted contributions to crystallography, including crystal structure analyses of organic molecules and proteins, charge-density studies, and the development of synchrotron radiation facilities. The ninth Erwin Felix Lewy Bertaut Prize awarded to young scientists was given to Matthias Zschornak from the Technical University Bergakademie Freiberg in recognition of his outstanding contributions to the development of resonant X-ray diffraction, his structural studies of perovskites and his extensive electronic calculations providing a thorough physical understanding of the properties of important materials.

Most of the SIGs had meetings in Oviedo including the first meeting of new SIG, SIG14 (entitled D3 – Dynamics, Disorder, Diffuse scattering). Overall, 1001 people attended the ECM, including 222 ECA individual members, 326 other regular participants and 175 students.

Several years ago the ECA introduced focus areas for the ECMs. At Oviedo there were 179 abstracts in Biological and Macromolecular Crystallography, 103 in Materials and Minerals, 117 in Physics and Fundamental Crystallography, 142 in Chemical Crystallography, 64 in Experimental and Computational Techniques and 17 in the General Interest sessions.

Two sessions of the ECA Council Meeting also took place, with the election of the new Executive Committee: Udo Heinemann (President), Alessia Bacchi (Immediate Past President), Marijana Đaković (Vice President), Arie van der Lee (Secretary), Jacob Overgaard (Treasurer), Jan Dohnálek, Della Haynes and Carl Henrik Gorbitz (Officers) and Consiglia Tedesco (Education Coordinator). Udo Heinemann, Alessia Bacchi, Marijana Đaković and Carl Henrik Gorbitz had served on the previous Executive Committee.

The Executive Committee's regular Winter Meeting was held in February 2018 in Vienna, Austria, because the 32nd ECM will be held there (18–23 August 2019, Chairs: Klaudia Hradil, Kristina Djinovic Carugo and Ronald Miletich). ECM-33 will be in Versailles in France, organized together with synchrotron Soleil (2021, Chair: Sylvain Ravy), and ECM-34 will be held in Padova, Italy, in 2022.

The ECA schools – European Schools of Crystallography (ECS) – are now a regular feature and are organized according to detailed ECA guidelines. The fifth European Crystallographic School (ECS5) was held under the auspices of the European Crystallography Association (ECA), the International Union of Crystallography (IUCr) and the South African Crystallographic Society (SACrS) in Stellenbosch, 8–14 July 2018. The school was attended by 86 participants, including 21 lecturers and tutors, from 13 different countries, primarily from Africa. The next school should be in Budapest in 2020.

An African Crystallography Steering Committee has been established and has defined six African regions. There is a plan to establish an African Crystallographic Association (AFCA) after 2020.

Schools and conferences were supported in 2018 (two in Croatia and three in Italy), but because of very limited finances the contributions to these were not very high.

The ECA members database has been cleaned to comply with GDPR. All records of members inactive for more than three years have been deleted. All personal data in the remaining records has also been deleted. Currently, the members database only contains information on user name, password, e-mail address and country.

The ECA is a member of the ISE (Initiative for Science in Europe, https://initiative-se.eu/), which has moved to Strasbourg and has 17 member organizations. The ISE appears to have solved many of its organizational problems and is ready to make its voice heard in the European science arena again. It was therefore suggested that the ECA maintain its ISE membership. The ISE meetings are usually attended by the ECA Vice President.

The ECA has two internet domains, http://crystallography.eu and https://ecanews.org, and a presence on the main social networks [@social_eca (Twitter) and ecanews (Facebook)].

Discussion continues on how to strengthen the position of the ECA as really European association; there are some legal issues (at present it is registered in the Netherlands according to Dutch law) and the possibility of professional management. There is also an option to include the organization of the ECM there, for example to have a core professional conference organizer. However, this option did not get support at the last council meeting in Oviedo.

R. Kuzel, IUCr Representative

11.4. Latin American Crystallographic Association (LACA)

Since its foundation in 2013 at the meeting of the Argentinian Crystallographic Association in Cordoba, Argentina, and its incorporation as a Regional Associate of the IUCr in 2014, LACA has consolidated as a vibrant regional organization. Many meetings and schools take place every year along with outreach activities to encourage children and teenagers to carry out studies in different disciplines in science.

The 1st LACA School 'Small Molecule Crystallography' took place 19–25 February 2018 at Facultad de Química, Universidad de la República, Montevideo, Uruguay. Organized by Natalia Alvarez, Gumán Peinado and Leopoldo Suescun, it offered approximately 40 participants one very intense week of lectures and practical sessions. The invited instructors were Florencia Di Salvo (Argentina), Hamilton Napolitano (Brazil), Javier Ellena (Brazil), Vojtech Jancik (Mexico), Anthony Linden (Switzerland), Silvina Pagola (USA) and Bruce Noll (USA). Later in the year, the Third LACA Meeting and First Meeting of the Chilean Crystallographic Association took place in Valparaíso, Chile, 10–12 October 2018, at Pontificia Universidad Católica de Valparaíso (PUCV). Prior to the meeting, an *Olex2* Workshop (8–9 October) was conducted at PUCV by O. Dolomanov and H. Puschmann. J. M. Delgado was the instructor of a Powder Diffraction Workshop on 9 October at Universidad Federico Santa María (UFSM). There was a good representation from Latin American countries at this meeting. A new Executive Committee was elected at the General Assembly, composed of José Reyes Gasga (México, President), José Miguel Delgado (Venezuela, Vice President), José Roberto Vega (Costa Rica, General Secretary), Mauricio Fuentealba (Chile), Natalia Álvarez (Uruguay) and Ingrid Benítez (Guatemala) Adjunct Secretaries, Iris Torriani (Brazil, Treasurer) and Diego Lamas (Argentina, Past President). A Deliberative Council was also established, formed by Sebastián Klinke (Argentina), Eduardo Granado (Brazil), Andrea M. Araya (Costa Rica), Ingrid Benítez (Guatemala), Abel Moreno Cárcamo (México), Mauricio Rodríguez (Uruguay) and Alexander Briceño (Venezuela). It is worth noting that a representative from the newly formed Guatemalan Crystallographic Association was included in the LACA Council. During the General Assembly of LACA, Professor José Antonio Henao (UIS, Colombia) presented a proposal to host the IV LACA

and the II LACA School in Bucaramanga, Colombia, in October 2019. The II LACA School will be 1–6 October and the IV LACA Meeting 7–10 October. The proposal was approved unanimously. The First Meeting of Colombian Crystallographers will also take place as part of the IV LACA Meeting, as efforts are being made to reorganize the Colombian Crystallographic Association, which was founded some 20 years ago. Professor Iris Torriani presented an update of the legalization of LACA's Statutes and By-Laws. Future LACA Schools were also planned and the Assembly agreed to support the III LACA School at UNAM, Mexico, in the first trimester of 2020, organized by V. Jancik, and the IV LACA School in December 2020, organized by C. Aguilar (Chile) and J. M. Delgado (Venezuela) in Valparaíso, Chile. It was also agreed to have future LACA Schools as satellite events of the LACA meeting.

Several IUCr commissions were involved in events in Latin America. The CrysAC Commission organized the 3rd CrysAC Workshop on Recent Advances in the Investigation of Ancient Mortars and Binders, 20 May 2018, before the 42nd International Symposium on Archaeometry (ISA 2018) in Mérida, Yucatán, Mexico, 20–26 May 2018. It also sponsored the CHEMFORS Workshop on 8–9 November 2018 as a satellite event of the XVI Seminar on Analysis by X-ray Techniques (SARX 2018) in Pucón, Chile, 4–7 November 2018. At the CHEMFORS Workshop, experts on X-ray diffraction and X-ray fluorescence presented advances on the use of these techniques to characterize materials related to cultural heritage and forensic investigations. It should be noted that SARX has been a very important interdisciplinary meeting in the region and over the years has incorporated more crystallography related topics. The next SARX meeting will take place in Puebla, Mexico, in November 2020 and will be a joint meeting with the Mexican Crystallographic Society. The Commission on Mathematical and Theoretical Crystallography organized an International School on Fundamental Crystallography, 26 November – 1 December 2018, in Bogotá, Colombia, with Mario Macías (U. de Los Andes, Colombia) leading the local organization. Before this, the IFSC/CCP4 Macromolecular Crystallography School 'From Data Processing to Structure Refinement and Beyond' took place in Sao Carlos, SP, Brazil, 14–24 November 2018. The local organizers were João Renato Muniz, Richard Garratt and Glaucius Oliva from Instituto de Física de São Carlos/USP, Brazil. The To.Sca.Lat.-1.0 Summer School 'Total Scattering Analysis for Nanoscience in Latin America', took place in Florianópolis, Brazil, 10–14 December 2018. Carlos Maduro de Campos (FSC-UFSC, Florianópolis, Brazil) led the local organization of this workshop.

Representatives from the IUCr, LACA and LAAAMP were present at the II Latin America and the Caribbean Open Science Forum (CiLAC) in Panamá City, 22–24 October 2018. Michele Zema, IUCr Outreach Officer, masterfully moderated the session Implementing Advanced Light Source Facilities in Latin America and the Caribbean for Sustainable Socio-Economic Development, with the participation of Richard Garratt (U. de São Paulo and LNLS, Brazil), Diego G. Lamas (U. de San Martín, Argentina, LACA President), Carlos Cabrera Martínez (U. de Puerto Rico, LAAAMP Representative), Abel Moreno (UNAM, México, President of Sociedad Mexicana de Cristalografía) and Graciela Díaz de Delgado (ULA, Venezuela, IUCr Executive Committee member). The panelists and moderator agreed that this was a very interesting meeting and that the IUCr should be present at the next CiLAC, which will be in Buenos Aires, Argentina, in 2020. The topics discussed included the almost completed new synchrotron facility in Brazil (Sirius), the project for the Mexican Synchrotron and the impact that scientific organizations such as the IUCr and LACA, through collaborative projects as the LAAAMP initiative, can have on the scientific, economic and (above all) social development in the region.

The work of some of our country members is worth mentioning. The Mexican Crystallographic Society (SMCr) had its IX Congress, jointly with the XII National Congress on Microscopy and the VII Synchrotron Users Meeting, 20–25 October in Oaxaca, Mexico. Sven Lidin (IUCr President) and Michele Zema (IUCr Outreach Officer) were among the invited speakers for the meeting. The SMCr alternates the scope of its annual meetings and in odd years holds the National Diffractometry Meeting. The Argentinian Crystallographic Association (AACr) had its XIV Annual Meeting, X School and VII Workshop 30 October – 9 November at Centro Atómico Constituyentes de la Comisión Nacional de Energía Atómica (San Martín, Buenos Aires). Mike Glazer (Oxford University, UK) participated as an Instructor at the school under the IUCr's Visiting Professor programme. The theme of the School was X-ray Diffraction in the Study of Phase Transitions.

Participation in the IUCr's crystal growth competitions continues to attract elementary-, middle- and high-school students. An Argentinian school obtained the Silver Medal in the 15–18 category and a Chilean school received an honorary mention for the best use of Personal Protective Equipment (PPE) in the 2018 competition. The work carried out by Argentinian and Uruguayan crystallographers, and now by Chilean crystallographers, has been highlighted at the general assemblies of LACA and all member countries are being encouraged to engage in this important outreach activity.

These are some of the events which took place in the LACA region in 2018. In these and other events, the participation of IUCr members from geographical regions outside LACA and the support of the IUCr must be gratefully acknowledged. The increased participation of Latin American crystallographers in IUCr committees is worth highlighting. Abel Moreno-Cárcamo (Mexico), Diego Lamas (Argentina) and Miguel Delgado (Venezuela) are part of the International Programme Committee for the Prague 2020 IUCr Congress. We should also point out that a very important characteristic of the crystallography-related events which take place in Latin America is the strong presence of women as organizers, as instructors and as participants. We hope to continue this trend in the coming years.

G. Diaz de Delgado, IUCr Representative

12. Representatives on Other Bodies

12.1. IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

There was only one activity during 2018 that related to crystallography or IUCr activities. In January 2018 a message was received from D. Brynn Hibbert, the incoming Secretary of the ICTNS. That message included the following:

'A few years ago I became involved in IUPAC's efforts to do something about the GoldBook. These are presently focused on the project Backup, Maintenance, and Redevelopment of the IUPAC Gold Book Website (https://iupac.org/projects/project-details/?project_nr=2016-046-1-024).'

Also from that website (which describes a project with a start date of 1 January 2017 and no end date):

'*Objective*. There are four primary goals of this project: (1) Create a stable, modern version of the current Gold Book website (https://goldbook.iupac.org/); (2) Create a downloadable vocabulary of Gold Book terms; (3) Create a simple website to administer updates to Gold Book terms; (4) Create a simple Application Programming Interface (API) to access the Gold Book terms. These activities are intended to stabilize and prepare the Gold Book website for future development via subsequent projects. In addition, the use of the existing Digital Object Identifiers (DOIs) assigned to the Gold Book terms will be leveraged to provide machine readability of the terms.'

No further message on this subject has been received from Hibbert or anyone else in the ICTNS. The most recent addition to the project website is dated January 2018.

C. P. Brock, IUCr Representative

12.2. International Science Council (ISC)

In October 2017, the International Council for Science (ICSU) and the International Social Science Council (ISSC) met in Taipei and voted to merge the two organizations. They met again in Paris in July of 2018 to create the International Science Council (ISC) as a non-governmental organization with a global membership of 40 International Scientific Unions and Associations and over 140 national and regional scientific organizations, bringing together natural and social scientists to form the largest global science organization of its type. The Council is governed by an international Governing Board, which provides scientific and strategic leadership for the organization, and is advised on key aspects of its work by a number of Advisory Bodies. The Council's global headquarters are located in Paris with regional offices in Africa, Latin America and the Caribbean, and Asia and the Pacific. A General Assembly of all members is convened every three years.

The vision of the ISC is to advance science as a global public good with a mission to act as the global voice for science – to articulate scientific knowledge on major issues of global concern in the public domain. In doing so, the ISC advocates that scientific knowledge, data and expertise must be universally accessible and its benefits universally shared, and that the practice of science must be inclusive and equitable.

As the ISC more clearly defines its goals, it is apparent that there are several activities of the ISC that have major overlap with the activities and interests of the IUCr:

(1) *ISC seeks to stimulate and support international scientific research and scholarship*: The IUCr partnered with IUPAP on a joint proposal supported by UNESCO, TWAS *etc.* and a number of large-scale facilities to obtain a grant for EUR 300 000 over three years. This project is known as LAAAMP (Lightsources for Africa, the Americas, Asia and the Middle East Project). The full title of the project is Utilization of Light Source and Crystallographic Sciences to Facilitate the Enhancement of Knowledge and Improve the Economic and Social Conditions in Targeted Regions of the World. This work is now supported by ISC, which supported the Pan African Conference on Crystallography (PCCr2) that took place at the University of Ghana, Accra, in 2018. This followed a successful conference held in 2016 in Cameroon and was aimed at bringing together African crystallographers, mineralogists, structural scientists and biologists to increase awareness of crystallography and improve the educational opportunities for African researchers and students of all levels. The variety of activities provided opportunities to engage with the scientific community, from expert crystallographers to young researchers and students of all ages, as well as government representatives and policy makers in Ghana. As part of maintaining relations with the ISC National Members, the ISC Regional Office for Africa visited the Ghana Academy of Arts and Sciences, had a fruitful discussion with the Executive Secretary and updated the Academy of the Council's activities at global and regional levels.

(2) *ISC advocates that scientific knowledge, data and expertise must be universally accessible and its benefits universally shared*: The ISC has been part of an active discussion related to the future of publishing as it relates to open access and article processing charges. In September 2018, a group of national research funding organizations, with the support of the European Commission and the European Research Council (ERC), announced the launch of cOAlition S, an initiative to push for full and immediate open access to research publications. It is built around *Plan S* with the aim that all scientific publications on the results of publicly funded research be made freely available by January 2020.

Part of the challenge in implementing *Plan S* is ensuring the trustworthiness of scientific and scholarly communication and the archiving of the results. There is a complicated interaction between the mode of publishing, research evaluation processes and career progression. Scholarly communications are managed by the scholarly community, with their own journal platforms and repositories, and supported by public funds as part of the public infrastructure needed for research. In 2012 during the Annual Meeting of the American Society for Cell Biology, the need to improve the ways scholarly research was evaluated was stated in the Declaration of Research Assessment (DORA). As a publishing Union, the

IUCr has a lot of interest in and expertise related to open access and publication.

(3) *ISC has a strong interest in data*: Web technologies are driving major changes as scientific research is more digital and more international than ever before. The ISC was a co-sponsor of the International Data Week 2018 (IDW 2018) held in Gaborone, Botswana, which brought together data professionals and researchers from all disciplines and all across the globe to explore how best to use the data revolution to improve knowledge and benefit society through data-driven innovations. A priority of ICSU was to seek ways to strengthen the voice of global science in international policy, *e.g.* the accord on Open Data in a Big Data World. The IUCr has been deeply involved in discussions on best practices to achieve the goals of open access in a way which is sustainable and 'FAIR' (Findable/Assessable (Accessible)/Interoperable/Reusable) data.

M. L. Hackert, IUCr Representative

12.3. ICSU Committee on Data for Science and Technology (CODATA)

CODATA is the interdisciplinary Committee on Data for Science and Technology of the International Council for Science (ICSU). Full details of CODATA activities are available from its website at http://www.codata.org.

As IUCr Representative I attended CODATA's biannual conference and general assembly in November 2018 in Gaborone, Botswana (IDW2018). This was part of an 'International Data Week' organized jointly by CODATA, the Research Data Alliance and the ICSU World Data System (http://www.internationaldataweek.org/). The IUCr worked with IUPAC and presented a talk in a session there entitled 'Data interoperability in chemistry, biology, and crystallography: Enabling multidisciplinary solutions to societal challenges'. A detailed report is available at http://forums.iucr.org/viewtopic.php?f=39&t=409.

During IDW2018 there were two plenary sessions. The plenary themes were: Science and Data in Africa; Data and Health; Science Policy and the Future of Science; Pan African Infrastructure; CODATA and WDS (World Data System) Initiatives; Data Science; and Data and Scholarly Communications. Within these, of direct interest to crystallographers was the citing of the CODATA–ICSTI Data Citation Standards and Practices Report, which was very warmly commended in the sessions and in which IUCr had been a participant (Brian McMahon, IUCr, UK). It was testimony that scientific data can be properly cited and that recognition of quality scientific data can thereby be gained.

The merger of the International Council of Scientific Unions and the International Council for the Social Sciences into the International Council for Science made its presence felt in the IDW2018 programme. Of especial note I felt was the keynote lecture by Professor Dr Fosca Gianotti (Italy) in which she stressed the need for data to be both 'FACT and FAIR'. FACT is an acronym from social scientists meaning Fair, Accurate, Confidential and Transparent. The FAIR acronym describes data which meet standards of Findability, Accessibility, Interoperability and Reusability. The public would expect no less, *i.e.* reproducibility, not irreproducibility, of her studies, Professor Dr Fosca Gianotti said. She is the coordinator of SoBigData, the European research infrastructure on Big Data Analytics and Social Mining, an ecosystem of ten cutting-edge European research centres providing an open platform for interdisciplinary data science and data-driven innovation (http://www.sobigdata.eu). There is then a difference between reusability of data, encapsulated within FAIR, and reproducibility of data, encapsulated within FACT.

At the CODATA General Assembly I noted three items.

(1) Crystallography's track record with preservation of its data and metadata along with its publications is frequently referred to as an exemplar for all science disciplines. A CODATA Task Group on Data Standards has been established to effect improvement in all science areas towards the ideal of the IUCr. Deputy Chair Lesley Wyborn, Adjunct Fellow at the National Computational Infrastructure Facility and The Research School of Earth Sciences in Australia, along with the CODATA President, reaffirmed to me as IUCr Representative the strong role that the IUCr has in this effort.

(2) The CODATA VAMAS Nanomaterials Uniform Description project, in which the IUCr was a participant (represented by John R. Helliwell, Reinhard Neder and Daniel Chateignier), was very warmly commended as both being well received by the science communities and testimony that scientific data integration towards a common good is possible. The common good in this case is society's need for guidance on the safety of nanomaterials and, first and foremost, a clear set of descriptors for them.

(3) The CODATA strategic initiative on Integration of Standards with the launch workshop in Paris in 2017 (in which I participated) has led to further workshops and the identification of three important themes for CODATA and the International Council for Science to focus on: (i) infectious diseases, (ii) resilient cities and (iii) disaster risks reduction. See http://www.codata.org/strategic initiatives/commission-on-standards.

J. R. Helliwell, IUCr Representative

12.4. ICSU 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). 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 42nd COSPAR Assembly was held in Pasadena, California, USA, 14–22 July 2018 (3230 participants, 4285 abstracts, 2845 oral presentations, 1049 posters, 370 withdrawn, 20 rejected).

The 43rd COSPAR Assembly will take place in Sydney, Australia, 15–23 August 2020. The 2022 one will be in Athene, Greece.

A big financial loss was reported this time to the Assembly (USD ∼1 000 000) owing to the Istanbul Congress in 2016 being called off. In 2019 the deficit is projected to be about USD 155 000, whereas the income from the membership is about USD 300 000. Capacity Building Workshops (CBWs) cost about USD 90 000.

During the Pasadena Congress there was a session COSPAR Capacity Building Initiatives: A Review of the Last 15 Years and How to Face the Next 10. The IUCr was invited to take part in this discussion as a follow-up to the very successful CBW on Crystallography for Space Science, in April 2016 (http://www.inaoep.mx). There is a strong chance for a similar future collaboration between the IUCr and COSPAR as a similar workshop/school is proposed for Ethiopia in 2020 (to be organized by Juan Manuel Garcia-Ruiz).

The official journal of COSPAR is *Advances in Space Research* (*ASR*, with an impact factor of 1.53 in 2017; http://ees.elsevier.com/asr/). *ASR* includes also COSPAR's information bulletin *Space Research Today*. The newest 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 space flight on the human body, radiation risks and other aspects of life sciences relevant in space research.

In 2018 COSPAR organized three CBWs, covering a large variety of new areas: Space Weather Capacity Building Workshop, 17–28 September 2018, Sao Jose dos Campos, Sao Paulo, Brazil; Coronal and Interplanetary Shocks: Data Analysis from SOHO, Wind, and e-CALLISTO Data, 21 May – 1 June 2018, Mekelle, Ethiopia; and Infrared and Submillimetre Astrophysics Data Analysis, 5–16 March 2018, Quito, Ecuador. The next one will be Broadband Spectral and Timing Studies with AstroSat, Chandra and XMM-Newton, 9–20 March 2019, Mohali, Punjab, India.

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

H. A. Dabkowska, IUCr Representative

12.5. International Organization for Standardization

There were no activities in 2018 related to crystallography.

C. P. Brock, IUCr Representative

12.6. International Organization for Crystal Growth (IOCG)

No formal meeting of the IOCG (http://www.iocg.org/) was planned or organized in 2018.

The IOCG President for 2016–2019 is K. Kakimoto (Japan). Co-Vice-Presidents are T. F. Kuech (USA) and E. Vlieg (The Netherlands), the Secretary is H. A. Dabkowska (Canada), and the Treasurer is J. Derby (USA). The members of the Executive Committee are S. Baldochi (Brazil), S. Krukowski (Poland), A. Voloshin (Russia), J. M. Garcia-Ruiz (Spain), Y. Mori (Japan), K. Roberts (UK), M. Heuken (Germany), J. Y. Wang (China) and J. De Yoreo (USA).

The connection with Commission on Crystal Growth and Characterization of Materials (CCGCM) is evident, as K. Kakimoto, T. F. Kuech, E. Vlieg, J. M. García-Ruiz, and J. Y. Wang are also members of or consultants for the CCGCM.

The 19th International Conference on Crystal Growth and Epitaxy (ICCGE-19) will be held in Keystone, Colorado, USA, 28 July – 2 August 2019. The week before, the 17th International Summer School on Crystal Growth in Granby, Colorado, USA, will be organized (with the support of the IUCr). It will be co-chaired by T. F. Kuech, who is also a member of the CCGCM. Members and consultants of the CCGCM are strongly involved in the work of the Programme and Advisory Committees of this meeting. Detailed information about both the conference and the school are available at https://www.iccge19.org andhttps://www.iccge19.org/isscg-17.

The next General Assembly of the IOCG will take place in Keystone, during ICCGE-19.

At the end of 2010 the European Network of Crystal Growth (ENCG) was formed. Part of the scope of the ENCG is the organization of an European Conference on Crystal Growth (ECCG). After ECCG4 in 2012 and ECCG5 in 2015, in 2018 the Sixth European Conference on Crystal Growth was organized in Varna, Bulgaria, together with the Second European School on Crystal Growth, co-chaired by myself. Many members and consultants of the Commission on Crystal Growth and Characterization of Materials were involved in the organization of these events, which are important to keep the crystal growth tradition alive in Europe.

A. Zappettini, IUCr Representative

12.7. 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

12.8. Worldwide Protein Data Bank (wwPDB)

The Protein Data Bank has been a key resource for macromolecular crystallographers for over 40 years, and its policies and development have been strongly influenced by the crystallographic community. Today the PDB is a partnership of four entities, referred to collectively as the Worldwide PDB (wwPDB). The partners comprise the RCSB-PDB in the USA, the PDBe in Europe, the PDBj in Japan and the BMRB (NMR database) in the USA. These centres collaborate intimately and share the load, maintaining a single archive that is freely accessible to researchers, educators and students throughout the world. In 2019 a fifth core partner will be added; the Electron Microscopy Database (EMDB), reflecting the rapid growth of structural data from this community.

Given the importance of this partnership to the crystallographic community, the wwPDB was formally designated a Scientific Associate of the IUCr in 2015. The IUCr has a representative on the wwPDB Advisory Committee (wwPDB-AC). This committee also has representatives from the NMR and cryoEM communities, as well as regional representation, and is currently chaired by Dr R. Andrew Byrd. The 2018 meeting of the wwPDB-AC was held in Cambridge, UK, 1–2 November. The following is a report on the activities of the wwPDB for 2018.

As of the end of 2018 the archive comprised nearly 150 000 macromolecular structures, of which about 90% were determined by crystallography. Some 11 230 structures were deposited in 2018, at a rate of increase that places increasing demands on the efficiency of annotation, checking and validation. Crucially, the size and complexity of the deposited structures – especially those determined by cryo-electron microscopy (cryoEM) – is also increasing. At the same time, much development work is being undertaken, both by the wwPDB partners and in the relevant communities as the range of techniques giving structural data continues to expand.

Some of the major issues from the past year are as follows:

(i) The number of structures being determined by cryoEM is increasing rapidly as new detectors and more powerful processing protocols are applied. The total number is now 2730, with 853 new structures deposited in the past year. These now outstrip the annual increase in NMR structures. A major effort is under way to develop robust validation tools, informed by the experience from crystallography and adapted for the special properties of EM maps and model building.

(ii) To cope with the increase in size of structures being deposited, both from cryoEM and crystallography, the old 'card image' format has been superseded to allow extremely large structures, such as ribosomes, to be presented in a single file. This necessitates a change in format to mmCIF-based PDBx/mmCIF files. All the major crystallographic software developers now produce output files in this format, and the PDBx/mmCIF dictionary has been extended to better represent serial femtosecond crystallography (SFX) and XFEL data. The change in format will be implemented in 2019 accompanied by announcements in the literature – including in *Acta Crystallographica* Section D.

(iii) On top of the growth in large cryoEM structures, crystal structures are also increasing in size; the number with molecular weight > 500 000 is growing significantly, as is the number with many chains and more than 100 000 atoms. This underscores the complexity of the data depositions and the demands on the wwPDB to adapt and integrate these data smoothly into the archive.

(iv) Validation reports, based on those previously implemented for crystal structures, have now been fully implemented for NMR-determined structures. Progress has been slower with the development of full validation reports for cryoEM structures, largely because of the difficulties of defining map quality, and because of the way the effective resolution can vary widely over different regions of a structure. It is hoped that a full validation suite will be in place by the end of 2019.

(v) Of particular relevance to crystallographers, there has been a delay in implementing more robust validation of bound ligands in crystal structures submitted to the PDB. This resulted from the unfortunate loss of a key staff member. As macromolecular crystallographers are aware, a small subset of published structures contain ligands that are almost certainly incorrect. These are a stain on our field. It is hoped that new ligand validation protocols, developed by a Taskforce led by Professor Randy Read, will be in place by late 2019/early 2020 and that these will help in addressing the problem.

(vi) It is pleasing to note that the lead taken by the IUCr in requiring that a PDB validation report be provided on submission of an article is now being followed by other journals, including those from the *Nature* stable. There is a clear and obvious need for referees to be given information that allows them to assess the quality of structural data.

(vii) A significant increase is taking place in the determination of hybrid structures, for example where parts of a structure have been determined by crystallography while other parts have been defined at lower resolution by small-angle scattering or other complementary techniques. A Hybrid Model Taskforce has been set up to develop protocols for representing such models appropriately in the PDB.

(viii) Work is also in progress to develop a Federated Databases model, in which structures in the PDB are linked to related data held in other databases. Relevant examples include the MX Images databases that are currently being set up – under IUCr auspices – to archive the full sets of unprocessed diffraction images for particular structures, and the SASB database that is being developed, in an initiative led by Professor Jill Trewhella, for archiving biological SAXS data.

(ix) The remediation of carbohydrate structures in the archive is continuing, to ensure that they conform to proper conventions of atom labelling and stereochemistry. Glycan chains on proteins are often poorly ordered and many archival entries violate stereochemical rules. Changes can only be

made with authors' consent, however, so remediation is a slow process.

With 1.8 million downloads per day across the three wwPDB sites, it is obvious that the archive is of enormous importance to the whole life sciences community. The IUCr can be proud of the contribution made by the crystallographic community, and I am happy to be able to report that the relationship between the IUCr and the wwPDB is strong, and is much appreciated by the wwPDB.

E. N. Baker, IUCr Representative

13. Finances

The Report and Financial Statements for 2018 are given as supporting information.

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

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

The virtual fund model that was used in previous years has been discontinued, as it created unnecessary complexity, increased accountancy costs and will make the eventual movement to electronic accounting software more difficult.

The balance sheet shows that the assets of the Union have increased during the year, from USD 3 289 014 to USD 3 314 038. The movement in market value of the investments was a reduction of USD 32 769 in 2018 (gain of USD 120 776 in 2017).

The administrative expenses were USD 426 781 in 2018 as compared with USD 325 311 in 2017, the difference being largely due to the costs associated with maintaining the IUCr website being recorded here rather than as part of the costs associated with the IUCr journals, as was done previously.

The expenses of the Union Representatives on other bodies were USD 11 269. The cost of the Finance Committee meetings held in 2018 was USD 13 569, while the Executive Committee meetings cost USD 42 179. The income from the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was zero as this agreement has now expired. The subscriptions from Adhering Bodies were USD 168 278. Interest on bank accounts and investments was USD 18 208.

The journals for 2018 show a surplus of USD 1 305 733, as compared with a surplus of USD 1 399 328 in 2017.

The cost of the technical-editing office has been divided between the journals and *International Tables* in percentages based on the staff time spent on each publication. The technical-editing costs for the journals were USD 1 344 401 as compared with USD 1 102 117 in 2017, which reflects the appointment of two new junior members of staff to begin to address the age profile in Chester, which is very much skewed towards the higher end.

Books showed a small deficit of USD 80, as compared with a profit of USD 80 131 in 2017. The net sales income was USD 118 336 in 2018 as compared with USD 210 896 in 2017.

The cost for the Union in producing the *IUCr Newsletter* in 2018 was USD 7196 compared to USD 73 865 in 2017, with the reduction being due to moving the operation to Chester.

USD 134 536 was provided for financial support to young scientists, to enable them to attend scientific meetings sponsored by the Union. Visiting Professorships (USD 11 313) and outreach and education costs (USD 111 798) in 2018 also contributed to the IUCr's good works.

An Outreach and Education Fund was established as part of the IYCr2014 legacy. In 2018 donations totalling USD 15 020 were received.