Appendix A. Appendices to the Agenda of the Twenty-Fifth General Assembly

A1. Report of Executive Committee

A1.1 Executive Committee and Finance Committee meetings

The Executive Committee met in Hyderabad, India, in August 2017 before and during the General Assembly, in Oviedo, Spain, in August 2018 at the time of the European Crystallographic Meeting, in Covington, USA, in July 2019 at the time of the American Crystallographic Association Meeting and virtually in August 2020. The Finance Committee met in March 2018, August 2018, March 2019, July 2019, March 2020, August 2020 and March 2021, to prepare its advice and recommendations on finances, establishment and staff matters.

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

appointment of a new Editor-in-Chief of IUCr Journals, editorial policy, pricing policy, review of work of Journals Management Board, development of *IUCrJ* and *IUCrData*, approval of appointments of Main Editors and Commissioning Editors, approval of appointments of Co-editors, Special Issues, open access, facility information pages, and other matters concerning the IUCr journals;

requirement for raw diffraction data images to be deposited in a publicly accessible database for all macromolecular X-ray diffraction structure publications;

review of contract with Wiley;

approval of audited accounts;

review of applications for membership of the IUCr;

the removal of the accounting funds as being a hinderance to transparency;

level of unit contribution, status of membership subscriptions;

investment policy;

revision of guidelines for the Sub-committee on the Union Calendar, sponsorship and financial support for meetings, young scientists' support, revision of internal guidelines, appointments of new members of the Committee;

establishment of a Gender Equity and Diversity Committee, a Code of Conduct and a Gender Equity and Diversity Statement;

review of a proposal to establish a Commission on Diffraction Microstructural Imaging;

progress with Volumes A, A1, B, C, D, E, F, G, H and I of *International Tables* and development of associated software, revision of Brief Teaching Edition of Volume A, appointment of Editors for Volume F;

IUCr Newsletter, *World Database of Crystallographers*;

marketing and promotional activities;

Outreach and Education;

LAAAMP and other activities;

OpenLabs and other activities;

appointment of the Selection Committee for the twelfth Ewald Prize;

appointment of the Selection Committee for the inaugural W.H. and W.L. Bragg Prize;

adoption of the Struchkov Prize by the IUCr;

sponsorship of other prizes;

discussion of arrangements for the Prague Congress;

discussion of the postponement of the Prague Congress;

discussion of the arrangements for the rearranged Prague Congress;

approval of membership of Programme Committee for the Prague Congress, approval of Programme for the Prague Congress;

level of financial support for the Prague Congress;

consideration of progress with arrangements for the Melbourne Congress;

review of nominations and election procedures for Officers of the IUCr and for Chairs and members of Commissions, proposals from National Committees for these positions.

Other items dealt with in this way were:

implementation of the Crystallographic Information File (CIF) for *Acta Crystallographica* and other uses of CIF, work of Committee for the Maintenance of the CIF Standard (COMCIFS), provision of checking services to other publishers, chemical information;

IUCr website;

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

Crystallography in Africa and other developing regions;

Visiting Professorship scheme;

review of activities of Commissions;

review of activities of Regional Associates;

review of reports of IUCr Representatives on other bodies;

merger of the International Council for Science with the International Social Science Council;

relations with other Scientific Unions.

Items concerning the Chester office were:

staffing requirements in the IUCr office in Chester;

retirement of, and appointment of successor for, the Research and Development Officer;

risk analysis;

refurbishment of premises and a new lease;

upgrading office technology in the IUCr office in Chester, provision of internet services.

A1.2 Publications

The subscription prices of *Acta Crystallographica*, the *Journal of Applied Crystallography* and the *Journal of Synchrotron Radiation* were increased in 2017, 2018 and 2019 but not in 2020. Open-access charges for the hybrid journals and for the fully open-access journals *Acta E, IUCrJ* and *IUCrData* were increased each year during the quadrennium.

The total annual number of pages published in 2017, 2018, 2019 and 2020 were:

	2017	*2018*	*2019*	*2020*
Acta Crystallographica Section A	488	713	918	783
Acta Crystallographica Section B	1,199	744	1,227	1,147
Acta Crystallographica Section C	1,159	1,782	1,697	1,107
Acta Crystallographica Section D	1,030	1,244	1,147	1,279
Acta Crystallographica Section E	1,980	1,929	1,952	1,875
Acta Crystallographica Section F	713	824	757	623
Journal of Applied Crystallography	1,852	1,776	1,468	1,631
Journal of Synchrotron Radiation	1,300	1,894	2,096	1,754
IUCrJ	823	879	1,133	1,215
IUCrData	1,021	688	459	405
Total	11,565	12,473	12,854	11,819

All the IUCr journals are available electronically through the **Crystallography Journals Online** service, including all back issues of the journals from 1948, and all the hybrid journals are also available through Wiley Online Library.

From January 2014 all journals have been available online only. *IUCrJ*, *Acta E* and *IUCrData* are fully open access.

The IUCr home page (http://www.iucr.org/) contains information in the following categories: The Union and its Components (including information on Adhering Bodies, Commissions, Regional Associates, Annual Reports, Congress Reports, sponsorship available *etc*.); Journals, *International Tables* and Other Publications; News (including the *IUCr Newsletter*, announcements, meeting reports *etc*.); People (including the photographic archive); Resources (including discussion lists); Education (including the *Online Dictionary of Crystallography*); and Outreach.

Full details on the publication of volumes of *International Tables for Crystallography* are given in the Quadrennial Report of this Commission (Section A8.2**)**.

The *World Database of Crystallographers* continues to undergo development to provide increased functionality and to allow online amendments and additions to be made by individual crystallographers.

The *IUCr Newsletter* is distributed electronically free of charge to 13 500 crystallographers and structural scientists worldwide. A. M. Glazer is the Editor with production done in the IUCr's Editorial Office in Chester. A report on the *IUCr Newsletter* is given in Section A10.

The IUCr/Oxford University Press Book Series continues to be successful. Details are given in Section A14.

A1.3 Sponsorship of meetings

The Sub-committee on the Union Calendar considers and advises the Executive Committee on requests for IUCr sponsorship and financial support of meetings. The Chair of the Sub-committee is G. Diaz de Delgado. A list of IUCr-sponsored meetings is given in Section A17.

Applications for sponsorship are considered if they are submitted at least nine months in advance of the date of the meeting. Applications will be considered by the Committee three times a year at the end of February, June and October. Applications for sponsorship should be timed accordingly. For example, for a meeting to be held in July an application should be submitted by October of the previous year at the latest.

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 except for virtual meetings. For any meetings scheduled to be held between one and two months before or after a Congress, except for virtual meetings, the application for sponsorship requires the approval of the Chair of the Congress Programme Committee. 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 the approval of the Chair of the Regional Associate Organizing Committee. Virtual meetings will be supported at a uniform, lower rate as travel and subsistence are not required. Virtual meetings organizers are expected to make a reasonable decision how the support is used so they mostly benefit young scientists.

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

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.

It is the policy of the IUCr that *strong emphasis should be given to provide a programme that is balanced with respect to gender and nationality.* IUCr support 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.

The IUCr continues to support and uphold ISC's procedures concerning free circulation of scientists. Organizers of any meeting seeking IUCr sponsorship and 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.

Explicit support from the Chairs of 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 or workshops (except for those organized by an IUCr Commission).

Travel support for young scientists is available for all meetings (including schools). This money should not be used for waiver of registration fees, except in the case of virtual meetings. It is recommended that the presentations of young scientists supported by the IUCr should be in English.

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

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

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

A1.4 Visiting Professorship scheme

The IUCr Visiting Professorship scheme aims to support some of the costs of having internationally recognized scientists as lecturers for short courses at workshops or schools organized in developing countries. These schools or workshops may have national or international character. Up to a maximum of three Visiting Professorships (VPs) 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. Support from at least one IUCr Commission is required.

Applications will be considered by the Sub-committee on the Union Calendar three times a year at the end of February, June and October. Applications should be submitted well in advance so that when considered at one of these deadlines, the date of the event should lie at least six months ahead. If the sponsorship of the IUCr is also requested for the school or workshop as a whole, both applications with their separate forms should be submitted together, and in this case the application should be timed according to the conditions for applications for IUCr sponsorship of meetings (*nine months in advance*).

A1.5 Commissions of the IUCr

Each Commission Chair is required to provide a written triennial report to the General Assembly. These reports are given in Section A8.

A1.6 Regional Associates, Scientific Associates, and other bodies

The reports of the Representatives on these bodies are given in Sections A15 and A16.

A1.7 IUCr staff

The present members of staff in the IUCr offices in Chester are: A.T. Ashcroft (Executive Secretary), C. Jones (Administrative Assistant to the Executive Secretary), P.R. Strickland (Executive Managing Editor), B. McMahon (Research and Development Officer), D. Holden (Head of IT), M. Zema (Executive Outreach Officer), A.J. Sharpe (Promotions Officer), C.A. Moore (Editorial Systems Developer), A.S. Berry (Technical Editor and Customer Support Officer), G.F. Holmes, L.E. Jones, S. Conway, A. Weight, N.J. Ashcroft and L. Stephenson (Managing Editors), S. Glynn (Deputy Managing Editor), S. Froggatt, A. Hill, M. Bates and J. Skade (Technical Editors), M.A. Hoyland, P. Gibson and Song Sang Koh (Systems Developers), L. Rathbone (Journals Production Assistant), C. Cook (Administrative Assistant).

A1.8 Acknowledgements

On behalf of the IUCr, the Executive Committee wishes to express its deep gratitude to the Czech and Slovak Crystallographic Association for the invitation to hold the Twenty-Fifth General Assembly and International Congress of Crystallography in Prague.

Finally, the Executive Committee wishes to thank all crystallographers who have assisted in the work of the IUCr in so many ways. This cooperation between crystallographers of different nationalities constitutes a most valuable aspect of the IUCr's activities.

A2. Financial Report

Extracts from the full financial statements for the three years 2017, 2018, 2019 and 2020 are summarized in Tables 1 and 2. All amounts are expressed in United States Dollars. The notations used in this report for the various currencies of the IUCr's activities are CHF = Swiss Franc, GBP = Pound Sterling, USD = US Dollar.

A2.1 General financial development

Table 1 shows a comparison of the balance sheets at the beginning and the end of the quadrennium. On advice from the IUCr's accountants, PM&M, the Finance Committee recommended abolishing the old system of sub-funds for several reasons. Firstly, the UK government was mandating electronic submissions of VAT returns, which would require accounting software to be introduced and it was PM&M's view that no software package would be able to handle the complexity of the IUCr accounts. Secondly, the separate funds made the accounts appear unnecessarily complex. Thirdly, the balances of the individual funds were never used to take decisions on spending – if an account was in deficit, money would be moved from the Journals Fund. Therefore, it was concluded that the individual accounts were no longer serving a useful purpose.
The total assets have increased by USD 1,654,995 from USD 3,042,669 to USD 4,697,664, or 54%, over the quadrennium. This cancels out the losses during the previous triennium. The great majority of the amounts under debtors and creditors have been settled since year-end.

The total holding of investments on 31 December 2020 was USD 2,501,896 at market value, as shown in Table 1. The IUCr bank accounts and short-term deposits are held with the Union Bank of Switzerland and the National Westminster Bank involving the currencies CHF, GBP and USD.

As an association incorporated in Switzerland, the IUCr is exempt from Swiss Federal and Geneva Cantonal Tax, although since 2019 the Swiss Tax Authorities have required the IUCr to provide a declaration of the number of hours that were donated without payment to non-commercial activities of the Union. The value of these hours was required to be similar in value to the income from IUCr Journals over the same period. With most schools and workshops being cancelled in 2020 due to the ongoing pandemic, a declaration of donated hours was not submitted for the 2020 tax year. Under the terms of the United Kingdom/Switzerland Double Taxation Agreement dated 8 December 1977, investment income arising within the UK under present circumstances is not subject to United Kingdom tax. Investment income received from other countries with which Switzerland has a Double Taxation Agreement is also exempt from tax. In October 1985 recognition of tax-exempt status in the USA was received from the Internal Revenue Service, Department of the US Treasury.

A2.2 Income and expenditure

In order to present an overall picture of the state of the Union's affairs, the income and expenditure for the quadrennium is included as Table 2. This shows that the Union was operating with surpluses in each year of the quadrennium. The profits are largely a result of cost-cutting measures, particularly in Chester, more realistic pricing for IUCr journals, the move of the Newsletter to Chester and better budgetary control that has been facilitated by the introduction of accounting software. The pandemic made it impossible for physical meetings to take place, which resulted in a reduction in costs in 2020, and this is also expected to be the case for much of 2021. The academic publishing market faces difficult challenges, with business models in flux and increased financial and regulatory pressure from funders and politicians. Wiley will be taking a larger share of the proceeds from IUCr Journals in the future, so it will be a challenge to remain in profit for the coming biennium.

A2.3 Outreach and Education Fund

This fund was established in 2016 so that initiatives begun during the International Year of Crystallography could be maintained. Donations that are not earmarked for a particular IUCr Prize are allocated to this Fund to support the IUCr's good works.

TABLE 1. BALANCE SHEET, ASSETS. US Dollars

	31 December 2016		*31 December 2020*	
FIXED ASSETS				
Tangible fixed assets		14,458		39,735
Investments at market value		2,594,950		2,501,896
		2,609,408		2,541,631
CURRENT ASSETS				
Stock	77,175		43,590	
Debtors	299,157		554,020	
Cash at bank and in hand	808,590		2,716,577	
	1,184,922		3,314,187	
Creditors: amounts falling due within one year	(751,661)		(1,158,154)	
NET CURRENT ASSETS		433,261		2,156,033
TOTAL ASSETS		3,042,669		4,697,664

TABLE 2. INCOME AND EXPENDITURE. US Dollars

	2017		2018		2019		2020	
I. INCOME								
Membership income		168,604		168,278		177,767		186,089
Journals, back numbers and single issues	2,892,487		2,637,924		2,573,585		2,442,914	
Open access income	253,431		371,197		580,318		857,553	
Books	210,896		118,336		118,153		112,360	
		3,356,814		3,127,457		3,272,056		3,412,827
Income from investments	22,313		17,104		28,408		31,349	
Bank interest	50		1,104		4,271		817	
Profit/(loss) on disposals of investments	(9,934)		(33,902)		42,363			
		12,429		(15,694)		75,042		32,166
Royalties and copyright fees	10,052		3,933		24,232		19,262	
Advertising income	73,044		53,645		22,068		20,056	
Checking services	14,668		28,853		9,899		31,162	
Associates programme	6,821		14,936		13,612		8,471	
Bragg Prize donation	6,727							
		111,312		101,367		69,811		78,951
TOTAL INCOME		3,649,159		3,381,408		3,594,676		3,710,033
II. EXPENDITURE								
Journals								
Publication costs	(340,126)		(243,703)		(347,547)		(378,245)	
Editorial expenses	(75,859)		(72,468)		(78,136)		(86,555)	
Technical editing	(1,102,117)		(1,344,401)		(1,149,447)		(1,150,451)	
Subscription administration	(108,488)		(42,816)		(40,621)		(40,500)	
Journal development costs	(537,437)		(462,716)		(499,281)		(542,464)	
Checking services	14,894						(34,295)	
		(2,149,133)		(2,166,104)		(2,115,032)		(2,232,510)
Books								
Publication costs	(17,252)		(13,177)		(21,023)			
Editorial expenses	(52,760)		(30,387)		(13,972)		4,416	
Technical editing	(60,753)		(74,852)		(93,569)		(102,926)	
		(130,765)		(118,416)		(128,564)		(98,510)
Outreach and education								
Outreach	(50,768)		(111,798)		(83,035)		(144,068)	
Presidenr's Fuand and other grants	(18,718)							
Young scientists' support	(133,853)		(134,536)		(111,772)		(17,517)	
Visiting professorship programme	(11,205)		(11,313)		(9,837)		(1,038)	
		(214,544)		(257,647)		(204,644)		(162,623)
General Assembly costs		(8,490)		(12,705)		(4,704)		(366)
Ewald Prize		(31,441)						
Promotion, advertising and marketing costs		(167,821)		(95,517)		(77,943)		(56,221)
Newsletter costs		(73,865)		(7,196)		(10,240)		(8,022)

Administrative expenses								
Committee meetings and expenses	(105,105)		(55,749)		(73,013)		(2,180)	
Subscriptions	(4,989)		(4,840)		(4,350)		(4,514)	
General Secretary and Treasurer expenses	(5,935)		(6,297)		(2,221)		(1,172)	
Audit and accountancy fees	(47,681)		(38,399)		(54,035)		(38,369)	
Legal and professional fees	(1,055)		(39,797)		(31,833)		(983)	
Bank charges	(4,498)		(18,949)		(15,529)		(41,708)	
Travel expenses	(14,026)		(17,274)		(7,152)		(95)	
Executive office salaries	(224,082)		(116,186)		(126,658)		(134,203)	
		(407,371)		(297,491)		(314,791)		(223,224)
Chester office expenses								
Office costs	(120,402)		(147,160)		(308,315)		(233,187)	
Staff overheads	(82,526)		(72,719)		(82,987)		(58,098)	
		(202,928)		(219,879)		(391,302)		(291,285)
Depreciation		(11,475)		(23,650)		(34,246)		(34,769)
TOTAL EXPENDITURE		(3,397,833)		(3,198,605)		(3,281,466)		(3,107,530)
SURPLUS OF INCOME OVER EXPENDITURE		251,326		182,803		313,210		602,503
Other gains and losses								
MOVEMENT IN MARKET VALUE OF INVESTMENTS	120,776		(32,769)		170,654		79,807	
EXCHANGE MOVEMENTS ON TRADING ACTIVITIES	(182,131)		(92,599)		41,185		138,074	
EXCHANGE DIFFERENCES ON INVESTMENT ACTIVITIES	56,375		(32,411)		36,738		1,454	
		(4,980)		(157,779)		248,577		219,335
TOTAL RECOGNISED GAINS RELATING TO THE YEAR								
		246,346		25,024		561,787		821,838
ACCUMULATED BALANCE AT 1 JANUARY		3,042,669		3,289,015		3,314,039		3,875,826
ACCUMULATED BALANCE AT 31 DECEMBER		3,289,015		3,314,039		3,875,826		4,697,664

A3. Ewald Prize

The establishment of the Ewald Prize, for outstanding contributions to the science of crystallography, was announced in February 1986. The name of the Prize was chosen with the kind consent of the late Paul Peter Ewald, to recognize Professor Ewald's significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography, especially their services as the President of the Provisional International Crystallographic Committee from 1946 to 1948, as the first Editor of the IUCr's publication *Acta Crystallographica* from 1948 to 1959, and as the President of the IUCr from 1960 to 1963.

Shortly after the death of Professor Ewald in 1985, their family informed the President that Professor Ewald had wished to make a bequest to the IUCr. After consulting Mrs Ewald, this generous bequest, together with a donation from the Ewald family and a donation from the IUCr, was used as starting capital for the Ewald Prize. Further donations from the IUCr are used to finance the Prize.

The Prize consists of a medal, a certificate and a financial award. It is presented once every three years during the triennial International Congresses of Crystallography. The first Prize was presented during the Perth Congress, being awarded jointly to J.M. Cowley and A.F. Moodie. The second Prize was presented during the Bordeaux Congress to B.K. Vainshtein. The third Prize was presented during the Beijing Congress to N. Kato. The fourth Prize was presented during the Seattle Congress to M.G. Rossmann. The fifth Prize was presented during the Glasgow Congress to G.N. Ramachandran, the sixth Prize was presented during the Geneva Congress to M.M. Woolfson. The seventh Prize was presented during the Florence Congress to P. Coppens. The eighth Prize was presented during the Osaka Congress to D. Sayre. The ninth Prize was presented during the Madrid Congress to E. Dodson, C. Giacovazzo and G.M. Sheldrick. The tenth Prize was presented during the Montreal Congress to A. Janner and T.W.J.M. Janssen. The eleventh Prize was presented during the Hyderabad Congress to T. Blundell.

The twelfth Ewald Prize has been awarded to

Dr Olga Kennard

for their invaluable pioneering contribution to the development of crystallographic databases, in particular the Cambridge Structural Database (CSD), which as they early foresaw, has led "… to the discovery of new knowledge which transcends the results of individual experiment". Their own surveys using the CSD were fundamental in the development of crystal engineering, and are outstanding examples of the use of crystallographic databases as an essential tool for analysis and prediction. As founder of the CSD, director of the Cambridge Crystallographic Data Centre (CCDC) over decades, and being involved in the founding of the Protein Data Bank (PDB), Olga Kennard has made a fundamental impact on the development of modern crystallography.

Suzanna Ward from the CCDC delivered Dr Kennard's Ewald Prize Lecture during the Opening Ceremony of the Congress.

A4. W.H. and W.L. Bragg Prize

In 2017 the IUCr established the W.H. & W.L. Bragg Prize to be awarded to up to two promising early-career crystallographers. The Prize will be awarded at IUCr Congresses. The awardee(s) will receive a certificate and a financial award, and will be invited to make a presentation at the Congress on a topic related to the prize citation. Research achievement relative to opportunity will define the eligibility of candidates for this award. For this purpose, an "early-career researcher" is defined as one who received their PhD no more than 10 years before the closing date for nominations. Academic interruptions, including periods of parental leave, will be taken into account if clearly indicated in the letter of support accompanying the nomination. The inaugural W.H. and W.L. Bragg Prize for outstanding early-career crystallographers has been jointly awarded to Dr James Fraser and Dr Jean-Philippe Julien as a recognition of their scholarly achievements as well as their strong commitment to serve the crystallographic community.

Dr Julien's research activities have been focused on the determination of crystal structures of macromolecules of high medical relevance. Their studies have made a huge impact on biological and medical sciences. In particular, they determined the first crystal structure of an intact HIV envelope trimer by X-ray crystallography as well as by cryo-EM. The insights gathered from this structure and the construct engineering now serve as the template in the worldwide community for HIV structure-based drug and vaccine design in the quest to curtail the HIV epidemic. Dr Julien has also determined the EM structure of a quaternary preferring antibody (PG9) in complex with the soluble SOSIP Env trimer. This work provided the first structural evidence that epitopes of broadly neutralizing antibodies are much more complex than thought. In this sense the corresponding publication in *PNAS* must be considered a paradigm-shifting publication. At present, Dr Julien's independent research programme is focused on two major areas: (*a*) structure-based immunogen design for the development of an anti-malarial vaccine, and (*b*) structural delineation of B-cell receptors. With respect to the latter, they embarked on a completely new direction of structural investigation of B-cell co-receptors, on nanoparticles engineered to target these receptors, and on characterising antibody responses to malaria antigens to aid in vaccine design.

Dr Fraser's research activities have been and are focused on studying the flexibility and conformational variability in macromolecules through experimental and computational methods. Their research has provided new insights into how we can understand the role of protein flexibility in function through the use of crystallographic data. They have made seminal contributions to advancing the analysis of diffraction data in new directions, including the analysis of room-temperature and temperature-dependent data to gain insights into protein dynamics, studies of diffuse scattering from proteins, and the development of new experiments to exploit X-ray free-electron lasers in this field. The two main developments, room-temperature X-ray data collection and structural ensemble modelling into weak electron density, contributed synergistically to help reveal the structural basis of protein dynamics, moving away from static representations towards more realistic descriptions of how proteins populate conformational space. Dr Fraser's innovative approaches contributed to translating fundamental discoveries in protein dynamics into improvement of protein engineering and drug design.

Drs Fraser and Julien shared the presentation of a Keynote Lecture during the Congress.

A5. Struchkov Prize

Professor Yuri T. Struchkov (1926-1995) was an outstanding Russian crystallographer who made substantial contributions to the structural chemistry of organic and organometallic compounds. They were the founder and longtime director of the X-Ray Structural Centre of the Russian Academy of Sciences, one of the most productive laboratories in the field of "small molecule" organic crystallography. They served as a member of the Executive Committee of the IUCr from 1990 to 1993 and were elected the Vice-President of the IUCr at the XVI General Assembly in Beijing in 1993. They did not finish their term as Vice-President, as they passed away in August 1995. In order to commemorate the life achievements of Professor Struchkov, their friends and former colleagues established the Struchkov Prize in 1997. Between 1997 and 2020, the Prize was awarded annually to a young (less than 35 years old) scientist from the Former Soviet Union (FSU) for the best research work in the field of X-ray crystallography. The winner received a diploma and a financial award. Since its inception, the Struchkov Prize Association has held 24 annual competitions, and has awarded almost 30 top and more than 50 secondary prizes. Since 2000, the Prize was funded by former colleagues and students of Professor Struchkov, researchers who used to know them personally

or were closely familiar and appreciative of their scientific achievements as well as their contributions to organization and development of chemical crystallography in Russia. The Struchkov Prize Association, a non-profit organization registered in the USA, was also supported by corporate sponsors. 100% of all donations collected during any current year were distributed among the winners of the Struchkov competition by the end of the same year. The Association were especially happy to see recent laureates among the supporters of subsequent Prizes. In order to ensure the longevity of the Prize, the Association asked the IUCr to administer the Prize.

After 2020, the Prize will be bestowed by the IUCr every triennium at the IUCr Congress and General Assembly beginning in Melbourne in 2023, with up to three winners being awarded Prizes at each Congress. The Association has endowed a Prize Fund. Any interest earned on the Fund, along with any donations received during the triennium, will be split equally between the winners. The principal of the Fund can never be used to supplement the Prize. The IUCr will select a committee that will consider nominations and determine the winners.

A6. Outreach and Education

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

Some initiatives are described below:

IUCr-UNESCO OpenLabs
Among the initiatives launched during IYCr2014, the IUCr-UNESCO OpenLabs (https://www.iucr.org/outreach/openlabs) proved to be one of the most successful and long-lasting actions. As many as 32 editions have been implemented in 24 different countries so far. In addition to UNESCO, the IUCr has partnered with many companies and institutions on this project. Recent editions since the last IUCr General Assembly held in Hyderabad in 2017 included Senegal, Costa Rica, Côte d'Ivoire, Turkey, Ghana and Benin. All editions planned in 2020 and 2021 were cancelled because of the pandemic. New editions are now on schedule including the first OpenLab Jordan, to be associated with the SESAME Users Meeting.

LAAAMP, Lightsources for Africa, the Americas, Asia, Middle-East and the Pacific
The IUPAP-IUCr *LAAAMP* project (https://laaamp.iucr.org) was originally funded with a EUR 300K grant by the International Science Council (ISC). The following tasks have been achieved: (1) Preparation and distribution of the brochure “Advanced Light Sources and Crystallography: Tools of Discovery and Innovation” (versions available: English, French, Spanish, Arabic and Portuguese); (2) Over 40 FAST (FAculty-STudent) teams from targeted countries visiting partnering advanced light source (AdLS) facilities for a period of two months; (3) Participation in strategic science policy meetings (e.g. World Science Forum 2017; CiLAC Forum 2018; World Science Forum 2019) and several other conferences (including the PCCr2/AfLS2 Conference); (4) Colloquium presentations given by experts in several targeted countries; (5) Strategic Plans for the development of AdLSs and crystallography in the targeted regions of the project published.

Given the success of the initiatives, the *LAAAMP* project has been continued and is in full swing. A new partner, the ICTP, has joined IUPAP and IUCr to run the project. The Executive Committee, presently chaired by the IUCr Executive Outreach Officer, has been extended by two new members with the aim of improving its gender and geographical representation. A close collaboration with the African Light Source initiative has been put in place and formalized with an MOU. The SPARC (Synchronizing Partners to Advance Research Characterization) initiative, a mail-in access programme to AdLSs for researchers from targeted areas of the project, has been launched to overcome problems related to the pandemic. New collaborations have been started, including one with the Canadian Light Source with initiatives directed to high-school science teachers.

X-TechLab, Benin
X-TechLab is a new X-ray techniques facility established in Benin (https://www.xtechlab.co/). It is one of the outcomes of the IUPAP-IUCr project *LAAAMP* and was initially developed under the framework of the IUCr-UNESCO OpenLab. It was very well received by local authorities, and funded by the government of Benin to be one of the flagship laboratories at Sèmè City (https://semecity.bj/en/), the International City of Innovation and Knowledge launched by the Government of Benin in 2016. The initial funding was used to acquire a single-crystal diffractometer, a cryostat and other lab equipment, and to organize some training sessions on crystallography and tomography, which were very successful and attracted participants from the entire Western African region. We plan to organize two such training sessions every year. The last session was held in a hybrid mode, with some students attending in person and lecturers and other participants attending remotely.

Given the success of the activities and the enthusiasm generated so far, new funding has been made available by the Sèmè City administration for instrumentation. The Scientific Committee, chaired by the IUCr Executive Outreach Officer, has recommended that the X-TechLab acquires a powder diffractometer, which is presently under negotiation.

International Years
The IUCr is actively participating in the organization of a few festival years to be celebrated in 2022, namely:

International Year of Basic Sciences for Sustainable Development 2022 (IYBSSD2022)
Main organizer: International Union of Pure and Applied Physics (IUPAP).
Status: approved by UNESCO in November 2019; expected to be approved by the United Nations General Assembly (UNGA) soon.
IUCr involvement: the IUCr Executive Outreach Officer has actively participated in all the preparatory steps, including the organization and co-chairing with the President of IUPAP of a session at the World Science Forum 2019, where the IYBSSD2022 was first announced. They are a member of the Steering Committee. The IUCr is formally a partner of IYBSSD2022.

Year of Mineralogy 2022
Main organizer: International Mineralogical Association (IMA).
Status: approved by IMA and seconded by UNESCO, not seeking for approval by the UN. It will be celebrated as part of IYBSSD2022.
IUCr involvement: all preparatory steps were conducted by IMA Past President Patrick Cordier and the IUCr Executive Outreach Officer. The IUCr Executive Outreach Officer is presently a member of the Steering Committee. The main event to celebrate the Year of Mineralogy will be the IMA 2022 Conference, Lyon (France), 18-22 July 2022.

International Year of Glass 2022 (IYOG2022)
Main organizers: International Commission on Glass (ICG), Community of Glass Associations (CGA), ICOM-Glass.
Status: approved by the UNGA on 18 May 2021.
IUCr participation: the IUCr Executive Outreach Officer and the IUCr Executive Secretary have worked with Professor David Pye (Past President, The American Ceramic Society and Past President, The International Commission on Glass), promoter of IYOG2022, and helped prepare the ground for submitting the proposal to UNESCO and the UNGA. They are now attending the preparatory meetings to evaluate possible involvement of the IUCr in the programme.

M. Zema, IUCr Executive Outreach Officer

A7. IUCr Associates Programme

The Executive Committee realized that the success of our IYCr2014 celebration highlighted the fact that more needed to be done to establish the professional brand of crystallographers and to serve better their needs. The Executive Committee was also very mindful of the changing financial climate in the publishing world, which further pointed out that the IUCr needed to identify ways to raise additional funds if the IUCr was going to be able to continue to fund many of the kinds of worthwhile activities that were initiated during the International Year.

Accordingly, the Executive Committee believed that a voluntary IUCr Associates Programme with a modest dues structure would help accomplish the dual goals of promoting a sense of belonging for our professional community and enable us to serve better our community and support worthy activities. Many scientific unions and societies operate similar programmes.

The National Committees for Crystallography were contacted concerning the proposed IUCr Associates Programme. Useful comments were received from the community (83% of respondents supported the proposal) and the proposal was modified taking into account these comments.

The IUCr officially launched its voluntary Associates Programme at the Hyderabad Congress. The Programme offers a series of benefits and tools to help Associates network, share ideas and discover more about crystallography. In addition, those who join will be supporting the IUCr in its many charitable activities, such as sponsoring international meetings and schools and its OpenLabs initiative.

The benefits of joining include, for example, a 20% discount on the open-access fee for publishing an article in an IUCr journal, the facility to download 6 free articles from Crystallography Journals Online, a 50% discount for individuals purchasing the print version of *International Tables for Crystallography*, and many others.

The Associates Programme welcomes individuals at any stage of their career, from undergraduates to postdoctoral and senior researchers (a reduced joining rate is available for students and retired scientists). The IUCr also offers three categories for Corporate Associates, each with different levels of benefits and visibility. We thank Dectris, Rigaku and Eldico Scientific for joining in Category 1, ThermoFisher Scientific for joining in Category 2 and Stoe for joining in Category 3.

A8. Reports of the Commissions of the Union

A8.1 Commission on Journals

Overview

	2015	2016	2017	2018	2019	2020
No. of submissions (all)	3278	2231	2685	2678	2424	2121
without Acta E or IUCrData	2006	1689	1694	1880	1732	1528
Rejection rate (%)	25	25	28	27	32	28
without Acta E or IUCrData	32	33	36	34	35	31
No. of published papers (all)	2557	2065	1880	1793	1710	1583
without Acta E or IUCrData	1390	1139	1047	1139	1153	1079
No. of open-access papers (all)	1534	1240	1129	999	923	936
without Acta E or IUCrData	366	273	296	345	365	430
No. of pages (all)	13867	12451	11565	12473	12854	11819
without Acta E or IUCrData	10936	9181	8564	9856	10443	9539

This quadrennial report on the IUCr journals must depart from previous triennial reports due to the effects of the global pandemic conditions throughout 2020 (and 2021) on scientific journal publication everywhere, not least making this a quadrennial report rather than the usual triennial one. The reports that follow below summarize the major developments for each journal over the quadrennium, and largely speak for themselves. They reflect the hard work and dedication of the respective Editorial Boards as well as the Managing Editors in Chester. As a preface to the individual journal reports, some major developments that encompass all of the journals are briefly summarized here.

The Journals Management Board (JMB) initiated by my predecessor has continued to act as the main forum guiding the long-term development of the journals. The JMB comprises the Main (Section) Editors of each journal, together with the Managing Editors and other relevant staff. It has also now been expanded to include the IUCr Journals Commissioning Editors. The JMB meets annually, but the meetings for 2020 and planned for 2021 have needed to be virtual. We hope that an in-person meeting will be possible for 2022. Meanwhile, virtual meetings of Section and Managing Editors with the Editor-in-Chief, and sometimes others, are encouraged to address individual journal developments, as needed. Such journal-specific virtual meetings have become more common, and this trend will likely continue even after in-person meetings are re-instated for the full JMB.

In order to assist the various journal Editorial Boards in commissioning new Feature and Lead Articles, new authors and editors, as well as new Special Issue proposals, or even new paper subject categories, three IUCr Journals Commissioning Editors have been appointed: Roberto Steiner (Kings College, London, UK) for Biological Sciences, Elena Boldyreva (Russian Academy of Sciences, Novosibirsk, Russia) for Chemical Sciences, and Thomas Proffen (Oak Ridge National Laboratory, Oak Ridge, TN, USA) for Materials, Methods and Instrumentation. As each Commissioning Editor works across several relevant journals, we anticipate future journal reports will include updates on their progress.

The increasing proportion of open-access papers across all of the (hybrid) journals is of note, and it is envisaged that some of these will transition to become fully open access over the next few years. Among the seven hybrid journals, the *Journal of Synchrotron Radiation* has one of the highest fractions of published open-access papers (43.5% in 2020), and it will transition to open access only from January 2022. This step has required considerable preparation in partnership with the IUCr's publishing partner, Wiley, including an expansion of the journal's Editorial Board leadership.

Finally, it should be noted that the IUCr's continuing commitment to furthering diversity has been, and continues to be, reflected as far as possible in the diversity of new Editorial appointment nominations. This includes diversity in geography, background and gender, subject to meeting the scientific scope, interest and range of expertise needs of a given journal's Editorial Board applicable at the time, as well as the commitment of that nominee to serve in the envisaged role on the Editorial Board.

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

	2015	2016	2017	2018	2019	2020
No. of submissions	95	120	93	150	115	94
Rejection rate (%)	27	38	40	29	38	35
No. of published papers	70	74	62	75	88	79
research papers – foundations advances	47 8	43 5	34 5	44 8	57 17	50 5
short communications	4	3	5 (1 advances)	2	0	4
lead articles	0	2 (advances)	0	0	0	2 (advances)
feature articles	1 (advances)	1 (advances)	0	1 (advances)	0	0
topical reviews	0	0	0	1 (advances)	0	1 (advances)
editorials	2	1	0	1	1	0
commentaries	2	2	3	3	1	2
abstracts	789	647	1864	1124	1217	0
other	6	17	15	15	12	15
No. of open-access papers	9	7	5	13	28	20
No. of pages	630	705	488	713	918	783
Average length (pages)	10.1	10.3	9.9	11.1	11.3	11.4
Average publication time (months)	4.8	5.6	5.6	5.7	6.1	6.2
Impact factor	2.3	5.7	7.9	1.9	2.0	
5 year impact factor	2.2	3.5	4.2	4.6	3.1	
Cited half life (years)	>10.0	>10.0	>10.0	>10.0	>10.0	

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

The journal has two sections: Advances and Foundations. Articles are selected for the Advances section based on their likely impact and broad interest. They benefit from rapid publication and may be highlighted by an accompanying scientific commentary, and (based on a review of paper downloads and citations carried out in mid-2017) tend to be our most read and most highly cited articles. A list of all the Advances papers we have published since the section was launched in 2014 can be found at https://journals.iucr.org/a/services/advances.html.

A few highlights of the quadrennium were:

- *Three-dimensional single-cell imaging with X-ray waveguides in the holographic regime* by M. Krenkel, M. Toepperwien, F. Alves and T. Salditt (https://doi.org/10.1107/S2053273317007902), the most highly-cited paper in 2017, with over 5800 views;

- W. Steurer's Topical Review *Quasicrystals: What do we know? What do we want to know? What can we know?* (https://doi.org/10.1107/S2053273317016540), the most highly cited paper in 2018 (and indeed the quadrennium);

- *XGANDALF – extended gradient descent algorithm for lattice finding*, by Y. Gevorkov, O. Yefanov, A. Barty, T. A. White, V. Mariani, W. Brehm, A. Tolstikova, R.-R. Grigat and H. N. Chapman (https://doi.org/10.1107/S2053273319010593), the most cited article in 2019; and

- Publication of a 'virtual' special issue featuring some highlights of the 9th Conference on Aperiodic Crystals (Aperiodic 2018), which is available at https://journals.iucr.org/special_issues/2019/aperiodic2018/.

In addition, the article *Comments on `A new theory for X-ray diffraction'* by J. T. Fraser and J. S. Wark (https://doi.org/10.1107/S2053273318003959) and P. F. Fewster's response (https://doi.org/10.1107/S2053273318007489) attracted a large number of readers, as did the article *The development of powder profile refinement at the Reactor Centre Netherlands at Petten* by B. van Laar and H. Schenk (https://doi.org/10.1107/S2053273317018435).

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

The impact factor for the journal started the quadrennium at 7.9, after the publication of two particularly highly cited articles, on *SHELX* and *OLEX2*, in 2015. As these articles passed out of the 'window' for inclusion in the impact-factor calculation, the impact factor dropped back down to around 2. This prompted us to carry out an in-depth analysis of why, when we are publishing many excellent articles in the Advances section, the impact factor was not higher. We found that while our Advances papers were doing very well, a significant number of articles had a very low number of downloads and were uncited within the required window. One reason for this might be that new methods take time to be adopted by the community, so articles describing these might not start to gather citations immediately. However, there were also a number of articles where little effort had been made to explain to potential readers why the work described in the article might be of interest to them. As a result, in an Editorial published in January 2021 (https://doi.org/10.1107/S2053273320016678) we reminded our readers of the great history of the journal and the wide range of articles that it accepts, but also outlined some simple steps that authors could take to help maintain its prominence and impact as the premier journal for foundational work in crystallography. These include making sure that the crystallographic context of the work is emphasized early on in the article (*e.g.* in the title, synopsis, keywords or abstract), thus making it clear who in the materials or structural communities will use it and what they will use it for. We strongly feel that this is important for maintaining the relevancy, vibrancy and broader impact of the journal at a time when, whether rightly or wrongly, journals are often judged by their impact factor rather than their long-term worth to the scientific community.

The Editorial Board has seen a number of changes over the last four years. In 2017 we were pleased to welcome Laure Bourgeois as a new Co-editor, followed by Paulina Dominiak, Uwe Grimm and Ivan Vartaniants in 2019. Also in 2019, after five years as a Co-editor, Angela Altomare became joint Main Editor alongside Simon Billinge. In 2020 we welcomed four more new Co-editors: Mois Aroyo, Irene Margiolaki, Lukas Palatinus and Amit Singer, along with Commissioning Editor Thomas Proffen, whose role is to attract new articles on materials, methods and instrumentation to the IUCr journals. Werner Kuhs, Laurie Marks, Kenji Tsuda, Henk Schenk and Jean-Guillaume Eon retired from the Board during the quadrennium and are thanked for their dedicated service and all their hard work for the journal.

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

Acta Crystallographica Section B

	2015	2016	2017	2018	2019	2020
No. of submissions	157	171	175	168	201	168
Rejection rate (%)	32	31	34	43	32	31
No. of published papers	93	106	134	75	136	117
research papers	72	81	118	63	120	107
short communications	3	3	0	1	0	0
lead articles	0	0	1	0	2	0
feature articles	5	5	0	1	1	0
topical reviews	0	0	0	3	1	0
editorials	2	1	3	1	1	0
commentaries	5	6	3	1	2	5
other	6	10	9	5	9	5
No. of open-access papers	9	10	8	8	12	17
No. of pages	813	933	1199	744	1227	1147
Average length (pages)	9.6	10.3	9.8	10.7	9.7	10.5
Average publication time (months)	4.4	5.3	5.7	5.0	5.2	4.6
Impact factor	2.9	2.0	6.5	6.7	2.0	
5 year impact factor	2.5	2.4	4.2	4.7	4.7	
Cited half life (years)	>10.0	>10.0	>10.0	>10.0	>10.0	

During the quadrennium 2017−2021 *Acta Crystallographica Section B* continued to publish six issues per year, the numbers of articles (pages) published in 2017, 2018, 2019 and 2020 being 134 (1199), 75 (744), 136 (1227) and 117 (1147), respectively. The annual numbers tend to depend on the number and size of special issues published in a particular year.

Over the period 2015−2020 the rejection rate has typically been just over 30%, with an outlier of 43% in 2018 which might have been related to the sudden increase in the impact factor for 2017. The average article length has alternated between about 9.5 and 10.5 pages during the quadrennium and there is no trend for ever-longer articles. The average time between submission and publication (around 5 months) previously rose and fell in response to the number of special issues published, but now appears more stable. There has been a slight increase in the number of open-access papers but there is no sustained trend and the proportion has never exceeded 15%.

The journal's base impact factor is around 2.0 but can be considerably higher (as seen for 2017 and 2018) when we publish very highly cited feature articles. Despite a strong programme of invited articles and special issues, it has not yet been possible to achieve a sustained increase in the impact factor. We look forward to working with the new Commissioning Editor, Professor Elena Boldyreva, in part to address this issue.

During the quadrennium *Acta B* has published special issues on *Halogen Bonding* (Guest Editors: Pierangelo Metrangolo and Mate Erdelyi) in April 2017 and one entitled *Charge Density, Photocrystallography and Time-Resolved Crystallography: a Tribute to Professor Philip Coppens* (Guest Editors: Claude Lecomte, Jason Benedict and Yu Sheng Chen) in August 2017. A special issue on *Mineralogical Crystallography* (Guest Editors: Sergey Krivovichev, Janusz Lipkowski and Stuart Mills) followed in December 2018 and *Electron Crystallography* (Guest Editors: Joke Hadermann and Lukás Palatinus) in August 2019. Future special issues include those on *Quantum Crystallography* (Guest Editor: Piero Macchi), *Structure Correlation and Dynamics in Crystals* dedicated to H.-B. Bürgi (Guest Editors: Simon Grabowsky and Mark Spackman) and a virtual special issue on *High-Pressure Crystallography* across *Acta B*/*C*/*D*, *JAC* and *JSR* (Main Guest Editor: Elena Boldyreva). A special issue on *Crystal Growth* is in the early planning stage. We record our thanks to all Guest Editors for their efforts in bringing about the special issues. Importantly, special issues represent a source of additional articles in the journal: they do not redirect or reclassify submissions that the journal would receive anyway. Invited articles are regularly sought from prominent scientists, including Keynote Lecturers at IUCr Congresses and Regional Associate Meetings.

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

We note the retirement from the Editorial Board of *Acta B* of long-serving Co-editors Simon Parsons and Richard Welberry. We thank them warmly for all their contributions to the work of the journal. We are also grateful to two Co-editors (Michal Dusek and Pierre Bordet) due to retire in 2020 who have agreed to serve until the Prague Congress.

The Editorial Board has not been sufficiently well balanced in terms of gender and geography, and we are pleased to welcome several new Co-editors to the Board: Joke Hadermann (Belgium), Tatyana Bekker (Russia), Karah Knope (USA), Piero Macchi (Switzerland), Reinhard Neder (Germany) and Olga Yakubovich (Russia). Crucially, these appointments also add significantly to the aggregate expertise available on the Board. *Acta B* is aiming to strengthen and emphasize its role as a route to publication for papers on crystal growth related to the scope of the journal (structural science, crystal engineering and materials) and some of the new appointments are in support of this initiative.

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

Acta Crystallographica Section C

	2015	2016	2017	2018	2019	2020
No. of submissions	407	335	367	441	406	227
Rejection rate (%)	52	47	47	43	49	41
No. of published papers	198	162	178	234	197	143
research papers	194	158	169	227	186	137
feature articles	2	0	1	3	3	0
topical reviews	0	0	2	0	0	0
editorials	1	1	3	1	0	0
commentaries	0	0	0	0	6	2
other	1	3	3	3	2	4
No. of open-access papers	3	0	3	6	9	22
No. of pages	1117	1011	1159	1782	1697	1107
Average length (pages)	5.7	6.4	6.7	7.7	8.2	8.0
Average publication time (months)	2.2	2.7	2.7	2.9	2.8	2.9
Impact factor	0.5	4.1	8.7	0.9	0.9	
5 year impact factor	0.4	1.7	3.0	4.4	6.3	
Cited half life (years)	>10.0	>10.0	9.2	3.9	4.8	

Since 2016 the transformation of *Acta Crystallographica Section C* towards making it a leading journal for reporting structural chemistry has continued, with an increasing emphasis on the published contributions telling a chemistry story and containing an increased amount of supporting spectroscopic and synthetic data. This has been successful to an extent as evidenced by the increase in the average number of published pages of each paper from 5.7 in 2016 to 8.2 in 2019 (and 8.0 in 2020). There is a view from the Main Editors that the quality of the papers has significantly improved and there has been an underlying increase in impact factor from 0.5 in 2016 to 1.09 in 2020. The impact-factor statistics have been highly variable in the period 2016-2020 with huge increases in 2016 and 2017, to 4.1 and 8.7, because of the publication of two papers: one by George Sheldrick on *Crystal structure refinement with SHELXL* [*Acta Cryst.* (2015). C**71**, 3] and one by Ton Spek on *PLATON SQUEEZE* [*Acta Cryst.* (2015). C**71**, 9]. The very high number of citations for these two articles was responsible for the substantial increase in impact factors for 2016 and 2017. Since then the impact factor for *Acta C* has returned to more normal values but with a significant increase on pre-2016 levels.

The number of articles received by *Acta Crystallographica Section C* has increased over the last five years and with the increased length of the articles the number of pages published each year has increased. The substantial drop in 2020 is, we

feel, a direct result of the global pandemic and we expect this reduction to continue through 2021 as research groups that have only been able to operate in a limited way build up their outputs again.

The journal has continued to try to broaden its readership within the chemistry community with the publication of feature articles and topical reviews on areas of particular research interest that we have identified. We achieved the publication of three feature articles in both 2018 and 2019 but, unfortunately, none in 2020, again owing to the effect of the pandemic on research outputs from our authors. We have plans for further feature articles and reviews to be published in late 2021 and early 2022, and are grateful to Professor Elena Boldyreva, in their role as Commissioning Editor, for their support in moving these ideas forward. There will be a particular focus on attracting features relating to work involving the Cambridge Structural Database and knowledge mining using small-molecule data sets.

Since 2019 *Acta Crystallographica Section C* has been publishing commentaries, with six in 2019 and two in 2020. These seem to have been successful and there is some evidence in the citations that these commentaries have highlighted high-quality structural papers.

Special issues on *NMR Crystallography* and on *Polyoxometallates* were published in 2017 and 2018, respectively. These issues were well received and have led to the submission of follow-up papers in the two areas, including a Feature Article. A special issue on *Non-Covalent Interactions Based on the Sigma Hole*, which Jonathan White is organizing with two Guest Editors, is currently being planned with a publication date early in 2022.

A pleasing feature over the last few years has been the increasing number of open-access papers that have been published in *Acta Crystallographica Section C*. In 2020 there were 22 open-access publications, which is a record high, and may reflect the increasing number of `read and publish' agreements that have been negotiated between Wiley and both individual university libraries and national organizations. We hope that this increase will continue.

The Review Board of referees that was set up in 2016 continues to work well and these crystallographers provide rapid and high-quality reports that help to maintain a reasonable average publication time of under three months. Members of the Review Board agree to review a certain number of papers each year. The Board is being refreshed and expanded to include a wider range of chemists to provide good-quality reviews of the non-crystallographic aspects of the papers that *Acta C* now publishes.

Acta Crystallographica Section C has an active and enthusiastic group of Co-editors who continue to do a splendid job for the journal. The current number of Co-editors stands at 22 with 11 new Co-editors having been recruited within the last two years to replace some of the long-standing Co-editors who have served the journal very well over the last decade. We are very grateful to all our Co-editors, old and new, for their outstanding service.

With Tony Linden's retirement at the end of the last triennium, Paul Raithby, Larry Falvello and Jonathan White have served as the Main Editors for the journal. We are extremely grateful to our Co-editors and to the whole team at the Editorial Office in Chester for their outstanding support over the last four years and through the pandemic. Their dedication and professionalism has been exceptional.

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

	2015	2016	2017	2018	2019	2020
No. of submissions	272	158	153	152	160	194
Rejection rate (%)	27	24	24	19	29	15
No. of published papers	239	132	105	120	112	129
research papers	230	123	95	110	98	115
short communications	0	0	0	0	0	0
feature articles	1	0	0	0	2	2
topical reviews	0	0	1	0	1	1
editorials	1	1	0	1	2	3
commentaries	1	2	0	1	1	1
other	6	6	9	7	8	7
No. of open-access papers	84	59	56	66	60	69
No. of pages	2542	1309	1030	1244	1147	1279
Average length (pages)	10.8	10.4	10.5	10.9	10.9	10.5
Average publication time (months)	5.2	5.6	4.9	5.6	4.9	4.7
Impact factor	2.5	2.1	3.1	3.2	5.3	
5 year impact factor	8.8	4.2	3.4	3.0	3.2	
Cited half life (years)	5.8	6.7	7.7	8.7	9.6	

There are encouraging signs that *Acta D* is gradually recovering from the effects of the impact factor having dropped in 2014 from over 7 to 2.7, when several highly-cited methods papers disappeared over the limited horizon of the impact-factor calculation. The number of submissions and published papers plateaued for 2017 to 2019 but increased significantly to over 190 in 2020, with 115 of these papers in the research category, the highest number since 2016. The impact factor for 2019 of 5.3 is a notable improvement on the 2018 value of 3.2 and is very good relative to the historic range of 2 to 3. The average rejection rate fluctuated between 24 and 15% over the 4-year period, being lowest in 2020 and again this resulted in the highest number of papers since 2016 being published in 2020. This was perhaps partly because of a number of special issues, including the held-over CCP4 Molecular Replacement issue. An average of one feature article per year and a total of 3 topical reviews and 3 commentaries were published in the 2017-2020 period, and there were no short communications. The number of editorials rose from 0 to 3 per year at an increase of one each year over the period. An average of 8 ‘other’ papers were included per year. Around 53% of all papers each year were open access, with this percentage staying constant over the 4 years.

Special issues continue to play a positive role for the journal, particularly the recurring series of annual CCP4 and (more recently) CCP-EM symposia. Ten special issues were published over the period 2017-2020. The timeliness of the papers was improved by the decision to publish them in regular issues as soon as they are accepted and typeset, rather than waiting until all the papers in preparation are ready. Once all papers for a special issue are available they are now collected in a ‘virtual special issue’.

Over the four-year period, two new Section Editors (Charlie Bond, July 2020, and Elspeth Garman, November 2018) and in May 2020 three new Co-editors (Kristina Djinović-Carugo, Ana González and K. R. Vinothkumar) were approved and appointed. The addition of these new Co-editors will cover an expansion into different areas of structural biology, particularly metalloproteins, integrative structural biology techniques that combine a variety of methods, cryo-electron microscopy and the use of XFELs.

Publication times have been somewhat variable with a lower than previous time for 2016, back to previous levels at 5.6 months in 2018 and then have decreased in 2019 and 2020 to 4.7 months. It is important to note that these are driven largely by the time required for refereeing and manuscript revision, rather than by the technical editing or typesetting, which are both highly efficient thanks to the excellent work by Louise Jones and Simon Glynn in the Editorial Office in

Chester, under the supervision of Executive Managing Editor Peter Strickland and Editor-in-Chief Andrew Allen. We are very grateful for their hard work, attention to detail and dedication.

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

Acta Crystallographica Section E

	2015	2016	2017	2018	2019	2020
No. of submissions	1273	542	551	506	497	438
Rejection rate (%)	15	17	15	17	20	16
No. of published papers	1168	450	458	411	392	365
Structure/data reports	768	0	0	0	0	0
research communications	395	441	456	408	392	362
editorials	0	1	0	1	0	0
other	5	8	2	2	0	3
No. of open-access papers	1168	450	458	411	392	365
No. of pages	2931	1874	1980	1929	1952	1875
Average length (pages)	2.5	4.2	4.3	4.7	5.0	5.1
Average publication time (months)	0.8	0.9	0.9	1.2	1.3	1.1

Quality of papers and general statistics

In the last few years, the quality of the submitted papers has increased, and the range of structures is far broader. Many papers now report two or more structures, discuss complementary techniques, and include extra tables and figures to illustrate their results. We are increasingly receiving papers describing measurements using synchrotron radiation, powder diffraction analyses and Hirshfeld surface analyses, energy frameworks and the results of complementary techniques such as DFT calculations. The Section Editors identify articles that do not contain sufficient scientific discussion at the pre-screening stage; these are either transferred to *IUCrData* or resubmitted after the authors have improved the content.

The number of submissions and of published papers has decreased slightly over the past three years, with a low for 2020, which, however, is probably due to the difficulties related to the global health emergency. On the other hand, the average length of the papers has increased, reflecting the more detailed discussion of the underlying science in the submitted papers. The average publication time remains close to a month, thanks to the efforts of our Co-editors. In 2019 and 2020, the number of downloads for Section E articles was 5.7 and 7.4 million, respectively, by far the largest number of the IUCr journals.

Geographical distributions of articles

	2017	2018	2019	2020
Top four countries	USA (15%, 62 papers)	USA (15%, 62 papers)	USA (14%, 69 papers)	USA (19%, 69 papers)
	India (9%, 39 papers)	India 12%, 51 papers)	India (12%, 45 papers)	India (9%, 33 papers)
	Germany (7%, 31 papers)	Germany (7%, 30 papers)	Germany (9%, 35 papers)	Germany (9%, 32 papers)
	China (6%, 27 papers)	Turkey (6%, 27 papers)	Morocco (7%, 28 papers)	Morocco (5%, 17 papers)

The distribution of papers by country has remained approximately constant in the past four years, with the top three countries always being the USA, India and Germany. Authors from 65-70 countries continue to publish with *Acta E*.

Editors

In the past four years, several changes have taken place to replace retired Main Editors and to recruit new Co-editors. In 2017, following the retirement of Bill Harrison and Matthias Weil, Elena Boldyreva (Russia; high-pressure crystallography) and Chiara Massera (Italy; organic molecular crystallography) were appointed and joined the two remaining Main Editors, Helen Stoeckli-Evans (Switzerland; crystallography of coordination compounds and organic/natural products) and Luc Van Meervelt (Belgium; biological and organic crystallography). In 2019, Sean Parkin (USA, chemical crystallography, cryocrystallography,

biocrystallography) and Graciela Díaz de Delgado (Venezuela; molecular crystallography, crystal engineering, polymorphism) were also appointed to succeed Elena Boldyreva, who had been selected as the IUCr Journals Commissioning Editor for Chemical Sciences, and the long-standing Section Editor Helen Stoeckli-Evans.

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

Special issues and themed articles

Following the suggestion of publishing Topical Reviews, a first collection of invited papers on Weak Interactions in Crystals: an Integrated Approach appeared in the May 2018 issue, edited by Chiara Massera and Helen Stoeckli-Evans. This issue was very well received and the papers in it have done well in terms of the number of citations and downloads. Since then, 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 [S. L. Tan, M. M. Jotani & E. R. T. Tiekink, *Utilizing Hirshfeld surface calculations, non-covalent interaction (NCI) plots and the calculation of interaction energies in the analysis of molecular packing*, *Acta Cryst*. (2019), E**75**, 308-318], followed in December 2019 by *Some reflections on symmetry: pitfalls of automation and some illustrative examples* [W. Clegg, *Acta Cryst*. (2019), E**75**, 1812-1819]. The series continued in 2020 with papers on *checkCIF* [A. L. Spek, *checkCIF validation ALERTS: what they mean and how to respond*, *Acta Cryst.* (2020), E**76**, 1-11] and tips and tricks for obtaining the best results [A. Linden, *Obtaining the best results: aspects of data collection, model finalization and interpretation of results in small molecule crystal structure determination*, *Acta Cryst*. (2020), E**76**, 765-766] and has been recently enriched by an educational paper on twinning [S. R. Parkin, *Practical hints and tips for solution of pseudo-merohedric twins: three case studies*, *Acta Cryst*. (2021). E**77**, 452-465].

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

As always, we are extremely grateful to our Co-editors for the excellent work they have done and cannot thank them enough. We are also extremely grateful for the excellent support that we receive from the staff in Chester, particularly Gillian Holmes, Sean Conway and Mike Hoyland, for their constant help and support, and to Peter Strickland for their sound advice and expert guidance.

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

Acta Crystallographica Section F

	2015	2016	2017	2018	2019	2020
No. of submissions	328	189	196	200	122	98
Rejection rate (%)	34	34	41	34	32	26
No. of published papers	251	136	108	116	105	85
research communications	247	130	106	113	95	76
topical reviews	0	0	1	2	1	0
editorials	2	0	0	1	5	3
commentaries	0	0	0	0	1	0
other	2	6	1	1	3	6
No. of open-access papers	41	27	22	28	16	27
No. of pages	1540	911	713	824	757	623
Average length (pages)	6.2	6.9	6.7	7.1	7.4	7.5
Average publication time (months)	3.2	2.7	2.6	3.4	3.9	2.8
Impact factor	0.7	0.8	1.0	1.2	1.0	
5 year impact factor	0.5	0.6	0.7	0.8	0.9	
Cited half life (years)	4.2	4.6	5.4	6.2	6.5	

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

In the years 2017-2020 the journal published 414 papers (2719 pages). This represents a large decrease in the number of papers compared with 2014-2016 - we need to attract more authors. The overall number of pages has also decreased but the average paper length has increased to 7.5 pages, probably owing to the extra scientific requirements for publishing in *Acta Cryst. F.* The average publication time had risen to over three months in 2019, but in 2020 dropped to an average of 2.8 months. Accepted papers undergo prompt final editing and usually appear published online in a matter of days, thanks to the efficient handling in Chester.

In 2017 six new Co-editors were recruited (Maria Romao, Matthew Bowler, Alok Mitra, Steven Sheriff, Gordon Joyce and Kyeong Kyu Kim) and a new Section Editor (Mark van Raaij). In 2018, an additional Section Editor was recruited (Janet Newman). In 2019, four new Co-editors were added: Jon Agirre, Yang Chen, Mike Hough and Linda Shimon. Together with the longer-serving Co-editors, this team of editors has good geographical diversity and subject diversity, and hopefully should be sufficient for 2021 and beyond. The referee panel continues to function well. This group of about thirty experienced scientists have agreed to referee twelve papers a year each, to reply to requests promptly, and to return reports within two weeks.

The strengths of the journal include the fast but high-quality scientific and technical editing, its standing in the crystallographic community and its goodwill, by virtue of it being a scientific society journal. However, the impact of the journal and its familiarity to non-crystallographic structural biology communities need to be increased further. The impact factor has been stable at around 1.0 between 2017 and 2019 (the number of citations suggests a similar impact factor for 2020). The five-year impact factor and citation half-life are both steadily increasing, a trend which will hopefully continue.

A new article type, Methods Communications, was introduced in 2019, with an August Editorial. This provides researchers with quick tips as well more detailed methods, and hopefully will obtain more citations for *Acta Cryst. F*. Three Methods Communications were published in 2019 and four in 2020. Two communications from the International Symposium on Diffraction Structural Biology (ISDSB) with a methods orientation have also been published. A special issue on protein/carbohydrate structures was published in August 2018 and a number of papers on cryo-EM were published in January 2019.

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

J. Newman and M. van Raaij, Editors

IUCrJ

	2015	2016	2017	2018	2019	2020
No. of submissions	82	74	133	138	147	151
Rejection rate (%)	25	24	34	33	38	41
No. of published papers	81	57	93	95	120	129
research papers	38	37	52	75	94	100
feature articles	16	1	4	1	1	1
topical reviews	5	1	12	1	3	1
research letters	0	4	7	5	6	8
editorials	6	6	6	4	6	5
commentaries	12	8	12	7	8	11
other	4	4	0	5	2	3
No. of open-access papers	81	57	93	95	120	129
No. of pages	690	467	823	879	1133	1215
Average length (pages)	10.9	10.5	10.8	10.5	10.7	10.8
Average publication time (months)	4.6	4.5	4.0	4.8	4.3	4.3
Impact factor	5.3	5.8	6.5	4.8	5.4	
5 year impact factor	5.3	5.8	6.6	5.4	5.7	
Cited half life (years)	1.3	1.8	2.6	3.1	3.0	

In the current quadrennium, *IUCrJ*, which was launched as an open-access journal in 2014 to coincide with the International Year of Crystallography, has been successful in establishing itself within the wider scientific communities that use results obtained from diffraction methods. It has made a strong impact in attracting high-quality science papers of wide scientific significance from these communities. Impressions from authors, readers, referees and commentators are very positive with a number of papers receiving high downloads and citations in line with high-impact publications.

The journal impact factor varied between 4.8 and 6.5 during the quadrennium. All submissions undergo preliminary screening by a panel consisting of the Main Editors (Dimitri Argyriou, Ted Baker, Richard Catlow, Gautam Desiraju, John Spence and Sriram Subramaniam) and the Editor-in-Chief (Andrew Allen), and this has helped to provide a rapid and efficient review process. Where appropriate, any articles that do not meet the journal's requirement for broad scientific significance are usually transferred, with the agreement of the authors, to another IUCr journal. Such transfers are seamless and do not require any further work by the authors.

The 24 issues of *IUCrJ* published in the quadrennium 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 increased from 133 in 2017 to 151 in 2020. Overall 437 papers were published in the quadrennium. A number of papers have been highlighted in each issue via an in-depth commentary in a manner similar to other comprehensive journals such as *Nature* and *PNAS*.

The Biology and Medicine section of *IUCrJ* continues to attract a wide variety of papers, with 109 research articles and 18 commentaries/letters in the quadrennium. Most report novel biological structures, with an emphasis on the binding of ligands and drug-related molecules, but innovative methods for obtaining structural data from biological systems continue to appear. These latter include new variations on serial crystallography, to better capture the dynamics of biological reactions, and approaches that further push the boundaries of crystallography, such as *in situ* imaging of cells. Other sections of the journal (*e.g.* the cryoEM, Neutron/Synchrotron and Physics/FELs sections) also address biological systems, making this a strong focus for the journal. Importantly, the current COVID-19 pandemic has galvanized structural biology to generate an outpouring of COVID-related structures. Most are not yet published, but we expect to be publishing many papers on this topic in the coming years; some outstanding examples have already appeared in *IUCrJ* and more are in the pipeline.

In 2017, we introduced a new section in *IUCrJ* to provide a forum for rapid publication of important results in the cryo-EM field. Over the last four years, we have published papers reporting both methodological advances as well as new biologically relevant findings that emerge from the use of cryo-EM and related techniques. The addition of this section has contributed to the overall doubling of research papers published annually in *IUCrJ* over this four-year period. Papers in the cryo-EM section have also featured prominently among the most downloaded articles in *IUCrJ* each year. The establishment of *IUCrJ* as a venue for publication of high-quality articles of relevance to technical and biological findings in cryo-EM, along with *IUCrJ*'s continued maintenance of a high and competitive impact factor, bode well for the future of publishing important cryo-EM studies in the coming four-year period.

The Chemistry and Crystal Engineering section of the journal has continued to grow in the quadrennium. There were 143 submissions of which 119 articles were voted for review. A total of 93 articles were accepted for publication. These numbers are satisfactory, but one might have expected around 50 submissions every year in this section (one per week). This section continues to pull its weight in contributing to the impact factor of the journal, but the impact factor seems to be flattening out and one would hope that this situation could be improved. It is important that the publication time competes with ACS and RSC journals where the proofs are available very quickly after acceptance and papers are online soon thereafter. The journal also needs to be aware of a potential identity problem: chemists might not want to submit to *IUCrJ* if the feeling is that the journal is too `crystallographic'. The present Co-editors of the Chemistry and Crystal Engineering section of the journal are M. Eddaoudi, P. Lightfoot, L. R. MacGillivray and C.-Y. Su. This number appears to be satisfactory given the number of submissions.

The 66 papers published in the Materials and Computation section of *IUCrJ* in the quadrennium illustrate well the challenges posed by structural problems in the science of materials and the key role that computation can play in this and related fields in structural science. They demonstrate the continuing developments in techniques and instrumentation and the increasingly complex structural problems which these developments now make accessible.

The other sections of the journal, covering Neutron and Synchrotron Science and Technology, and Physics and Free Electron Laser Science and Technology, published 39 and 47 papers, respectively, in the period 2017-2020 and have illustrated the rapid advances that are being made in these fields.

During the quadrennium, Professor Samar Hasnain retired as Editor-in-Chief and was replaced by Dr Andrew Allen. The Board and the Union express their gratitude to Professor Hasnain for the role they have played in establishing the journal. In addition, three Co-editors (E. E. Lattman, C. Lecomte and J. Trewhella) stepped down and are thanked for their hard work for the journal. Additional Co-editor appointments were made to cover cryo-EM (E. Bullitt, L. A. Passmore, S. Raunser and F. Sun) and FELs (F. Maia), and the Editorial Advisory Board was boosted by the appointment of S. S. Hasnain and J. Trewhella. The journal also welcomes the appointment of three Commissioning Editors (E. V. Boldyreva, Th. Proffen and R. Steiner).

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

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

	2015	2016	2017	2018	2019	2020
No. of submissions	360	380	330	299	284	297
Rejection rate (%)	29	30	37	33	32	33
No. of published papers	249	271	211	201	172	188
research papers	183	197	165	152	121	132
short communications	11	9	4	5	5	4
feature articles	1	0	0	1	0	0
computer programs	25	38	18	20	21	26
editorials	3	2	1	2	1	0
commentaries	2	0	1	0	0	2
other	24	25	22	21	24	24
No. of open-access papers	55	60	55	38	33	55
No. of pages	2044	2282	1852	1776	1468	1631
Average length (pages)	9.2	9.3	9.8	9.7	9.7	9.8
Average publication time (months)	5.5	5.4	5.2	5.5	5.6	5.7
Impact factor	2.6	2.6	3.4	2.9	3.0	
5 year impact factor	5.1	4.7	4.3	3.4	3.4	
Cited half life (years)	>10.0	>10.0	>10.0	>10.0	>10.0	

Over the past four years, the number of submissions to *Journal of Applied Crystallography* has hovered around 300 per year, of which about 200 are accepted for publication, accounting for around 1700 published pages. These values are roughly 75% those of the preceding (triennial) period. The impact factor has fluctuated, being slightly higher in the second half of the four-year period than in the first half. The five-year impact factor has decreased gradually, possibly reflecting the dip in impact factor in the first half of the four-year period. The citation half-life continues to exceed 10 years. The number of computer program submissions, which generally attract above-average citations and which we do actively seek, remains at a healthy level. The fraction of published papers that are open access has fluctuated between 19 and 30% over the four-year period.

Several virtual special issues have been published in the period 2017-2020. The first, featuring some highlights of the 13th Biennial Conference on High-Resolution X-ray Diffraction and Imaging (XTOP 2016) held in Brno, Czech Republic, in September 2016, was published in June 2017, with Guest Editors Václav Holý and Virgine Chamard. A special issue not associated with a conference, *Advanced Neutron Scattering Instrumentation*, was published in August 2018 with Guest Editors Dimitri Argyriou and Andrew Allen, and Guest Co-editors Masatoshi Arai, Kenneth W. Herwig, Flora Meilleur, Kenji Nakajima and Dan A. Neumann. All articles in the special issue on ptychographic software and technical developments that was initiated by the Ptycho Developers 2019 Workshop held at Berkeley Laboratory in June 2019 were published in the second half of 2020. The Guest Editors were Stefano Marchesini and David Shapiro from Lawrence Berkeley National Laboratory, and Filipe Maia from Uppsala University. An editorial closing the issue was published in April 2021. Further special issues are planned.

The Editorial Board underwent several major changes during the four-year period 2017–2020. Anke Kaysser-Pyzalla passed on their baton as Main Editor to Garry McIntyre in 2017, while Andrew Allen, following their promotion to Editor-in-Chief of IUCr Journals in 2019, passed their baton on to Karena Chapman, who was previously a Co-editor. Thomas Proffen, a Co-editor since 2014, was promoted to be the new IUCr Commissioning Editor for Materials, Methods and Instrumentation in 2020. During the four-year period we also bade farewell to three long-serving Co-editors: Gernot Kostorz, Gilles Renaud and Satoshi Sasaki. These promotions or retirements were compensated by the appointments in 2020 of five new expert Editorial Board members to ensure full coverage of the broad scope and reach of the journal: Helen Brand, Jan Ilavksy, Arthur Haozhe Liu, Stephen Moggach and Taku Sato.

We thank all members of our Editorial Board, whether retired or current, who have served the journal during this review period for their hard work and dedication to the continued success of the journal. We are especially thankful for the tireless

support of the staff of the Editorial Office in Chester, who keep us on the straight and narrow to ensure that each issue is of the highest quality.

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

Journal of Synchrotron Radiation

	2015	2016	2017	2018	2019	2020
No. of submissions	258	262	247	334	297	299
Rejection rate (%)	19	28	25	20	25	24
No. of published papers	210	198	156	222	249	209
research papers	164	157	121	172	203	158
short communications	9	10	6	6	10	14
feature articles	2	1	0	4	0	0
lead articles	2	1	0	0	0	0
beamlines	15	16	13	17	27	23
editorials	2	1	2	2	1	2
commentaries	0	1	0	0	0	0
other	18	11	14	21	6	12
No. of open-access papers	84	53	54	88	87	91
No. of pages	1560	1563	1300	1894	2096	1754
Average length (pages)	8.1	8.3	8.8	8.9	8.7	9.0
Average publication time (months)	5.1	5.0	5.6	5.6	5.7	5.3
Impact factor	1.9	3.0	3.2	2.5	2.3	
5 year impact factor	2.3	2.9	3.0	2.8	2.8	
Cited half life (years)	8.3	7.4	7.1	8.0	7.8	

During the 2017-2020 quadrennium, *Journal of Synchrotron Radiation* (*JSR*) continued to publish six issues per year. The number of articles published each year has risen since the last triennium, with an average of 209 papers over the last four years compared with 198 in the previous triennium. The rejection rate slightly increased to an average of ~24%.

There have been changes to the Editorial Board over the last four years. We gratefully acknowledge the work of Mikael Erikssen and Ilme Schlichting who stepped down as Main Editors during this time, while Co-editors Aldo Craievich, Piero Pianetta and David Reis retired after also reaching their nine-year term of service on the journal. We were pleased to welcome several new Main and Co-editors to the board: Anna Bergamaschi, U-Ser Jeng, Kristina Kvashnina, Andrew Stevenson and Meitian Wang all joined the team of Co-editors in 2019, with Kristina promoted to Main Editor in 2020 where they were joined by new Main Editor Dibyendu Bhattacharyya. We would like to thank our Main Editors and Co-editors, retired or current, who have served the journal during this quadrennium for their hard work and dedication.

JSR published a number of special issues during the last quadrennium. In 2017, a special issue on *X-ray Radiation Damage to Biological Crystalline Samples* was published in the January issue (Guest Editors Elspeth Garman and Martin Weik); this is a recurring special issue, with papers taken from the corresponding workshop held every two years. 2018 saw two special issues, the first, published in the January issue, on papers from the *PhotonDiag2017 Workshop* (another recurring special issue, again published every two years; Guest Editors Elke Plönjes, Marco Zangrando and Daniele Cocco), and the second, in July, on papers from the *Q2XAFS2017 Workshop* (Guest Editors Sofia Diaz-Moreno and Richard W. Strange). This was followed by the next installment of the *X-ray Radiation Damage to Biological Crystalline Samples* special issues, published in the July issue of 2019 (Guest Editors again Elspeth Garman and Martin Weik). In 2020 we saw the first `virtual' issues published in *JSR*, where papers are published as soon as they are ready and are then all brought together as a virtual issue online. Two such

issues were published: the first was on papers taken from the *PhotonDiag2018 Workshop* (Guest Editors Elke Ploenjes, Daniele Cocco, Jan Grünert, Kai Tiedtke and Marco Zangrando) and the second was organized and brought together by Main Editor Ilme Schlichting on *X-ray Free-Electron Lasers* (Guest Editors Paul Fuoss, Ilme Schlichting, Thomas Tschentscher and Makina Yabashi). We wish to record our thanks to these Guest Editors for their exceptional efforts in bringing about the special issues.

Facility Information pages continued to be published in *JSR* over the last quadrennium, providing an opportunity for facilities to communicate important news and updates to the international community of synchrotron radiation users. Our three long-standing contributers, Advanced Photon Source, Paul Scherrer Institute and MAX IV, were joined from 2018 to 2019 by LAAAMP (Lightsources for Africa, the Americas, Asia and Middle East Project). We kindly thank all of these facilities for their support during this time.

The number of open-access papers published in *JSR* has increased since the previous triennium, with an average of 80 per year over the last quadrennium compared with 63 per year for 2014-2016. In view of this, and with the current climate in journal publishing, following discussions between the IUCr and Wiley we look forward to *JSR* becoming a fully open-access journal from the beginning of 2022.

Y. Amemiya, I. Lindau, I. Schlichting, K. Kvashnina and D. Bhattacharyya, Editors

A8.2 Commission on International Tables

International Tables for Crystallography is a book series published by the IUCr in conjunction with Wiley. Eight volumes designated A (and A1) through G were in print at the beginning of the triennium. A ninth (H, *Powder Diffraction*) was published in 2019, and a tenth (I, *X-ray Absorption Spectroscopy and Related Techniques*) is being written. Printed volumes can be purchased individually; online access is by subscription to the entire series. A new, considerably revised edition of the low-cost, printed *Brief Teaching Edition of Volume A* (*Space-Group Symmetry*) should appear in 2021.

Symmetry information is covered in Volumes A (*Space-Group Symmetry*), A1 (*Symmetry Relations between Space Groups*), and E (*Subperiodic Groups*). Information about the influence of symmetry on the physical and tensor properties of crystals is found in D (*Physical Properties of Crystals*). Information on superspace symmetry is, for now, split between B (*Reciprocal Space*) and C (*Mathematical, Physical and Chemical Tables*). An extensive electronic Symmetry Database is available to subscribers to the online version of the series.

Additional information of a general type is included in Vols. B and C, which can be traced back to Vol. II of the original series (1937) and Vols. II – IV of the series with red covers (1959-74). The other volumes of the current series can be described as comprehensive handbooks that cover more specific areas. These volumes are D, F (*Crystallography of Biological Macromolecules*), G (*Definition and Exchange of Crystallographic Data*), H, and the future I.

Historically the series has been composed of print volumes but online versions started appearing in 2006. While printed copies of all volumes are still available for individual purchase they may not all remain so indefinitely because economic considerations so greatly favor annual online subscriptions to the entire series. The symmetry tables (*e.g.*, Vols. A and E) are, however, expected to remain available in both formats. So far the *Brief Teaching Edition* has appeared in print only.

A series that is largely electronic allows greater flexibility; parts of new and revised volumes can appear online in advance of completion of the entire volume and problems identified after publication can be fixed quickly. This scheme was first used during this triennium (*e.g.*, for the new Vol. H) and has been well received. Authors who complete their chapters promptly appreciate not having to wait for all articles to be finalized. This approach also makes it easier to meet Wiley's annual target of 10% new or revised content.

Developments in the triennium 2017-19 include:

(1) Completion in 2019 of the new Vol. H on powder diffraction, which is selling well. It is a great pleasure to thank Chris Gilmore, Jim Kaduk and Henk Schenk for all their work bringing this major project to fruition. An article about the new edition appeared in the 3rd issue of the *IUCr Newsletter* (https://www.iucr.org/news/newsletter/etc/articles?issue=143731&result_138339_result_page=11).

(2) Near completion of the material for a revision of the *Brief Teaching Edition* (Mois Aroyo). The new version is designed to be more useful for inexperienced readers. The revision will also serve as an introduction to Vols. A1 and E of *International Tables*, to magnetic space groups, and to the Symmetry Database, *i.e.*, to a broad set of topics in crystallographic symmetry, some of which are still being developed.

(3) Continued expansion of the Symmetry Database (also edited by Mois Aroyo). This electronic resource simplifies use of non-standard space-group settings, which are often appropriate when phase sequences are being considered, and facilitates identification of group/subgroup/supergroup relationships. Visualization tools are also being developed.

(4) Work on revised editions of Vols. B (Gervais Chapuis) and C (Richard Welberry). These two volumes are the successors of Vol. II of the original series (1937) and Vols. II–IV of the `red' series (1959-74). Much of the material in Vol. B (current edition dated 2010) remains up to date but Vol. C (dated 2006) is in serious need of revision. Articles for the revisions of the two volumes are in various stages of completion; some of them are expected to be online before the end of 2020.

(5) Substantial progress on the new Vol. I (*X-ray Absorption Spectroscopy and Related Techniques*) being edited by Chris Chantler, Federico Boscherini and Bruce Bunker. The first set of completed articles should be made available electronically before the end of 2020.

(6) Plans for a revised version of Vol. F (*Crystallography of Biological Macromolecules*). The outline for the revision was completed before the untimely passing of Editor Michael Rossmann but was put on hold at the request of the Executive Committee. The two remaining Editors, Liang Tong and Eddy Arnold, expect to start contacting prospective authors by the end of 2020. The revised edition will be dedicated to Rossmann.

(7) Planning for a revised Vol. G (*Definition and Exchange of Crystallographic Data*) by Editors Brian McMahon and James Hester. Drafts of chapters describing the new standards for dictionaries are near completion, and an automated process for updating dictionary chapters from the first edition to meet the new standards has been developed.

(8) Extension of the text and the tables of reflection conditions in Vol. A (Chapter 1.6) to include the so-called `diffraction symbols' (also known as `extinction symbols') that were present in the previous edition. Many readers had requested that these symbols be restored. The typesetting of the new text and tables has been completed but additional checking is needed before the new chapter can be put online.

Attempts continue to find a new Editor for Vol. A1 (to join Ulrich Müller) and new Editors for Vols. D (now that André Authier has retired) and E (after the 2020 retirement of Danny Litvin). Also continuing are discussions with the Commission on Magnetic Structures about a volume covering their field.

Plans for the futures of all volumes have been discussed with their Editors and with the staff in Chester. Further information about all the volumes can be found at the home page of the Commission, http://www.iucr.org/resources/commissions/international-tables. Access to the Tables of Contents of all the volumes is free, as are sample pages (including author lists and prefaces).

Central to the success of this series are the contributions of the staff in Chester, and especially of Nicola Ashcroft. As always they have applied their considerable expertise in layout, typesetting and insertion of hyperlinks. They have helped authors and Editors by answering questions about standard practices and by tactfully suggesting ideas for clarifying text. Having technical editors with writing as well as technical skills is a very great asset. The Chester staff has also been very helpful in finding ways to take advantage of advances in electronic publishing while at the same time working to preserve print publication.

C. P. Brock, Chair

A8.3 Commission on Aperiodic Crystals

The Commission (the CAC) continued during the last four years to actively promote aperiodic crystallography, in organizing, supporting and promoting meetings, workshops and educational activities worldwide.

The past four years were marked by the loss of two pioneers of aperiodic crystallography. Professor Ted Janssen passed away on 29 September 2017 at the age of 81; they were one of the founders of the symmetry description of aperiodic crystals. Professor An-Pang Tsai, leader in the field of quasicrystal and complex intermetallic research, passed away on 25 May 2019 at the age of 61.

The CAC has supported regular workshops and schools, including the 9th Workshop on Structural Analysis of Aperiodic Crystals in Bayreuth, Germany, 23–26 March 2017 (aperiodic.unibayreuth.de/workshop_2017, local organizer Professor Sander van Smaalen). This provided young scientists with an overview of the methods of structural analysis of incommensurately modulated crystals and composite crystals. The 10th edition scheduled for March 2020 had to be cancelled owing to the COVID-19 pandemic.

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

In 2019, the CAC also organized the 4th International School on Aperiodic Crystals in Portbail, Normandy, France, with the support of the CNRS, the Normandy Council, the European C-MetAC network and other sponsors. The IUCr provided six grants for promoting women in science. The school attracted 32 participants from 13 different nations. Teaching at the school was provided by nine lecturers. This school is our central educational activity, with the objective of providing an overview of

aperiodic order, of the basics of the mathematical description of both modulated structures and quasicrystals, and of physical properties and chemical understanding of aperiodic crystals, as well as a working knowledge of structural analysis of aperiodic crystals. The fifth edition of the school is expected to take place in Prague in 2022.

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

These last four years have also been very rich in conferences and workshop-type events. The events organized by the IUCr or the ECA allow us to meet a wider community. Thus the 24th Congress and General Assembly of the IUCr, Hyderabad, India, 21–28 August 2017, and the 31st and 32nd European Crystallography Meetings (22–27 August 2018, Oviedo, Spain, and 18–23 August 2019, Vienna, Austria) all had good coverage of aperiodic crystals, with microsymposia and keynote lectures related to aperiodic crystals.

However, two series of triennial conferences specific to our community are organized under the auspices of the CAC conferences. The first one is the International Conference on Aperiodic Crystals. Our flagship scientific event in 2018 was the 9th edition of this congress (Aperiodic 2018), which was held on the campus of Iowa State University in Ames, USA (8–13 July 2018). The conference was chaired by Patricia Thiel, Alan Goldman and Gloria Borgstahl, and was attended by about 100 delegates from more than 20 countries. 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. The programme also included a public lecture given by the Nobel Prize winner Professor Danny Shechtman on `The role of TEM in the discovery of the quasi-periodic materials'. The 10th edition of this conference, planned for Sapporo in 2021, has been postponed to 2022 owing to the COVID-19 pandemic.

The second specific conference of the CAC is the International Conference on Quasicrystals. The 14th edition (ICQ14) was held at Kranjska Gora, Slovenia, 26–31 May 2019. The conference was chaired by Janez Dolinšek, with the Jožef Stefan Institute, the Ljubljana Faculty of Mathematics and Physics and the University of Ljubljana Institute of Mathematics, Physics and Mechanics, Ljubljana, as the local organizers. The conference was attended by 84 delegates from more than 20 countries. A broad range of topics were covered, including formation, growth and phase stability; structure and modelling; mathematics of aperiodic order; physical properties; surfaces and thin films; quasiperiodic soft matter; new frontiers; and applications. At ICQ14 the 2019 Jean-Marie Dubois Award for Excellence in Quasicrystals was presented to Professor Alan Goldman of Iowa State University. The award was given for `elucidating the relationship between quasiperiodicity and magnetism, particularly through the ground-breaking discovery of a series of binary Cd–rare earth icosahedral quasicrystals, measurement of their magnetic properties, and comparison with the parent 1/1 periodic approximant'. For more details, see the conference website at http://icq14.ijs.si/. The next edition of this conference is expected to be held in Tel Aviv (Israel) in 2022, but is under discussion owing to the probable overlap with the 10th edition of the International Conference on Aperiodic Crystals.

Finally, to develop the connection between structure and properties, the workshops Open Space Between Aperiodic Order and Strong Electronic Correlations took place in Annecy (France), 19–22 June 2017, and in Tohoku University (Tokyo, Japan), 23–27 June 2019. This international workshop aims to explore the frontiers between aperiodic order and strongly correlated electron systems, and brings together specialists of the two communities to explore the open space between aperiodic order and strong electronic correlations to promote the exchange of ideas. This series of workshops led in 2020 to the formation of an international research network `Aperiodic'; its objective is to foster collaborations between the aperiodic crystal community and those who work on the chemical and physical properties of materials.

O. Perez, Chair

A8.4 Commission on Biological Macromolecules

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

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

(1) The CBM and CommDat submitted a memorandum to the IUCr Executive Committee and proposed a mechanism for making the results of diffraction experiments publicly available. The goal of this action was to achieve better reproducibility of scientific discoveries and ensure that the structures and subsequent publications are of the highest possible quality. A paper that was jointly authored by the editors of all relevant IUCr journals and the Chairs of the Committee on Data and the Commission on Biological Macromolecules that encourages researchers to deposit diffraction images was published in several crystallographic journals [*e.g.* Helliwell, J. R. *et al.* (2019). *IUCrJ*, **6**, 341–343]. Thus, IUCr Journals are taking the lead by encouraging authors to provide a digital object identifier (doi) for their deposited original raw diffraction data when they submit an article describing a new structure or a new method. An extensive discussion of the issues is available in the

following publications: Grabowski *et al.* (2016). *Acta Cryst.* D**72**, 1181– 1193; Kroon-Batenburg *et al.* (2017). *IUCrJ*, **4**, 87–99; Meyer *et al.* (2016). *Nat. Commun.* **7**, 10882; Baker, E. N. (2017). *IUCrJ*, **4**, 1–2; and Grabowski, M. *et al.* (2019). *Struct. Dyn.* **6**, 06430.

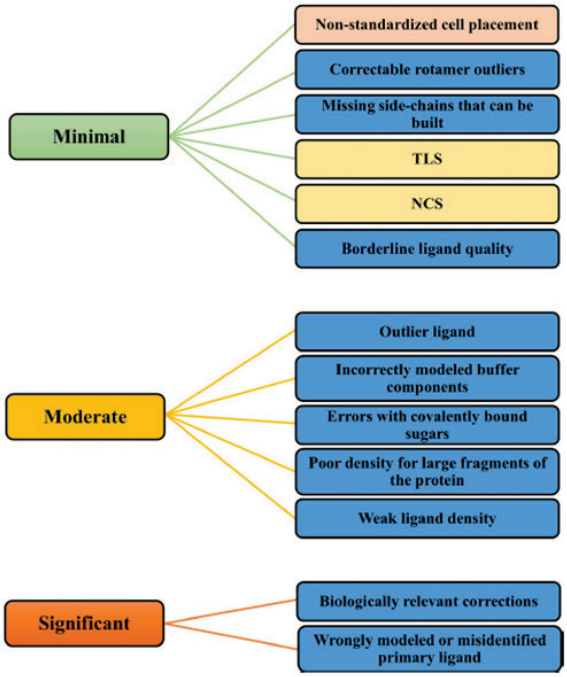
(2) CommDat and the CBM jointly addressed the long-standing and growing issue of deposits that have the phrase `To be published' as their primary citation. As of 12 June 2020, there were over 26,000 such PDB deposits, and over 9,000 deposits have held this status since 2010, *i.e.*, for up to twelve years. When a researcher is working on a similar structure, they may often need additional information that is impossible to get from the PDB deposit alone. It was proposed that every PDB deposit should include the e-mail address of the senior author at their work institution in the metadata. This suggestion has been approved by the wwPDB and awaits full implementation. Currently, the PDB provides the ORCID number, which in some cases has alleviated the problem. More than 30 senior crystallographers, including Nobel Laureates and US National Academy members, supported this initiative.

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

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

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

The Commission members and other interested crystallographers have continued to discuss standards of PDB and data depositions that would help *consumers of the PDB who are not structural biologists* receive information that is easier to understand. The COVID-19 pandemic sped up the process of developing quality standards due to several groups who were carefully watching the quality of COVID-19 related structures [Croll, T. I. *et al*. (2021). *Biophys. J.* **120**, 1085–1096]. A classification of common problems that occur in macromolecular structures can be visualized in the following way [Grabowski, M. *et al.* (2021). *IUCrJ*, **8**, 395–407]:



These problems, which do not represent an exhaustive list, may be difficult or even impossible to correct. Some criteria are case- and resolution-dependent, such as NCS and TLS (indicated in a different color). The classification may depend on who is looking at the structure, *i.e.*, a crystallographer or a biologist. Non-standardized cell placement should be avoided because it makes it more challenging to compare two or more similar structures (also indicated by color) by scientists without a crystallographic background.

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

W. Minor, Chair

A8.5 Commission on Crystal Growth and Characterization of Materials

During the 2017-2019 triennium the composition of the Commission (the CCGCM) did not change with respect to that approved during by the General Assembly at the 24th IUCr Congress in Hyderabad.
Members and consultants of the Commission had the chance to meet three times: in 2017 during the IUCr Congress in Hyderabad, in 2018 in Varna, Bulgaria, during the 6th European Conference on Crystal Growth, and in 2019 in Keystone, Colorado, USA, during the 19th International Conference on Crystal Growth and Epitaxy (ICCGE-19). All the reports of these meetings can be found on the Commission website. Apart from these events, discussion among members was carried out by e-mail. The next Commission meeting will take place during the 25th IUCr Congress in Prague.
The Commission was very active in the organization of the 24th IUCr Congress in Hyderabad. All the microsymposia organized by the Commission at the Hyderabad Congress were quite successful. I would like to thank J. Kumar, R. Mosca, Abel Moreno, S. Cuffini, Jaime Gomez Morales and G. Mezzadri for their enthusiastic efforts in the organization of these sessions. Jim De Yoreo, Affiliate Professor, Materials Science and Engineering, University of Washington, USA gave excellent plenary and keynote lectures.
One of the main tasks for our Commission in the last triennium was to promote crystal-growth-related conferences and schools. This was also done by strengthening further cooperation with the International Organization for Crystal Growth (the IOCG). Many of the CCGCM members/consultants (K. Kakimoto, T. Kuech, J. Wang, A. Moreno and E. Vlieg) are also active within the IOCG.
Of course, the organization of IUCr Congress catalyzed many activities of the Commission and of the crystal growth community. However, other events were organized and supported by the IUCr with the backing of the Commission, in particular the 6th International School on Biological Crystallization (ISBC2017) organized in Granada, Spain, 29 May – 2 June 2017. This event, although not directly organized by the Commission, was organized and supported by many Commission members and consultants.
In 2018 the Sixth European Conference on Crystal Growth and the Second European School on Crystal Growth in Varna, Bulgaria, took place. Many Commission members and consultants were involved in the organization of these events, myself for example, as Co-chair of the School. It has been decided that both the European School and Conference will take place in 2021 in Paris. We are very happy that the tradition of European Crystal Growth Conferences has been established again and together with it also the tradition of European Schools on Crystal Growth.
In 2019, the most important meeting for the crystal-growth community was the 19th International Conference on Crystal Growth and Epitaxy, ICCGE-19, 28 July – 2 August 2019, in Keystone, Colorado, USA. Twenty-four general sessions were

organized. The Conference was successful and well organized, even if the number of participants was lower than in the previous edition. The week before the conference, from 21 to 27 July, the 17th International Summer School on Crystal Growth, ISSCG-17, was held, with the participation of about 100 students. Both the conference and the school were supported by the IUCr. Many members and consultants of the CCGCM were involved in the organization of the conference and the school, but I would like to mention in particular the contribution of Thomas F. Kuech, Chair of ISSCG-17 and member of the CCGCM.

The work of the Commission in 2019 was mainly devoted to the organization of the IUCr 2020 Congress that was to be held in Prague. Our Commission suggested and supported the organization of several microsymposia, including: The Mineral/Life Interface: From Prebiotic Chemistry to Biomineralization and Advanced Biomimetic Materials, co-chaired by Professor García-Ruiz (Spain) and G. Falini (Italy); Facets and Twinning in Bulk Crystal Growth, chaired by Professor Thierry Duffar (France); Applications of Electron Crystallography to Functional Materials; Novel Techniques and Insights into In Vitro and In Situ Crystallization for X-ray and Electron Diffraction, co-chaired by Professor Louisa Meshi (Israel) and Professor Janet Newman (Australia); Layered 2D Type Crystals with Varying Polytypes, co-chaired by Professor Matteo Bosi (Italy); and Frustrated Magnetic Order and Emerging Science, chaired by Professor Geetha Balakrishnan (UK). A keynote speaker was also suggested: Juan Manuel Garcia Ruiz, who was selected.

As part of preparations for the IUCr Congress, the Commission was asked to produce a document about the future trends of crystal growth. Most of the members and consultants contributed to this paper, a revised version of which will be submitted to one of the IUCr journals.

In this triennium the Commission recommended that the IUCr should also support the following conferences and schools (most of them organized by Commission members and consultants):

- Second European School on Crystal Growth (ESCC2), Varna, Bulgaria, 13-16 September 2018;
- 6th European Conference on Crystal Growth (ECCG6), Varna, Bulgaria, 16-20 September 2018;
- 6th International School on Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials (ISC2018), Granada, Spain, 20-25 May 2018;
- 17th International Conference on the Crystallization of Biological Macromolecules (ICCBME17), Shanghai (China), 27-31 October 2018;
- 7th International School on Biological Crystallization (ISBC2019), Granada, Spain, 26-31 May 2019;
- International Summer School on Crystal Growth ISSCG17, Colorado, USA, 21-27 July 2019;
- 2019 Gordon Research Seminar on Crystal Growth and Assembly;
- 19th International Conference on Crystal Growth and Epitaxy (ICCGE-19), Keystone, Colorado, USA, 28 July – 2 August 2019;
- 6th Directionally Solidified Eutectics Conference (DSEC VI), Department of Physics of the University of Salerno in Salerno, Italy, 10-13 September 2019; and
- 7th International School on Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials (ISC2020), to be held in Granada, Spain, 24 –29 May 2020.

Finally, on a personal note, I wish to say that it has been a great pleasure and honor for me to chair the Commission during the period 2014-2017. I believe that promoting understanding of crystal growth is essential for progress in materials science, and I wish the Commission the best in the future challenges.

A. Zappetini, Chair

A8.6 Commission on Crystallographic Computing

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

Activities

(1) Organization of a Computing School as a satellite to the IUCr Congress in Prague in 2021. The planned location was the castle of Nove Hradi (Czech Republic). A list of speakers and a complete programme had been drawn up. Because of the COVID pandemic, the school was postponed to 2021 and is now scheduled as a virtual event for 1-3 September 2021. Most of the speakers are still participating, and a preliminary scientific programme has been prepared. The organizers of the school are Claudia Millán Nebot, Jan Rohlicek and Martin Lutz.
(2) Preparation of microsymposia for the IUCr Congress in Prague. Our representative on the programme committee is Thomas Proffen.
(3) Organization of a Software Fayre at the IUCr Congress in Prague. The Software Fayre is a daily event where developers can present their software. Nearly all the time slots have been filled. Because the Congress has been postponed to 2021, the Software Fayre is being re-planned. The organizers are Claudia Millán Nebot and Martin Lutz.
(4) Members of the Commission contributed to the conferences of the Regional Associates.

M. Lutz, Chair

A8.7 Commission on Crystallographic Nomenclature

The members of this Commission (the CCN) are the editors of the Union's journals and the editors of the volumes of *International Tables*, the Chair of the IUCr/OUP Book Series Committee, the Chair of the Teaching Commission, the Chair of the Committee for the Maintenance of the Crystallographic Information File Standard, and both the IUCr President and General Secretary. The total number of members and appointed consultants is around 50. This number is somewhat unwieldy but there seems to be no good way to reduce it. 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.

(1) *Nomenclature problems*

The Commission's web page invites crystallographers to bring nomenclature problems to the attention of any Commission member. The one matter that came up concerned the definition of screw axes, particularly screw axes (*e.g.*, 5_1, 11_3) that are incompatible with the space groups listed in Vol. A of *International Tables for Crystallography*. This matter arose in connection with an article for the revised edition of the *Brief Teaching Edition of Vol. A* (the BTE). So far only informal discussions between Ulrich Müller (Editor, Vol. A1), Mois Aroyo (Editor, Vol. A and the BTE) and Carol Brock (CCN Chair) have taken place.

(2) *The Online Dictionary of Crystallography (ODC)*

The editor of the ODC is Gervais Chapuis. The CCN is responsible for maintaining this dictionary, which was established in 2006 as a wiki and continues to be run as such, *i.e.*, as a website of definitions that qualified members of the crystallographic community can add to or modify. Snapshots of the ODC were published in paperback form in 2014 and 2017 (*i.e.*, on the occasion of the two most recent IUCr Congresses).

The ODC has never generated much activity even though the IUCr Commissions were charged by the Executive Committee during the 2017 Congress in Hyderabad to provide definitions for their areas of expertise. The ODC still has only 316 definitions, with only a dozen or so having been added in the last three years. At least some of the new definitions were sent to the Editor, who then entered them into the ODC. The number of authors who created new entries or revised existing definitions remained very small.

Some new definitions related to powder diffraction were added in connection with the publication of the new Vol. H of *International Tables for Crystallography*. New definitions are also being generated in connection with development of the new Vol. I on X-ray absorption spectroscopy and related techniques.

In an attempt to increase the number of entries in the ODC, Gervais Chapuis and Carol Brock wrote an article about it that appeared in the first 2019 issue of the *IUCr Newsletter* (see https://www.iucr.org/news/newsletter/etc/articles?issue=141171&result_138339_result_page=13). That article generated a few requests for a permission to contribute but no new definitions.

It is noteworthy that IUPAC is also having problems with its dictionaries (the Color Books, including the Gold Book). The Chair of the CCN is a member of the IUPAC Interdivisional Committee on Terminology, Nomenclature, and Symbols (the ICTNS). That committee has been circulating documents and meeting electronically to set up procedures for adding new definitions to the Gold Book. Considerable time is being contributed to this effort by some of the other ICTNS members but progress has been slow.

(3) *Other*

Four articles related to CCN activities appeared in the 2019 issues of the *IUCr Newsletter*. The article about the Online Dictionary of Crystallography is described above. The intent was to increase interest and activity.

Consultant Massimo Nespolo contributed engaging articles to the 2nd, 3rd and 4th issues of the *IUCr Newsletter*. *The Lattice Sickness Pandemic* discusses the difference between a crystal lattice (a mathematical construct) and a crystal structure (https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=7). *The Super-Sub Schizophrenia* points out that a superstructure is associated with a sublattice rather than with a superlattice (https://www.iucr.org/news/newsletter/etc/articles?issue=143731&result_138339_result_page=9). *Crystallographic Flatland* argues that the widely used adjective low-dimensional should be replaced by subperiodic (https://www.iucr.org/news/newsletter/etc/articles?issue=145052&result_138339_result_page=6). Each of Nespolo's articles was highlighted in the issue's Editorial written by *Newsletter* Editor and CCN Consultant Mike Glazer.

C. P. Brock, Chair

A8.8 Commission on Crystallographic Teaching

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

Overview of activities
Action items from the last report have been addressed, specifically the reorganization and updating of web resources are ongoing and CCT web pages are now current. In addition to the 2017 Zoom meeting, the CCT met via Zoom in December 2020 and April 2021, and communicated regularly via e-mail. Planning is underway on educational and crystallography teaching activities in the age of COVID-19.

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

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

IUCr Congress
The CCT is sponsoring the following sessions at the 2021 Congress:
MS-202 Machine learning in biological and structural sciences
MS-117 Social media and new frontiers for spreading crystallographic
MS-116 Crystallography schools to promote interdisciplinarity in science
MS-205 Online crystallography: tools, apps and web services
Special session: Using crystallography for education during the pandemic

O. A. Asojo, Interim Chair

A8.9 Commission on Crystallography in Art and Cultural Heritage

The Commission members are Gilberto Artioli (Italy) (Chair), Petr Bezdička (Czech Republic), Miguel Delgado (Venezuela), Koen Janssens (Belgium), Izumi Nakai (Japan), Fermin Otalora (Spain), Patrick Ravines (US) and Elena Tereschenko (Russia), and the consultants are C. Abad-Zapatero (USA), J.M. Castera (France), E. Dooryhée (USA), E. Makovicky (Denmark), S. Mande (India), S. Quartieri (Italy), A. Rafalska-Lasocha (Poland), A. Thalal (Morocco) and A. Zürn (Switzerland).

During the triennium, the Commission (CrysAC) continued to pursue the mission of spreading crystallographic knowledge related to artworks and ancient materials.

In 2017, thanks to the work of Gilberto Artioli and Alicja Rafalska-Lasocha, the CrysAC representatives on the International Programme Committee, the programme for the 24th Congress and General Assembly of the International Union of Crystallography in Hyderabad, https://www.iucr2017.org/, featured a plenary lecture by Giacomo Chiari, `Crystallography in art and cultural heritage', and a keynote lecture by Jean-Marc Castera, `Indian geometric patterns, compared to Persian and Moroccan styles', along with four microsymposia: MS-047: Crystalline Materials Characterization with Combined Techniques, chaired by Koen Janssen and Alejandro Ayala; MS-071: Crystallographic Patterns in Art and Cultural Heritage, chaired by Louise De Las Penas and Rima Ajlouni; MS-104: Synchrotron Measurement in Conservation and Cultural Heritage, session prepared by Eric Dooryhee, chaired by Alison Edwards and Gilberto Artioli; and MS-114: Crystallography and Cultural Heritage: From Microsampling to Noninvasive Techniques, chaired by Manfred Schreiner and Serge Cohen.

The CrysAC Commission, in collaboration with Professor Bernardo Cesare (University of Padua), was involved in the preparation of an exhibition Beauty Hidden in Rocks, which accompanied the Congress. The IUCr also prepared some beautiful postcards showing photographs from the exhibition, which were distributed during the Congress.

During the triennium we organized the following four CrysAC workshops:

2nd CrysAC Workshop, Applied Crystallography in the Study of Pigment Degradation, Brno, Czech Republic, 31 May 2017, https://www.alma-lab.cz/eng/conference-programme--invited-speakers.

3rd CrysAC Workshop, Recent Advances in the Investigation of Ancient Mortars and Binders, Mérida, Yucatán, Mexico, 20 May 2018.

4th CrysAC Workshop, CHEMFORS, Pucon, Araucania, Chile, 8-9 November 2018. https://sarx-jfmf-2018.ufro.cl/en/chemfors-sarx-2018/.

5th CrysAC Workshop, The Crystallography of Ancient Metals and Metal Corrosion, Vienna, 17 August 2019, https://ecm2019.org/satellites/crysac/.

CrysAC also co-organized two international scientific conferences:

6th ALMA Conference in Brno, 1-2 June 2017 (P. Bezdička, G. Artioli, A. Rafalska-Lasocha and Koen Janssens), https://www.alma-lab.cz/userfiles/files/ALMA2017_final_programme.pdf.

7th Meeting X-ray and Other Techniques in Investigation of the Objects of Cultural Heritage, Krakow, 17-19 May 2018, http://www.biurokarier.chemia.uj.edu.pl/conf/x-ray18.

In May 2019, Jose-Miguel Delgado and Petr Bezdička participated in the meeting Current Trends and Future of Crystallography in Chemistry, Physics, Biology and Materials Science as representatives of the CrysAC Commission. This workshop was organized to prepare the scientific programme of the 25th General Assembly and Congress of the IUCr in Prague. As a result, it was decided that the CrysAC Commission will organize (1) or co-organize (2) microsymposia during the Congress: Global Cultural Heritage Challenges and Crystallography: Where Do We Stand?, co-chaired by Dr Alicja Rafalska-Łasocha; X-ray Spectrometry and X-Ray Diffraction in Art and Archaeology, co-chaired by Dr Petr Bezdička; and Science Meets Art: Crystallography and Cultural Heritage.

Jean-Marc Castera delivered six lectures and workshops on geometric art in India in 2017 and five lectures and workshops on geometric art in Iran in 2018.

Koen Janssens (University of Antwerp, Belgium) delivered a Public Lecture during the European Crystallographic Meeting ECM32: `Examining old paintings with new X-ray methods: A fresh look at and below the surface'.

Petr Bezdička attended the Jahrestagung `Archäometrie und Denkmalpflege 2019' AK Archäometrie der GDCh in Vienna, Austria, and presented an invited talk `The role of laboratory X-ray diffraction techniques in the provenance analysis of historical paintings'.

Gilberto Artioli delivered a series of lectures: (1) March 2017, Archeometria: La materialità della storia umana. `Scienza e tecnica nell'Antropocene – Rischi e benefici' Accademia Nazionale delle Scienze detta dei XL, Orto Botanico, Università di Padova; (2) July 2017, Metallurgy in the Copper Age. `Nights of Archaeology'. Museo Archeologico, Massa Marittima; (3) October 2017 `Tools, weapons, money: metals in human history'. TeRRRa: Risorse, Rischi, Rispetto. QuarantaScienza Scienziati online. Accademia Nazionale delle Scienze XL, Roma; (5) July 2018 `The contribution of geosciences to cultural heritage investigations', Materials Research Laboratory, Univerza v Novi Gorici, Ajdovščina, Slovenia; (6) August 2018, `Technical advances in cultural heritage analysis: potential and needs', Istituto Italiano di Cultura, Sydney, Australia. Round Table `Science and technology for cultural heritage'; (7) August 2018 `Crystallography and cultural heritage: science and passion', Istituto Italiano di Cultura, Melbourne, Australia; (8) November 2018, `Ancient metals provenancing', Université Paris 1 - Panthéon-Sorbonne, UFR d'Histoire de l'Art et d'Archéologie, Paris, France; (9) December 2018, `Materials science for cultural heritage', VI Giornata di Formazione `Geologia e geofisica applicate ai beni culturali', Rovereto, Fondazione Museo Civico Rovereto, Italy; (10) June 2019, `Blue colour from lapislazuli to Klein', Open Workshop `Colour in science', Dipartimento di Beni Culturali, Università di Padova; (11) Invited talk at the Mineralogical Society of America Centennial (1919-2019) Symposium, `Modern mineralogy and ancient pots: The archaeometry of ceramics', Carnegie Institution for Science Building, Washington, DC, 20-21 June 2019, https://youtube/Kv9mK7bKxWU.

Elena Tereschenko helped organize a number of events in Russia aimed at the formation and consolidation of the humanitarian and natural-science community in the field of cultural heritage research: (1) Intermuseum International Festival (in 2017 and 2019, Moscow), including the seminar `Principle of the convergence of sciences in museum practice' (May 2019), (2) microsymposium Natural-Scientific Methods in the Study of Cultural Heritage at the 7th European Conference on Neutron Scattering ECNS 2019 (July 2019, St Petersburg), (3) session `Interdisciplinary research and natural-scientific methods of studying history: new opportunities for historians' at the First International St Petersburg Historical Forum (October 2019, St Petersburg), (4) Users Meeting of the Kurchatov synchrotron-neutron complex of research (November 2017), as well as a number of specialized seminars and meetings held at the Institute of Archaeology, Russian Academy of Sciences, State Historical Museum *etc*. As part of the development of the lifelong education system for children, special courses were

organized at the international children's center `Artek' under the programme `Physics and Art' (2019) and scientific Saturdays at the Kurchatov Institute (2019).

Members and consultants of the Commission contributed to many publications during the triennium, including a chapter *Powder diffraction in art and archaeology* in *International Tables for Crystallography* [Artioli, G. (2019). *International Tables for Crystallography*, Volume H, ch. 7.4. ISBN: 978-1-118-41628-0, doi: 10.1107/97809553602060000115] and the article *CrysAC activities towards a crystallography-based knowledge of archaeometry and conservation* [Artioli, G., Cotte, M., Delgado, M. & Rafalska-Lasocha, A. (2019). *Materials Structure*, **26**, 94-96].

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

G. Artioli, Chair, and A. Rafalska-Lasocha, past Secretary

A8.10 Commission on Crystallography of Materials

Our Commission was formally approved by the General Assembly of the IUCr in Hyderabad (August 2017). The members of the Commission are Changqing Jin (Chair, China), B. Albert (Germany), E. Antipov (Russia), Wenhui Duan (China), V. Blatov (Russia), M. Eremets (Germany), Y. Gogotsi (USA) and M. Petrukhina (USA), and the consultants are Tian Cui (China), V.L. Solozhenko (France), A.R. Oganov (USA), H. Maynard-Casely (Australia), O. Yaghi (USA), S. Qiu (China), Nan Zhang (China) and Y. Sugawara (Japan). The Commission website is at https://www.iucr.org/iucr/commissions/crystallography-of-materials.

Conferences and symposia

The 26th International Conference on High Pressure Science & Technology (AIRAPT 26), joint with the 8th Asian Conference on High Pressure Research (ACHPR 8) and the 19th China High Pressure Research (CHPC 19), Beijing, China, 19-23 August 2017 (http://www.airapt26.org/). Conference Chair: Changqing Jin. Number of participants: 800-900.

International Symposium of New Emergent Materials at Extreme Conditions, joint with the National Conference on Crystallography of China, Tianjin, China, 25-28 September 2018 (http://uhp.iphy.ac.cn/2018iucrcm/). Conference Chair: Changqing Jin. Number of participants: ~80.

The 2nd International Fusion Conference `From Carbon Rich Molecules to Carbon-Based Materials', The Bahamas, 7-10 June 2018. Conference Chair: M.A. Petrukhina. Number of participants: ~70.

Workshop on Crystal Structure Prediction: Exploring the Mendeleev Table as a Palette to Design New Materials, Grignano, Trieste, Italy, 14-18 January 2019. Organizer: Artem Oganov. Number of participants: ~60.

17th USPEX Workshop, Rennes, France, 4-6 July 2019. Conference Chair: Artem Oganov. Number of participants: ~70.

Symposium of China Materials Research Society, Chengdu, China, 10-14 July 2019, https://cmc2019.medmeeting.org/newsinfo/23414. Conference Chair: Changqing Jin. Number of participants: ~80.

MXene Conference 2020, 3-5 August 2020, https://mxeneconference.coe.drexel.edu. Conference Chairs: Michel Barsoum, Yury Gogotsi. 2400 registered participants (online).

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

25th IUCr Congress, Prague, Czech Republic (postponed to 2021), http://www.xray.cz/iucr/. Conference Chair: Radomír Kužel. Number of participants: >1000.

Organization of workshops to disseminate knowledge and technical skills

Workshops on computational materials discovery, Poitiers, France, 11-13 January 2017, organizer Artem Oganov, No. of participants: ~35; and Shanghai, China, 16-20 June 2017, organizer Artem Oganov, No. of participants: ~90.

Workshops on crystal structure prediction, Skoltech, Moscow, Russia, 17-19 September 2018, organizer Artem Oganov, No. of participants: ~70; and Tianjin, China, 24-26 September 2018, organizer Artem Oganov, No. of participants: ~70.

Computational Materials Science Program of Excellence, Skoltech, Moscow, Russia, 7-8 September 2019. Organizer: Artem Oganov. Number of participants: ~70.

19th ONLINE USPEX Workshop: Crystal structure prediction with the USPEX code, 11-13 November 2020. Organizers: Vladimis S. Baturin and Artem R. Oganov. Number of participants: >200 researchers worldwide.

Three week-long online courses on MXenes (last weeks of July 2020, February 2021 and March 2021 to about 60 participants in each session), https://nano.materials.drexel.edu/mxene-course/. Organizer: Yury Gogotsi; ten instructors from Drexel University lectured. Number of participants: 180.

Changqing Jin, Chair

A8.11 Commission on Electron Crystallography

During 2017-2019 a major increase in the number of publications in our field was noted and interest in electron crystallography as a tool for structure solution of any crystalline matter (inorganic, organic and biological) has increased. This is seen in an increasing number of microsymposia, conferences and schools with large numbers of attendees, as reported here. Each item denotes an activity that members and/or consultants of Commission on Electron Crystallography (CEC) have organized, sponsored or were involved in. The wide geographic spread of our activities is an important achievement.

2017

- 24th Congress and General Assembly of the IUCr (Hyderabad, India). Prior to the Congress, the CEC organized a satellite workshop on Electron Diffraction for Materials Science and Pharmaceutical Applications (sponsored by Nanomegas), in which several of the CEC consultants were involved. The Gjønnes Medal in Electron Crystallography was awarded to Professors Richard Henderson and Nigel Unwin. Subsequently Professor Henderson and co-workers were awarded a Nobel Prize.
- At the annual meeting of the Brazilian Society of Microscopy and Microanalysis in Búzios, RJ, Brazil, 4-7 June 2017, courses on electron diffraction and electron back scattered diffraction (EBSD) as well as symposia on electron diffraction mapping in materials characterization in SEM and TEM were held.
- Professors Lukas Palatinus and Damien Jacob organized and participated in the electron diffraction session of the Quantitative Electron Microscopy European School in 2017 (QEM2017, Balaruc-les-bains, France), 21 May - 2 June 2017. The school was attended by 98 students and 33 lecturers.
- Professor Joke Hadermann was a speaker at the International Autumn School on Fundamental and Electron Crystallography (IASFEC), 8-13 October 2017, Sofia, Bulgaria, organized by the Commission on Mathematical and Theoretical Crystallography.
- Professor Joke Hadermann was also involved in the organization of the biannual EMAT Workshop on Transmission Electron Microscopy, where they gave classes on electron diffraction (12-23 June, University of Antwerp, Antwerp, Belgium).
- Professor Xiaodong Zou and colleagues organized an International Symposium on Cryo-EM - Past and Future Challenges on 9 December in Stockholm, Sweden. The speakers include pioneers in cryo-EM and microED, present/former collaborators of the Nobel Laureates, and young researchers in the field. There were 120 participants.
- The K. H. Kuo School in 2017 was held in Xi'An, China, 30 May - 2 June. Professor Xiaoadong Zou attended the school and gave a talk.
- At the 2017 ACA meeting in New Orleans, USA, Professors Jim Ciston and Olaf Borkiewicz organized a symposium on Electron Diffraction of Solid-State Materials. There were 30-40 participants.
- Professor Gianluigi Botton was involved in the organization of the 9th Advanced Electron Microscopy School and a one-day Advanced Microscopy Methods for Materials Research workshop at the Canadian Centre for Electron Microscopy, Hamilton, Canada. The workshop had over 100 participants.

2018

- The 51st Course of the International School of Crystallography: Electron Crystallography, 1 - 10 June 2018, Erice, Italy, was directed by Professors Lukas Palatinus (member of the CEC) and Joke Hadermann (consultant of the CEC). The course had 74 participants. In addition, the vast majority of CEC members and consultants participated as lecturers.
- A two-day UK-Israel Workshop on Nano-Scale Crystallography for Bio and Materials Research on 18-19 June was held at Tel Aviv University, Israel. It was supported by the CEC, and the Chair of the CEC as well as some members and consultants of the CEC (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 plenary lecture, Professor Joke Hadermann (consultant of the CEC) gave a keynote lecture and three microsymposia on different electron crystallography related subjects were held.
- The 2018 Kuo Symposium on 3D-EM of Macromolecules and Cells and The 11th K. H. Kuo Summer School on Electron Microscopy & Crystallography were held in Zhejiang University, which houses a newly established state-of-the-art cryo-EM facility for structural studies of macromolecules and cells. It was fully supported by the CEC.
- 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 around 60 participants.

- A Workshop on Cryo-Electron Microscopy was held at the ACA meeting in Toronto.

2019

- In August 2019, *Acta Crystallographica Section B* published a special issue on electron crystallography containing reviews and original papers. This issues' Guest Editors were Professors Joke Hadermann and Lukas Palatinus, who are active members of the CEC and the IUCr.
- At the Microscopy and Microanalysis 2019 conference held in Portland, USA, in August, the X-13 workshop Modern Electron Crystallography for Materials Sciences and Biology was organized by Professors Sergei Rouvimov, Roberto Reis and Peter Moeck (member of the CEC). Approximately 50 participants attended the workshop.
- Professor Xiaodong Zou (member/consultant of the CEC) and Dr Hongyi Xu (member of the ECA's SIG4 on electron crystallography) gave lectures at the eBIC MicroED Workshop at the Diamond Light Source, UK, 6–8 November 2019. There were 20-30 participants.
- Drs Tom Willhammar and Hongyi Xu (both members of the ECA's SIG4) gave lectures at the Electron Diffraction Workshop at the NTNU in Trondheim, Norway, 15-16 May 2019, with approximately 20-30 participants.
- Professor Karla Balzuweit (member of the CEC) organized the 1st Electron Crystallography School in Brazil, 14-17 January, at the Universidade Federal de Minas Gerais, Brazil. The school had 31 attendees.
- Professor Lukas Palatinus (member of the CEC) organized the 37th *ad hoc* Workshop on *Jana2006* - Electron Diffraction, 2-3 December, at the Institute of Physics, Prague, Czech Republic. The workshop had 20 attendees.

L. Meshi, Chair

A8.12 Commission on High Pressure

Members: Haozhe Liu (Chair, People's Republic of China), Narcizo Marques Souza-Neto (Brazil), Boris A. Zakharov (Russia), Natalia Dubrovinskaia (Germany), Nandini Garg (India), Kamil Filip Dziubek (Italy), Stephen Moggach (Australia), Yasuo Ohishi (Japan), Jean-Paul Itie (France) and Guoyin Shen (USA).

Consultants: Ross Angel (Italy), Stefan Klotz (France), Amy Lazicki (USA), Malcolm I. McMahon (UK), John B. Parise (USA) and Andrzej Katrusiak (Poland).

The role of the Commission on High Pressure (CHP) in this multidisciplinary and dynamically evolving field is to facilitate and enable the efficient exchange of new ideas and cutting-edge developments worldwide. The main activities available to the CHP to achieve these goals are annual workshops on high-pressure crystallography. The CHP also helps to shape a strong high-pressure programme at the triennial IUCr Congresses. In addition, Commission members and consultants are involved in organizing summer schools for high-pressure crystallography, and in other dedicated meetings for high-pressure science and techniques. Our activities in each year of the quadrennium are listed below.

2017

The main event in 2017 was the 24th Congress and General Assembly of the IUCr at Hyderabad, India, 21-28 August. The CHP was represented on the International Programme Committee by Professor Andrzej Katrusiak. The following keynote lecture and microsymposia were sponsored by the CHP:

Keynote lecture: `Progress in high-pressure methodology and applications', presented by Jon Eggert, Lawrence Livermore National Laboratory, USA.

MS023: Synchrotron and XFEL for Materials at Ambient and Extreme Conditions (Chairs: Yasuo Ohishi and John Tse).

MS060: XAS at Extreme Conditions (Chair: Giuliana Aquilanti).

MS078: Advances in High Pressure Crystallographic Methods (Chairs: Goutam Dev Mukherjee and Kamil Dziubek).

MS119: Interactions in Solids Under Stress (Chairs: Boris Zakharov and Shanti Deemyad).

The new Commission members and consultant who were present in Hyderabad (Haozhe Liu, Boris Zakharov, Narcizo Marques De Souza-Neto, Jean-Paul Itie, Andrzej Katrusiak and Kamil Filip Dziubek) held a closed lunchtime meeting during the Congress, and discussed the mission of and future activities and challenges for the CHP.

Two major conferences organized by current and previous chairs of this Commission were held in 2017:

Haozhe Liu co-chaired the 26th International Conference on High Pressure Science and Technology (AIRAPT-26), which was held in Beijing, China, 19-23 August, and reached a record high attendence of 983. The Bridgman Gold Medal Award winner was Mikhail Eremets (Max Planck Institute for Chemistry, Germany) and the Jamieson Award winner was Philip Dalladay-Simpson (HPSTAR, China).

Andrzej Katrusiak chaired the 55th European High-Pressure Research Group Meeting (EHPRG-55), which was held at Poznan, Poland, 3-8 September, with 220 attendees from 26 countries.

2018

We had an informal meeting during Gordon Research Conference for High Pressure at Holderness, NH, USA, on 20 July 2018. Four CHP Commission 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 CHP took place in Honolulu, USA, 29 July - 2 August, at the Ala Moana Hotel. 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.

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-hour hands-on practical tutorial sessions.

The main workshop event was attended by 104 participants from 16 countries, and included four full days of programme, organized into nine scientific sessions, featuring a total of 52 session talks. 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, one special session, `Women under high pressure', was added to the agenda one evening, and many participants expressed support for this.

Five CHP Commission members, Haozhe Liu, Kamil Dziubek, Amy Lazicki, Guoyin Shen and Andrzej Katrusiak, attended this workshop and met on 1 August 2018. The Chair of the CHP, Haozhe Liu, briefly introduced the history of the IUCr and the history of CHP workshop 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 efforts on data formats during the workshop.

2019

We had an informal meeting during the AIRAPT Conference in Rio, Brazil, on 6 August 2019. Six CHP committee members, Haozhe Liu, Kamil Dziubek, Guoyin Shen, Jean-Paul Itie, Narcizo Souza-Neto and Andrzej Katrusiak, met and briefly exchanged ideas for future workshop bidding *etc*.

The 2019 workshop of the IUCr Commission on High Pressure took place in Vienna, Austria, 13-17 August 2019. The Chair of the Local Organizing Committee was Professor Ronald Miletich-Pawliczek from the University of Vienna, who was one of the local hosts for the 32nd European Crystallographic Meeting (ECM), 18-23 August 2019. This was first time we have had a back-to-back arrangement for the CHP workshop and the ECM. Workshop participants had the opportunity to join talks and lectures in other satellite workshops held in the same building (the Faculty of Electrical Engineering and Information Technology, Vienna Technical University). This workshop was jointly organized by the Commission (chaired by Haozhe Liu) and the European Crystallographic Association (ECA) Special Interest Group SIG-11 (chaired by Dr Yaroslav Filinchuk).

The workshop was attended by over 50 participants from 15 countries and regions, and included three full days of programme, organized into nine scientific sessions, featuring a total of 35 talks. The three plenary talks were presented by Dr Eva Zurek (State University of New York at Buffalo, USA), Dr Stewart McWilliams (University of Edinburgh, UK) and Dr Takanori Hattori (J-PARC Center, Japan). The poster session featured 11 short lighting talks in the afternoon of 14 August, right before the poster presentations.

Five Commission members, Haozhe Liu, Kamil Dziubek, Amy Lazicki, Boris Zakharov and Yasuo Ohishi, attended this workshop and acted as session conveners or session chairs. The Commission members who were present met on the evening of 14 August 2019, and discussed future workshop bidding *etc*.

Other activities: Commission member Dr Narcizo Souza-Neto organized a workshop on PRESSYNC: Synchrotron Techniques under High Pressure, held 31 July – 2 August 2019 at the Brazilian Synchrotron Light Laboratory, Campinas, Brazil. Commission members Haozhe Liu, Kamil Dziubek and Jean-Paul Itie joined this workshop and delivered invited talks. At the end of this workshop, the local organizers hosted a facility tour of the high pressure lab and the dedicated high pressure beamline at Sirius, the new Brazilian synchrotron light source.

As Commission representative, Haozhe Liu attended the workshop on Current Trends and Future of Crystallography in Chemistry, Physics, Biology and Materials Science in Prague, Czech Republic, 14-16 May 2019. This workshop was organized by the International Programme Committee in preparation for the 25th Congress of the IUCr, and it summarized the main topics of modern crystallography represented by every IUCr Commission.

2020

In July 2020, three Commission members, Haozhe Liu, Kamil Dziubek and Boris Zakharov, held a long Zoom meeting with Professor Elena Boldyreva, the Chair of the local organizing committee for the 2021 IUCr High Pressure Workshop. After

discussions of all the possibilities including hybrid modes, the Commission members decided to hold the upcoming workshop via Zoom meeting from Novosibirsk, Russia, in February 2021.

Despite the lack of the regular workshop organized by the Commission in 2020 because of the international travel ban, two small related workshops/summer schools were held:

(1). Commission member Professor Natalia Dubrovinskaia organized the IUCr/DGK (German Society of Crystallography) International Summer School on Novel Methods of Atomic and Electronic Structure at High Pressure at Bayreuth, Germany, 31 August – 4 September 2020. This school was attended online via Zoom by 25 participants from seven countries, and co-organizers included Dominique Laniel, Thomas Meier and Leonid Dubrovinsky.

(2). Commission consultant Professor Andrzej Katrusiak organized The 13th Frolic Goats Workshop on High Pressure Diffraction at Poznan, Poland, 19-21 April 2020. This was part of a continued effort from Professor Katrusiak's group with the primary goal of disseminating practical skills, allowing newcomers to perform high pressure experiments in an X-ray lab and outlining possibilities for further studies at dedicated high pressure beamlines at synchrotrons and neutron sources worldwide.

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

H. Liu, Chair

A8.13 Commission on Inorganic and Mineral Structures

This report summarizes the activities of the Commission (CIMS) during the period 2017-2021.

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) and N. Zubkova (Russia). Consultants: K. Byrappa (India), C. Cahill (USA), R. Carbonio (Argentina), G. Ferraris (Italy), T. Gesing (Germany), S.V. Krivovichev (Russia), C. Ling (Australia), D. Pandey (India), J.B. Parise (USA), I. Pignatelli (USA), J. Rocha (Portugal) and M. Welch (UK).

Upon its establishment at the Geneva Congress in 2002, CIMS was founded to promote and achieve the following aims:

- To strengthen links and interactions among mineral, inorganic and materials scientists and between these scientists and the crystallographic community.
- To promote the presence at the IUCr meetings of scientists working in `inorganic-crystallographic' and `geoscience-crystallographic' institutions.
- To present at the same meetings common aspects of the inorganic structures independently from their natural or synthetic origin.
- To favour the historical influence that mineral structures have played on developing inorganic materials of technological interest.
- To promote and encourage the publication of inorganic and mineralogical papers in the journals of the Union.
- To promote the development and dissemination of methods, computing programs and databases of interest for the inorganic crystallographic community.
- To promote and organize symposia of interest to the inorganic community on the occasion of the IUCr meetings, also in cooperation with other Commissions.
- To promote and organize workshops and schools of interest to the inorganic community, also in cooperation with other Commissions.

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

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

CIMS also maintains strong links with the new Commission on NMR Crystallography and Related Methods, with J. Rocha the liaison person and also consultant for that Commission.

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

Strong links exist between CIMS and the European Crystallographic Association: Frédéric Hatert (CIMS member) was a representative for ECM32 (https://ecm2019.org/home/), Marie Colmont (CIMS member) was Chair, and Sergey V. Krivovichev (CIMS consultant) was Co-chair.

There are very good relationships between CIMS and the European Mineralogical Union (EMU, http://eurominunion.org/); R. Oberti is a member of CIMS and was also Commissioning Editor of the *EMU Notes in Mineralogy* until January 2021.

Sergey Krivovichev served as President of the IMA in 2015–2016.

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

In 2019, 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). C. Ling is a member of the Australian Synchrotron's User Advisory Committee and BRIGHT Advisory Committee, and a member of the Australian National Committee for Crystallography (ANCCr).

P. Mercier was Chair of the Canadian National Committee for Crystallography from August 2015 until December 2020.

R. Oberti was Chair of the Committee on the participation of CNR (Consiglio Nazionale delle Ricerche) in the IUCr until the end of 2018, and is presently a member of the same Committee until the end of 2022.

P. Mercier (CIMS) represented CIMS interests at the International Programme Committee meeting for the upcoming IUCr Congress, which was held in May 2019 in Prague, Czech Republic.

Co-organization of scientific meetings/conferences and special publications

The following meetings, conferences and special publications have been proposed/organized by CIMS members and/or consultants. The activities of members and/or consultants of CIMS as organizers/conveners/lecturers are indicated.

(1) C. Ling (CIMS consultant) was Chair of Crystal-33, the 33rd meeting of SCANZ, held in early 2020.

(2) R. Oberti (CIMS member) was Co-editor (with Gilberto Artioli) of the volume *The Contribution of Mineralogy to Cultural Heritage*, *EMU Notes in Mineralogy*, Vol. 20 (2019), 448 pp., published by the European Mineralogical Union and the Mineralogical Society of Great Britain & Ireland. ISSN: 1417 2917; ISBN: 978-0903056-61-8.

(3) R. Oberti was a member of the scientific committee for the 2019 EMU School Naturally Occurring Asbestos (NOA): From Geological to Medical Aspects, Casale Monferrato, Italy, 9-13 September 2019.

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

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

(6) 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.

(7) J. Rocha (CIMS consultant, past Chair) was involved in the organization of SMARTER6, Ljubljana, Slovenia, 2-6 September 2018 (https://smarter6.ki.si/index.php/committees/).

(8) M. Nespolo (CIMS member) was Ambassador at the 22nd Meeting of the International Mineralogical Association (13-17 August 2018, Melbourne), and main convenor of the session on Modular Aspects of Mineral Structures (co-convenors Isabella Pignatelli and Sergey Krivovichev, both CIMS consultants).

(9) 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 insufficient registrations, the workshop did not take place.

(10) J. Rocha (CIMS consultant, past Chair) was involved in the organization of the SMARTER5 meeting in Bayreuth, which for the first time was held as a satellite meeting of the 30th Meeting of the European Crystallographic Association (http://www.smarter5.uni-bayreuth.de/de/index.html). This event was promoted jointly by CIMS and the Commission on NMR Crystallography and Related Methods.

(11) R. Oberti (CIMS member) was a member of the scientific committee of the 2017 EMU School Mineral Fibers: Crystal-Chemistry, Chemical Physical Properties, Biological Interactions and Toxicity, held in Modena, Italy, 19-23 June 2017, http://emu2017.unimore.it. The school received support from the IUCr after CIMS sponsorship.

(12) The volume *Mineralogical Crystallography*, co-edited by J. Majzlan, Sergey Krivovichev (CIMS consultant) and J. Plasil, was published in 2017 by the EMU.

CIMS support of applications for financial funding by the IUCr, or 'moral' support

(1) American Crystallographic Association Annual Meeting 2019, 20-24 July 2019, Cincinnati, Ohio, USA.
(2) XIX International Meeting on Crystal Chemistry, X-ray Diffraction and Spectroscopy of Minerals, 2–5 July 2019, Apatity, Russia.
(3) 17th European Conference on Solid State Chemistry (https://ecssc17.com/), 1–4 September 2019, Université de Lille, France.
(4) 17th European Powder Diffraction Conference (EPDIC17) (https://www.epdic17.org/), 26–30 May 2019, Šibenik, Croatia.
(5) Sixth SMARTER Crystallography Conference, 2–6 September 2018, Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia.
(6) The 4D Workshop: Deep-Time Data-Driven Discovery and the Evolution of the Earth, 4-6 June 2018, Carnegie Institution for Science in Washington DC, USA. https://www.4d-workshop.net/.
(7) Gordon Research Conference 2018: Crystal Engineering, 24-29 June 2018, Newry, Maine, USA. https://www.grc.org/crystal-engineering-conference/2018/.

P. H. J. Mercier, Chair

A8.14 Commission on Magnetic Structures

Following the Montreal Congress in August 2017, the voting members of the Commission are Branton Campbell (Chair, USA), Maxim Avdeev (Australia), Maria Teresa Fernandez-Diaz (France), Ovidu 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). The Commission's consultants are: Mois Aroyo (Spain), Javier Campo (Spain), Daniel Litvin (USA), Alexander Pirogov (Russia) and Wieslawa Sikora (Poland). Following the Congress in Hyderabad, it was decided that in the coming term J. Manuel Perez-Mato would serve as Secretary of the Commission, Danny Litvin would continue to serve as liaison to the Commission on Nomenclature and Maria-Teresa Fernandez-Diaz would continue to serve as liaison to the Commission on Neutron Scattering.

53rd International School of Crystallography

The Commission organized and conducted the 53rd course of the International School of Crystallography at the Ettore Majorana Research Foundation in Erice, Italy, on the subject of Magnetic Crystallography (https://crystalerice.org/2019/welcome.php), during the ten days from 31 May to 9 June 2019.

Commission members who participated in organization and/or lectures and workshops:
Branton Campbell (Brigham Young University, USA) – Science Director
Maria Teresa Fernandez-Diaz (Institut Laue-Langevin, France) – Science Director
Manuel Perez-Mato (Unversidad del Pais Vasco, Spain) – Science Director
Maxim Avdeev (ANSTO Australian Center for Neutron Scattering, Australia)
Ovidiu Garlea (ORNL Neutron Scattering Division, Oak Ridge, USA)
Margarida Henriques (CAS Institute of Physics, Prague, Czech Republic)
Vaclav Petricek (CAS Institute of Physics, Prague, Czech Republic)
Juan Rodriguez-Carvajal (Institut Laue-Langevin, Grenoble, France)
Taku Sato (Tohoku University, Tohoku, Japan)
Andrew Wills (University College London, London, UK)
Oksana Zaharko (Paul Scherrer Institut, Villigen, Switzerland)
Others who contributed lecture and workshop presentations:
Laurent Chapon (Diamond Light Source, Didcot, UK)
Luis Elcoro (University of the Basque Country, Bilbao, Spain)
Oscar Fabelo (Institut Laue-Langevin, Grenoble, France)
Dmitry Khalyavin (RAL ISIS Facility, Didcot, UK)
Harold Stokes (Brigham Young University, Provo, USA)
Robert Von Dreele (ANL Advanced Photon Source Argonne, USA)

The local organizing team was led by Annalisa Guerri (University of Florence, Italy) and Paola Spadon (University of Padova, Italy), and included computing and technical support from Andrea Giaccherini (University of Florence, Italy), Andy Stewart (University of Limerick, Ireland) and Erin Davis (USA).

The school was advertised internationally, with a special emphasis on reaching out to researchers in countries that are not typically well represented at such meetings. There were no restrictions on geographical affiliations of the participants. From among the roughly 100 applicants, 64 participants (not including the presenters) were selected based on their preparation and

ability to benefit from attendance; this was the maximum number that facility-space limitations allowed. The participants and presenters came from 25 different nationalities and country affiliations, more than half of which were outside of Western Europe or North America. There were significant numbers from each of Russia and Eastern Europe, Asia, South America and India. More than one third of the attendees were women.

The magnetic-crystallography programme was organized to address key advances in magnetic-structure research, as well as the foundational and state-of-the-art theoretical, experimental and computational capabilities that made these advances possible. The school included a roughly 50/50 combination of lectures and hands-on workshops. Three hours of workshops were held each morning, with two sessions conducted in parallel. The state-of-the art computational tools represented in the workshops included *FullProf*, *JANA 2006*, *SARAh*, the Bilbao Crystallographic Server, the ISOTROPY Software Suite, *GSAS-II*, and *TOPAS*. Both introductory and advanced tutorial exercises were provided, in order to fully engage beginners and experts alike. Three hours of lectures were presented each afternoon. Topics included the experimental determination and communication of magnetic structures, the theoretical and mathematical foundations of magnetic symmetry and representational analysis, and a wide variety of applications. Each of the 17 presenters, in addition to contributing a lecture, also provided lecture notes in manuscript form. The technical programme ended with a one-hour panel discussion of questions submitted by the participants.

Of 40 submitted participant abstracts, ten were selected for oral presentations (22 minutes or 15 minutes), including Shivani Sharma (JNCASR, Bengaluru, India), Anna Matveeva (Petersburg Nuclear Physics Institute, Gatchina, Russia), Jose Luis Garcia-Munoz (ICMAB-CSIC, Barcelona, Spain), Stephanie Gneuwuch (University of Maryland, USA), Anuradha Vibhakar (University of Oxford, UK), Elena Solana Madruga (University of Edinburgh, UK), Stefanie Siebeneichler (Stockholm University, Sweden), Fernando Pomiro (University of Warwick, UK), Claire Colin (Institut Néel, University of Grenoble-Alpes, France) and Francoise Damay (Laboratoire Léon Brillouin, Gif-sur-Yvette, France). The two poster sessions for participant research were also of very high quality and were well attended during the school. Three of these posters were selected by a panel of judges for awards, which were presented during the closing ceremony to Premakumar Yanda (JNCASR, Bengaluru, India), Rebecca Scatena (University of Bern, Switzerland) and Guru Khalsa (Cornell University, USA).

To facilitate interaction between and among the participants and presenters, the school included a rich social programme. In the relaxed atmosphere, the organizers attempted to become personally acquainted with each participant. We are confident that the school initiated many long-term friendships and collaborations.

Preparations for the IUCr Congress in Prague

In preparation for the IUCr Congress in Prague, the Commission met online to brainstorm, select and prioritize potential topics. Then, in May 2019, Oksana Zaharko, our representative to the International Programme Committee (IPC), travelled to Prague to negotiate the final programme. Oksana's outstanding efforts and negotiation skills made it possible to organize 15 sessions with magnetic-structure themes or components, among which nine microsymposia and three keynote lectures were sponsored or co-sponsored by the Commission (listed below). Oksana's invaluable service on the IPC is greatly appreciated by all.

Methods and Software Developments for Magnetic-Structure Analysis (MS-22)
Magnetic Structures of Novel and Functional Materials (MS-30)
Topological Magnetic Order and Quasiparticles (MS-87)
Magnetic Structures at Extreme Conditions and in Extreme Samples (MS-61)
Symmetry Aspects of Magnetic Order and Magnetic Properties (MS-68)
Frustrated Magnetic Order and Emerging Science (MS-45)
Molecular Magnets and Metal-Organic Frameworks, Including Quantum Crystallography Approaches (MS-51)
Structural, Electronic and Magnetic Ordering: From Fundamental Physics to Functionality (MS-38)
New Applications of Coherent Scattering (MS-40)
The Science of Symmetry Breaking, Harold Stokes (KN-35)
Quantum Crystallography and Spintronic Materials, Piero Macchi (KN-15)
Dithiadiazolyl Radicals as Building Blocks for Molecular Magnetic Materials (KN-12)

For the IPC meeting in Prague, Oksana, together with B.J. Campbell, J.M. Perez-Mato and T. Sato, submitted a manuscript on *Magnetic Structure Research, Future and Future Trends*, which was subsequently published in *Materials Structure* (2019), **26**(2), 97-100 (http://www.xray.cz/ms/bul2019-2/cms.pdf).

In early 2019, the Commission advertised the IUCr Congress actively and widely within various magnetic-structure research communities, with special emphasis placed on identifying researchers in developing nations. Because the Congress was postponed for a year owing to the COVID-19 pandemic, this advertising thrust was repeated again in early 2020.

Standard development

The magCIF working group actively discussed a variety of revisions to the standard magCIF dictionary that was developed by the Commission in previous years: (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. (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 regarding the development of extended CIF standards for the communication of magnetic structures, the Commission began work on the symmetry-mode CIF (smCIF) dictionary, which will standardize the concise and unambiguous description of magnetic and other symmetry-lowered crystal structures in terms of symmetry modes (basis functions of matrix representations of the parent symmetry group, often referred to as representation analysis). The most efficient and complete approach to the description of a magnetic structure simultaneously employs both a magnetic symmetry group and symmetry-mode information, which are fully compatible. The smCIF dictionary will facilitate such descriptions. A first draft of the smCIF dictionary, including some examples, was proposed by Branton Campbell, and is now under discussion by an *ad hoc* working group of interested people among the membership and the consultants of the Commission. In accordance with our terms of reference, these CIF-related activities have included communication with the Chair of COMCIFS, James Hester.

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

Software development and reference materials

Software and reference materials supporting the modeling, solution, refinement and visualization of magnetic structures have seen significant development during the years 2018-2020. Commission participants contributed to much of this development.

The Bilbao Crystallographic Server upgraded the *MTENSOR* program to include magnetic phases, as reported in *Acta Cryst*. (2019) A**75**, 438-447. It now calculates the symmetry-adapted forms of physical-property tensors that include magnetic properties.

The Bilbao Crystallographic Server has continued to add to the MAGNDATA database of magnetic structures, which has grown rapidly to include roughly 1500 structures. Their team estimate this to be approximately 25% of the magnetic structures in the scientific literature which are sufficiently complete and unambiguous to catalog. An author-search feature has been added to the user interface, and a structure-submission feature for new structures is expected soon.

The first version of *FullProf* (version 7.00) able to refine magnetic structures (powder and single crystals) having up to three independent modulations within the superspace formalism was distributed in May 2019. The symmetry constraints on modulation functions were fully implemented for an arbitrary set of propagation vectors and harmonics. Spherical coordinates can be used to describe modulation amplitudes facilitating the use of extra constraints beyond symmetry. Presently, only magnetic modulations are available, though displacive, occupational and ADP modulations will be also implemented in the future. The program outputs a magnetic *P*1-symmetry CIF file that can be directly read by *VESTA* to visualize a user-selected supercell. A conventional modulated mCIF file is also output with the refined magnetic structure. This file can be read by *JMOL/MVISUALIZE* to plot the magnetic structure.

Le Bail fits using superspace groups were also fully implemented in *FullProf* with an output adequate to perform, in a second stage, a simulated-annealing run working with the full powder profile to solve magnetic structures *ab initio*. All modulation functions are included in the simulated-annealing method with all kind of constraints compatible with the symmetry.

The program *mCIF_to_PCR* from the Bilbao Crystallographic Server has been extended to accommodate incommensurate structures with superspace-group symmetry. After importing a CIF from *ISODISTORT*, *mCIF_to_PCR* automatically allows one to prepare the input file for *FullProf* using a superspace group in whatever setting.

The program *WinPLOTR-2006* in the *FullProf* suite has been modified in order to identify the different kind of reflections: nuclear, magnetic or mixed (up to six integer indices), when using the superspace description.

SARAh was recently launched as a web application in order to stabilize its development base and move away from issues related to legacy Windows operating systems. As part of a goal to bring representational analysis calculations closer to the two-colour groups, the web version now determines isotropy groups and related magnetic point groups of the little group of the wavevector and also determines the corresponding magnetic basis vectors, as well as those of the kernel calculations. Calculations can be done for commensurate and incommensurate structures alike.

GSAS-II now fully supports magnetic structures, including those with one incommensurate modulation. The search for a correct description of a magnetic structure is simplified in *GSAS-II*, where a special version of the *k-SUBGROUPSMAG* tool from the Bilbao Crystallographic Server is called with the parent chemical space-group operations, selected **k** vectors and some option flags. The result is parsed by *GSAS-II* to extract the generated magnetic space groups, transformation matrices, origin shift vector, conjugacy classes (if any) and supergroup lists. *GSAS-II* also examines the magnetic atom positions to determine if any or all can carry a nonzero moment, flagging those space groups with atoms that can.

JANA2006 performs representation analysis for **k** = 0 and commensurate cases based on the irreducible representation data published by H. T. Stokes, B. J. Campbell and R. Cordes, *Acta Cryst.* (2013). A**69**, 388-395. This allows it to use the same symbols as in *ISODISTORT*. The procedure for importing the models from *ISODISTORT* was considerably improved. Furthermore, *Jana* was upgraded to the new version, *Jana2020*, which allows parallel refinement of several models. The graphical interface for the new *Jana2020* has also been further developed.

In the ISOTROPY Software Suite, the symmetry-allowed forms of Wyckoff sites are now presented for magnetic and non-magnetic incommensurate structures. Magnetic and non-magnetic incommensurate symmetry groups have been fully implemented in both *FINDSYM* and *ISOCIF*, so that it is possible to detect the actual or pseudo symmetry (with tolerances on atomic parameters and Fourier coefficients) of an incommensurate structure. The magnetic superspace groups (MSSGs) with up to three modulations have now been fully enumerated for the first time, and have been incorporated into all of the modulation-capable software tools in the suite.

Scientific meetings

During the years 2018-2020, the Commission has encouraged high-quality magnetic-structure research through the support of roughly 30 national and international conferences, schools and workshops. This support by the Commission and its individual members and consultants has included sponsorship, direct meeting organization, grant writing, organization and/or chairing of conference sessions, workshop presentations, and both invited and contributed lectures.

Future plans

Other plans or interests of the Commission include the following:
(1) Expand efforts to educate the crystallographic and broader structural-science communities in the art of unambiguously and concisely describing a magnetic structure.
(2) Continue to promote the widespread adoption of the magCIF standard amongst crystallographic software developers.
(3) Extend magCIF to support magnetic structure factors, magnetic reflection conditions, low-dimensional magnetic order, short-range magnetic order *etc*.
(4) Expand the MAGNDATA database of magnetic structures into an exhaustive resource.
(5) Support the development of tools that convert between OG and BNS presentations of a commensurate magnetic structure (in magCIF format), and between commensurate-supercell and incommensurate-wave descriptions of a commensurate magnetic structure.
(6) Develop long-term strategies for supporting and preserving computational tools and data resources relevant to the determination and communication of magnetic structures.
(7) Prepare a new volume of *International Tables for Crystallography* that focuses on magnetic symmetry, magnetic diffraction and magnetic structures.

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

A8.15 Commission on Mathematical and Theoretical Crystallography

During the 24th Congress and General Assembly of the IUCr held in Hyderabad in August 2017, the membership of the MaThCryst Commission for the triennium 2017-2019 was approved as follows: D. Pandey (Chair, India), M.L.A.N. De Las Peñas (Secretary, Philippines), V.A. Blatov (Russia), D. Gratias (France), J. Hadermann (Belgium), G. McColm (USA), H.B. Napolitano (Brazil), R. Oishi-Tomiyasu (Japan), Wei Ren (People's Republic of China), P. Zeiner (Malaysia) and L. Suescun (Uruguay), with 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) acting as consultants. This membership changed, however, when the Executive Committee asked the Commission Chair D. Pandey to step down during 2019. This led to the appointment by the Executive Committee of interim Co-chairs Professor M.I. Aroyo and Professor M. Nespolo, who are responsible for re-organizing the Commission membership and activities until the election of a new Chair at the 25th General Assembly. They remain in these positions at the time this report is written owing to the postponement of the Congress and General Assembly to August 2021.

During the period 2017-2019, e-mail and the internet were the main communication tools used by the members and consultants of MaThCryst, supplemented by personal contacts at occasional events, meetings, conferences or schools. MaThCryst's home page has been maintained by M. Nespolo, and can be found at http://www.crystallography.fr/mathcryst/index.php. G. McColm is developing and maintaining a blog on mathematical crystallography, called Crystal Mathematician, which can be found at http://blogs.iucr.net/crystalmath and is devoted to the mathematics of crystal design and analysis.

The main educational and scientific activities of MaThCryst during the triennium 2017-2019 can be summarized as follows:

Educational and scientific events

International Schools
One of the main activities of the members of MaThCryst is the organization and participation in International Schools devoted to the Commission's multiple areas of interest. In addition, many Commission members organize and participate in general schools devoted to techniques (X-ray/neutron single-crystal/powder diffraction) or materials characterization, where they teach symmetry and the use of *International Tables for Crystallography* Volume A, topology *etc*. This is a list of such events developed in the triennium.

(1) International Schools on Fundamental Crystallography
These are the flagship educational events of the Commission, where the basics of symmetry and the use of *International Tables for Crystallography* are taught. These schools, the first of which was held in Havana in 2007, are sometimes combined with applied schools or workshops in related areas, such as the use of the Bilbao Crystallographic Server, phase transitions, twins *etc*. The schools have been held annually in different parts of the world and they have turned into an essential educational event for students interested in crystallography. During the period two editions of the school took place:

(i) International School on Fundamental Crystallography and Workshop on Structural Phase Transitions (satellite event to the XXIV IUCr Congress), 30 August – 4 September 2017, at Rourkela, India, organized by D. Pradhan (consultant of the Commission) as the local organizer and M.I. Aroyo, M. Nespolo, B. Souvugnier, D. Pandey and R.N.P. Choudhary as members of the International Programme Committee. The speakers included one member of the Commission (L. Suescun) and four consultants (M.I. Aroyo, M. Nespolo, B. Souvignier and D.K. Pradhan). There were 72 participants and the event was financially supported by the IUCr, which included Visiting Professorship funds for one speaker (http://www.crystallography.fr/mathcryst/satelliteIUCr2017.php).

(ii) The International School on Fundamental Crystallography (Sixth MaThCryst School in Latin America), followed by a one-day Workshop on the Applications of Group Theory in the Study of Phase Transitions, took place in Bogotá, Colombia, from 26 November to 1 December 2018. This event was organized by Mario A. Macías-López, A.P. Reiber, E. Vargas, W. Baumann and E. Jimenez with M.I. Aroyo, M. Nespolo (consultants of the Commission), L. Suescun (Commission member), A. Penton-Madrigal and M. Glazer as speakers. There were 39 participants at the school, 25 from Colombia and 14 from eight other Latin-American countries. The event was financially supported by the IUCr, and included Visiting Professorship funds for two speakers (http://www.crystallography.fr/mathcryst/bogota2018.php).

(2) Training courses on symmetry and group theory in Japan
For the International Year of Crystallography a series of training courses in symmetry and group theory were started in Japan, coordinated by and with lectures by M. Nespolo (Commission consultant). The schools have been running regularly since 2014. Since 2017 the training course has been included in the curriculum of the Graduate University for Advanced Studies in Japan, and participants have been able to get corresponding credits after passing a written examination. During this period four courses took place (the 2020 courses were cancelled because of the COVID-19 pandemic):

(i) and (ii) Training courses on Symmetry and Group Theory (ongoing series in Japan); fifth course 6–10 March 2017, sixth course 31 July – 4 August 2017, both at KEK Tsukuba, MaThCryst coordinator and lecturer: M. Nespolo. There were 45 participants. (See https://www.iucr.org/gallery/2017/5th-tsukuba-training-course and https://www.iucr.org/ gallery/2017/6th-tsukuba-training-course for photographs.)

(iii) Training Course on Symmetry and Group Theory (seventh course) –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.

(iv) Eighth Training Course on Symmetry and Group Theory, Tsukuba, 22–26 July 2019 (in English), 29 July – 2 August 2019 (in Japanese), special session Mount Koya, 4–9 August 2019. Local Organizing Committee: T. Kamiyama, N. Igarashi and Y. Takahashi. Speaker: M. Nespolo. http://www.crystallography.fr/mathcryst/TrainingCourseJapan.php.

(3) International Schools on Topological Methods in Materials Science
A series of schools on topological methods in materials science have been organized by D. Proserpio (Commission consultant) and V. Blatov (Commission member). These were mainly held at Samara State University, Samara, Russia, during the previous triennium. However, during 2017-2019 these schools moved away from Russia and were held in China and Spain.

(i) The International School on Topological Methods in Materials Science 2017 was held in Beijing, China, 13–15 October 2017, with MaThCryst coordinator and main speaker V.A. Blatov (Samara University, Commission member). There were 20 participants (http://www.crystallography.fr/mathcryst/beijing2017.php).

(ii) International School on Topology and Group Theory, San Sebastian, Spain, 23–26 August 2018, with Dario Bercioux, M. Reyes Calvo, Jerome 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.

(4) Shanghai International Crystallographic School: Working with the Bilbao Crystallographic Server was held at Shanghai University, 11–17 June 2017, with MaThCryst consultant M.I. Aroyo (University of Basque Country, Spain), and local organizers A. Stroppa and Wei Ren (Commission member). There were 88 participants and the speakers were M.I. Aroyo, I.

Errea, M. Nespolo (Commission consultant), A. Stroppa and Q. Zhu. The school was financially supported by the IUCr (http://www.crystallography.fr/mathcryst/shanghai2017.php).

(5) The International Autumn School on Fundamental and Electron Crystallography was held at Sofia, Bulgaria, 8–13 October 2017, with MaThCryst coordinators J. Hadermann (Commission member) and M.I. Aroyo (Commission consultant), and local organizer D. Karashanova (Bulgaria). The speakers included M. Nespolo, M.I. Aroyo, J. Hadermann (all members or consultants of the Commission) and B. Ranguelov. There were 48 participants including speakers and 12 local organizing committee members, and the school was financially supported by the IUCr (http://www.crystallography.fr/mathcryst/sofia2017.php).

(6) Second Shanghai International School on Crystallographic Groups and Representations, and Their Application in Magnetic Structure Descriptions and Topological-Insulator Studies, Shanghai University, Shanghai, 1–7 July 2019, http://www.crystallography.fr/mathcryst/shanghai2019.php. Organizers: M.I. Aroyo (Commission interim Co-chair), A. Stroppa and W. Ren (Commission member). Lecturers: M.I. Aroyo, B. Andrei Bernevig, B. Bradlyn, J. Cano, L. Elcoro, M. Nespolo (Commission interim Co-chair) and B. Souvignier (Commission consultant). There were 110 participants from China and abroad, and all the lectures were broadcast live on the Koushare academic platform, a platform that aims to spread science widely by using new technologies. A total of 9854 people watched online via this platform.

(7) Summer School on Mathematical Crystallography, Nancy, France, 3–7 June 2019. Local Organizing Committee: M. Nespolo (Commission interim Co-chair) and I. Pignatelli. Lecturers: M. Nespolo, B. Guillot and G. de la Flor Martin; tutors: I. Pignatelli, B. Stöger and V. Richalet, http://www.crystallography.fr/mathcryst/nancy2019.php.

Workshops, courses and meetings

During the period 2017-2019 the Commission actively continued to promote mathematical and theoretical crystallography by organizing, supporting and promoting worldwide scientific events such as workshops and meetings. The main scientific activities can be summarized as follows:

(1) XXIV IUCr Congress. The Commission actively participated in the organization of the 24th Congress and General Assembly of the IUCr held in Hyderabad, India, 20–29 August 2017, with L. Suescun as member representative of MaThCryst on the International Programme Committee (IPC) of the Congress. Thanks to our representative's successful negotiations, one keynote lecture (M. Nespolo, Nancy, France) and two microsymposia (MS-035 Crystal-Structure Relationships and their Applications and MS-026 A Bridge between Two Worlds: Graphs as Standard Descriptors) sponsored by the Commission and five more co-sponsored microsymposia (MS-007 Topology and Symmetry of Modular Structures, MS-017 Extending the Boundaries of Crystallography, MS-071 Crystallographic Patterns in Art and Cultural Heritage, MS-103 Methods for Characterizing Commensurate and Incommensurate Magnetic Structures and MS-115 Polymorphism and Structural Transformations in Crystalline Materials) were held at the Congress. M.L.A.N. De Las Peñas co-chaired the MS-071 microsymposium, M.I. Aroyo co-chaired MS-017, H. Napolitano and B. Souvignier co-chaired MS-026, and K. Momma co-chaired MS-115. All these microsymposia were well attended and there were lively discussions after the talks.

(2) The Second Philippine Workshop on Mathematical Crystallography with M.L.A.N. De Las Peñas (Commission Secretary) as the main local organizer was held in Manila, 20–25 May 2017. The speakers were M.L.A.N. De Las Peñas, J.G. Eon (Commission consultant), M. Nespolo (Commission consultant), E. Schulte, S. Hyde (Commission consultant), M.I. Aroyo (Commission consultant), D. Frettloeh, S. Akiyama and M. Senechal. There were 65 participants, including 14 members of the local organizing committee. The event was financially supported by the IUCr (http://www.crystallography.fr/mathcryst/manila2017.php).

(3) ECM32, XXXII European Crystallographic Meeting, MaThCryst Satellite Conference on Graph Theory and Modular Structures, Technische Universität Wien, Vienna, Austria, 18–23 August 2019. Organizers and Programme Committee: B. Souvignier (Commission consultant), M. Nespolo (Commission interim Co-chair), B. Stöger (Commission consultant). Lecturers: B. Souvignier, M. Nespolo and B. Stöger, with oral contributions by participants S.I. Ben-Abraham and V. Kurlin. There were 15 participants, of which four were from Austria and 11 from abroad (http://www.crystallography.fr/mathcryst/wien2019.php).

(4) A Hands-On Workshop on Density Functional Theory First-Principles Simulations in Materials Science, Baoshan Campus, Shanghai University, 17–22 November 2018, with W. Ren (Commission member), A. Stroppa, C. Draxl and P. Pavone as organizers. The speakers were H. Guo, J. Hong, M. Liu, H. Jiang, A. Gulans, P. Pavone, F. Caruso, L. Reining, M. Scheffler, W. Yang, C. Draxl, M. Troppenz, C. Vorwerk, S. Lubeck and A. Stroppa. There were 100 participants from the home country and 15 from abroad. This event was financially supported by the IUCr.

(5) 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 M.I. Aroyo (Commission consultant), J.M. Perez-Mato and G. de la Flor in Oviedo, Spain, 20–21 August 2018. There were 16 participants from ten different countries, including four from Spain.

(6) 2019 AMS Sectional Meeting – Special Session on Crystallographic and Highly Symmetric Structures, University of Florida, Gainesville, USA, 2–3 November 2019. Organizers: M. Krajčevski and MaThCryst member G. McColm. Speakers:

M.L.A.N. De Las Peñas (Commission secretary), E. Flapan, A. Mohammed, M.M. Ferrari, C. Goodman-Strauss, E. Schulte, I. Streinu, M. Cramer Pedersen, N.C. Carter and M. Nespolo (Commission interim Co-chair).
http://www.crystallography.fr/mathcryst/ams2019.php, http://www.ams.org/meetings/sectional/2264_progfull.html.

Preparation for the 25th IUCr Congress and General Assembly
Discussions of lists of speakers and keynotes for the IUCr Congress in Prague (Czech Republic, planned for August 2020 but postponed until 14-22 August 2021) were held by e-mail, moderated by the International Programme Committee representative for the Commission, M.L.A.N. De Las Peñas. Thanks to the hard work and very successful and efficient negotiations of our representative, the Commission is responsible for a keynote lecture (D. Gratias) and for the organization of three microsymposia (MS-111 Graphs, Tilings and Crystal Structures, MS-112 Generalizations of Crystallographic Groups and Their Applications and MS-114 Beyond Pure Point Diffraction: Theory and Application of Diffuse Scattering), and co-sponsored another three (MS-53, MS-66 and MS-95).

Publishing activities
Members and consultants of the Commission contributed actively to different IUCr publishing activities:
(i) M.I. Aroyo is the Editor of the 6th edition of Volume A (*Space-group symmetry*) of *International Tables for Crystallography*, published by the IUCr and Wiley, prepared during the previous triennium but published in February 2017.
(ii) A series of articles devoted to the Training Courses on Symmetry and Group Theory in Japan were published in the *Journal of the Crystallographic Society of Japan* (in Japanese) [Nespolo, M. (2017). *Hierarchy and classification of space groups*. *J. Crystallogr. Soc. Jpn*, **59**, 51-63; Nespolo, M. (2017). *Miller indices, Laue indices and the reflection conditions. J. Crystallogr. Soc. Jpn*, **59**, 150-158; Nespolo, M. (2017). *Subgroups of point and space groups. J. Crystallogr. Soc. Jpn*, **59**, 210-222; Nespolo, M. (2018). *Structure relations and construction of structural models. J. Crystallogr. Soc. Jpn*, **60**, 80-87; Nespolo, M. (2019). *A brief introduction to the Bilbao Crystallographic Server. J. Crystallogr. Soc. Jpn*, **61**, 82-94].
(iii) A Special Issue on Mathematical and Theoretical Crystallography 2019 was prepared during the period and published in the 5 May 2020 issue of *Crystal Research & Technology*, edited by M. Nespolo, with contributions from M. Nespolo; A. Umayahara & M. Nespolo; M. Nespolo, M. Tokuda & A. Yoshiasa; M. Rotter & B. Stöger; M.M. Mosca & V. Kurlin; R.D. Svetogorov, P.V. Dorovatovskii & V.A. Lazarenko; and B. Stöger, M. Weil, O.P. Missen & S.J. Mills.
(iv) M.I. Aroyo is the Editor of the 6th edition of the *Teaching Edition of International Tables for Crystallography*. Mois is also responsible for the development of the Symmetry Database server of the Online Edition of *International Tables for Crystallography* (on the IUCr website) and participated in work on the enhancement of the Symmetry Database, including additional computer tools for the analysis of group-subgroup relations of space groups.

Contributions to general courses from MaThCryst Commission members

(i) Mois I. Aroyo was a member of the Scientific and Programme Committee for the International Crystallography School 'Crystallographic Information Fiesta', Naples, Italy, 29 August – 3 September 2019 (organized by the Italian Crystallographic Association and supported by the IUCr). Mois gave a Plenary Lecture on 'Space-group symmetry - Understanding *International Tables for Crystallography*, Vol. A', a lecture on magnetic and incommensurate CIF extension dictionaries and a tutorial on Crystallography Online by the Bilbao Crystallographic Server.
(ii) Ma. Louise Antonette De Las Peñas attended the IPC meeting of the 25th IUCr Congress in Prague, 15–16 May 2019, to prepare the Congress programme and the list of keynote and invited speakers, and gave a talk on 'The future of mathematical crystallography' at the Workshop on Current Trends and Future of Crystallography in Chemistry, Physics, Biology and Materials Science, 14 May 2019, in the Prague Congress Center.
(iii) S. Hyde co-organized and delivered a lecture at the International PhD School on Geometry and Topology in Contemporary Materials Science - 2017 at the Niels Bohr Institute (https://indico.nbi.ku.dk/event/938/).
(iv) H. Napolitano gave a talk on 'Structural analysis and biological profile of a novel hydroxychalcone' in the session Solid State Supramolecular Chemistry and Crystal Engineering Part II at the 2019 ACA Annual Meeting in Covington, Kentucky, USA, 20–24 July 2019.
(v) L. Suescun acted as a member of the Consejo Consultivo of the Latin American Crystallographic Association (LACA) and lectured at the LAAMP Open Lab Costa Rica on Symmetry and the Use of *International Tables for Crystallography* (https://openlabcr2017.webnode.com/).
(vi) L. Suescun and H. Napolitano organized the 1st Latin American Crystallographic Association School on Small Molecule Crystallography, Montevideo, Uruguay, 19-25 February 2018, with L. Suescun, N. Alvarez and G. Peinado as organizers. L. Suescun lectured on Symmetry and *International Tables*. Thirty students from 11 countries participated, including 11 from Uruguay (http://lacassmc.fq.edu.uy/).

Activities in 2020 and in the near future

Owing to the COVID-19 pandemic, activities planned by the Commission (as well as most of the IUCr-sponsored activites) for 2020 were cancelled or postponed. A few that were performed in virtual mode and those that were postponed are listed below.

Contributions to general courses from MaThCryst members in 2020
H. Napolitano and L. Suescun co-organized and lectured at the 3rd LACA School: Small Molecule Crystallography – Virtual Edition, UNAM, Mexico City, DF, Mexico, Part 1: 23–27 November 2020, Part 2: 7–11 December 2020 (originally organized for 23-30 March 2020 but postponed because of the COVID-19 pandemic). Organizers: V. Jancik, N. Alvarez, F. Di Salvo, J. Ellena, H. Napolitano, M. de J. Rosales Hoz and L. Suescun. Lecturers: M. de J. Rosales Hoz, L. Suescun (`Symmetry and

International Tables for Crystallography Volume A'; `Symmetry of the diffraction pattern'), F. Di Salvo, J. Ellena, H. Napolitano (`Methods for structure determination'), V. Jancik, B. Noll, D. Martínez-Otero, G. Alvarado and N. Alvarez. The school had 65 students from 13 countries (including 30 from Mexico). This event was sponsored by the IUCr (https://www.iquimica.unam.mx/LACA/).

Postponed educational events for 2021
(i) The International School on Fundamental Crystallography (Seventh MaThCryst School in Latin America) was planned for November 2020 at Universidad Nacional Mayor de San Marcos, Lima, Peru, organized by J. Quispe with M.I. Aroyo, M. Nespolo, L. Suescun (Commission members), A. Pentón-Madrigal and E.E. Estevez-Rams (Commission consultant) as lecturers, has been postponed to November 2021 at the same location. If problems persist there, the School will take place in 2022 in Goiás, Brazil, organized by H. Napolitano (Commission member)
(https://www.crystallography.fr/mathcryst/lima2021.php).
(ii) SIAM conference on Mathematical Aspects of Material Science, 17-28 May 2021, Bilbao, Spain. M.I. Aroyo (MaThCryst interim Co-chair) is co-organizer of minisymposium MS25: Computational Geometry, Topology and Symmetry Meet Material Science (MaThCryst contributors: M.L.A.N. De Las Peñas and M.I. Aroyo).
(iii) Crystallography Online: Workshop on the Use and Applications of the Structural and Magnetic Tools of the Bilbao Crystallographic Server, University of the Basque Country (UPV/EHU), September 2021, Leioa, Spain. Organized by M.I. Aroyo, MaThCryst interim Co-chair.

L. Suescun, *Commission Member*

A8.16 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.

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

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

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

The CSNS started operation in 2018 with three instruments.

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

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

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

The Japanese Research Reactor (JRR-3) restarted operation from February 2021 after a ten-year shutdown.

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

On 23 March 2020 ANSTO moved to an essential and critical operations mode with all scientific research infrastructure being shutdown, including the Australian Centre for Neutron Scattering (ACNS). ACNS re-commenced user operations on 23 June

2020 with a focus on clearing the backlog of proposals unable to be run due to COVID-19 travel restrictions and the ANSTO shutdown, and the recently approved 2020-2 round proposals, initially using mail-in services and then progressively to Sydney-basin users and interstate users. Since then, the OPAL reactor has continued to operate, with the long shutdown scheduled for June 2020 now postponed to June 2021. Unfortunately, international borders have not opened and are not planned to until early 2022. However, recently (April 2021) a travel bubble between Australia and New Zealand has opened up, allowing New Zealand researchers to visit ANSTO to undertake measurements. The ACNS provided additional support to early-career researchers (ECRs) in 2020/2021, and prioritized discretionary beamtime proposals to backfill COVID experiment cancelations, undertaking 51 discretionary proposals supporting ECRs. The ACNS also opened the Spatz neutron reflectometer to the user community in 2020. The BioRef neutron reflectometer was transferred from the BER-II reactor in Berlin to ANSTO in February 2017 and renamed `Spatz', which is German for sparrow. Spatz adds significant capability and capacity to the existing suite of neutron-scattering instruments at the OPAL reactor, and is ideally suited to the investigations of soft matter, biomedicine, energy and materials science.

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

In this quadrennial period, a notable neutron conference was the 11st International Conference on Neutron Scattering (ICNS2017), held in South Korea in 2017. A total of 758 scientists, engineers and aspiring students from 36 countries participated in this conference.

Also prior to COVID-19 restrictions, the 6th Design and Engineering of Neutron Instruments Meeting was held in Sydney in 2017, the Neutrons and Food 5 meeting was also held in Sydney in 2018, and the World Conference on Neutron Radiography, also in Sydney, in 2018. In 2019, two regional neutron conferences, the European Conference on Neutron Scattering (ECNS2019) in St Petersburg in Russia (with more than 700 attendees) and the 3rd Asia-Oceania Conference on Neutron Scattering (AOCNS2019) in Taiwan took place. The three continental associations ENSA, AONSA and NSSA met in Taiwan for the first time and discussed creating a world union together which could be announced at the next ICNS. On the other hand, the 12th International Conference on Neutron Scattering (ICNS2020) in Argentina had to be postponed because of the COVID-19 situation.

Several neutron schools at many facilities and crystallographic seminars were supported by Commission members in each year in many countries or regions. The 1st ANSTO-HZB Neutron School was held at the ACNS in 2019, a Neutron Radiography Workshop in 2018, and the 10th AONSA Neutron School was held at ANSTO in 2018. In 2020, some of these schools and seminars were held in virtual classrooms. These included the annual Powder Diffraction Workshops held jointly by the ACNS and the Australian Synchrotron, which ran in person in 2017, 2018 and 2019, and then remotely in 2020. The annual Small Angle Scattering Workshop organized by the ACNS with the Australian Synchrotron was held remotely in 2020.

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

T. Ishigaki, Chair

A8.17 Commission on NMR Crystallography and Related Methods

In this reporting period, the Commission entered its second triennium. A new list of members of the Commission was approved at the 24th IUCr Congress in Hyderabad, India. As the Commission's existence became better known in the NMR and diffraction communities, we saw increased interest in our various activities.

2017
In early 2017, David Bryce (University of Ottawa, Canada) and Francis Taulelle (KU Leuven, Belgium) guest-edited a Special Issue of *Acta Crystallographica Section C* on NMR crystallography. The 23 papers in the issue captured the growing breadth of NMR crystallography in the interrogation of the crystalline state of matter. At the one-year anniversary of the issue, the citation metrics for articles were reported to be roughly three times the average for papers in that journal, indicating heightened interest in the subject.

We continued to strengthen our ties with the American Crystallographic Association (ACA). The 2017 Annual Meeting of the ACA in New Orleans, USA (26-30 May 2017) featured a first-of-a-kind half-day session on NMR crystallography, co-chaired by Tomislav Friscic and Manish Mehta. Five speakers formed a compelling and complementary set to present a good cross section of a growing field. They were James Harper (University of Central Florida, USA), Mhialis Arhangelskis (McGill University, Canada), Leonard Mueller (University of California, Riverside, USA), Kenneth Harris (Cardiff University, UK) and Darren Brouwer (Redeemer University, Canada). The session exceeded everyone's expectations. The participants felt momentum coming out of the meeting, as well as a certain relevance to the crystallography community. The session's attendance of approximately 50 was strong, relative to the meeting size of 500, and the science presented was of the highest quality.

The 24th IUCr Congress in Hyderabad, India, featured a microsymposium on NMR Crystallography, featuring six leading practitioners in the field. Held on 23 August 2017, it came on the heels of a successful keynote lecture by David Bryce on 22 August. Both the keynote and microsymposium were the first of their kind at an IUCr Congress. At its peak, the microsymposium had nearly 60 members in the audience. While an emerging discipline, NMR crystallography is broad in its scope, ranging from technique development to applications in a variety of areas. The six presentations reflected this breadth in an impressive way. The talks were broadly accessible to the mixed audience. The presentations were of complementary nature and gave a good feel for the questions that are being addressed and the tools employed to tackle those questions. P.K. Madhu gave an excellent overview of cutting-edge NMR capabilities and their potential application to crystallography, while Yusuke Nishiyama showed what can be accomplished with proton chemical shift tensors. Sachin Chaudhari, having completed a postdoc with Lyndon Emsley in Lyon, spoke about the utility of dynamic nuclear polarization, while James Harper spoke about the possibility of determining crystal structures using NMR data alone. Gerd Buntkowski and Jurgen Senker spoke about powerful applications of NMR crystallography in the study of enzymes and polymer additives, respectively. In all, this was a highly successful microsymposium, which made a valuable addition to the overall scientific programme.

2018

Now in the middle of the triennium, the bulk of the Commission's activities continued to involve work with regional crystallographic associations and helping to organize themed sessions on NMR crystallography at their annual meetings, and to support the SMARTER conference.

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 deepening relevance to the larger crystallography community.

The Commission has supported 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 SMARTER conference after Aveiro in 2007 and 2011, Versailles in 2012, Durham in 2014, and Bayreuth in 2016. At Ljubljana there were 80 participants. The programme followed a regular scheme of organization with the goal of leaving enough time for discussion between people from different disciplinary fields: solid-state crystallography, diffraction crystallography, topological crystallography and crystal modeling. The invited speakers were of a high scientific level and none refused the invitation to participate. 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, modeling) and this meeting was an ideal forum 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.

2019

In the final year of the triennium, the Commission's activities continued 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 ACA continue to strengthen. The 2019 Annual Meeting of the ACA in Cincinnati/Northern Kentucky, USA (20-24 July 2019) featured a half-day session on NMR crystallography, co-chaired by Tomislav Friscic and Manish Mehta. Three speakers were part of a programme representative of the NMR crystallography community in North America. They were Robert Schurko (University of Windsor, Canada, now at Florida State University, USA), Roderick Wasylishen (University of Alberta, Canada) and Aaron Rossini (Iowa State University, USA). The session enjoyed good attendance and again delivered on the high expectations set by the previous year's session. The session sustained the momentum generated in sessions at previous ACA meetings. In anticipation of the IUCr Congress in Prague in 2020, it was decided that there would be no session on NMR crystallography at the 2020 ACA meeting. The Commission had already planned to have a full session and a keynote on NMR crystallography at the Prague Congress. Collaborative efforts between our Commission and the ACA will serve as a model for future efforts of the Commission to connect with other regional crystallographic associations.

M. Mehta, Interim Chair

A8.18 Commission on Powder Diffraction

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

Since its formal appointment at the Hyderabad meeting, the current Commission on Powder Diffraction nominated Professor Brendan Kennedy as its representative on the International Programme Committee (IPC) for the IUCr Prague Congress. Professor Kennedy's membership of the IPC was subsequently confirmed, and their involvement in due course resulted in the following 16 microsymposia proposed or supported by the CPD forming part of the final programme (see https://www.xray.cz/iucr/ms-powder.asp for details and Chairs):

Ab Initio Powder Structure Analysis for Polymorphism and Phase Transformation Studies with Pharmaceutical Applications
Combination of X-rays and Electrons for Structure Characterization
Combining X-ray Diffraction and Spectroscopy to Characterize Materials
Diffraction Imaging, Grain Mapping in Materials and Art
Disordered Materials: Spectroscopic and Scattering Techniques
In Situ and *In Operando* Studies of Battery Materials
Integrative Methodologies for Novel Thin Film Structures
Materials for Energy Conversion and Storage
Matter at Extreme Conditions at SR and XFEL: Complementarity of Spectroscopy and Diffraction
Perovskites
Phase Transitions in Complex Materials (Structure and Magnetism)
Structure Solution and Poorly Crystalline Materials
Symmetry Aspects of Magnetic Order and Magnetic Properties
Texture, Strain and Structure in Metals and Ceramics
Total Scattering
XAS and Crystallography Applied for Geomaterials and Environmental Problems

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). Then, as always, the primary conference for powder diffractionists was the 16th European Powder Diffraction Conference (EPDIC16) that took place in Edinburgh (1-4 July).

The biannual nature of many of the established meetings means odd calendar years are generally quieter years. Unfortunately, the pandemic that started in 2020 also resulted in EPDIC17 in Croatia as well as the 25th Congress and General Assembly of the IUCr being rescheduled (the Prague meeting to 2021 and EPDIC17 to 2022). Professor Brendan Kennedy continues as the CPD representative on the IPC for the IUCr Prague Congress.

Also of great significance to the CPD was the eventual publishing of Volume H of *International Tables for Crystallography*, and it is understood from the Editorial Office that approximately 200 copies have already been sold.

The CPD is also pleased to confirm that the 59th International School of Crystallography in Erice will be devoted to powder diffraction and has been scheduled for 31 May - 8 June 2024.

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

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

Ongoing CPD projects include:

- Recommended Practice and Publication Guidelines: Most members are concerned about the poor quality of data published in many journals and the fact that this is generally exacerbated by poor reporting and/or poor interpretation of the data.
- QPA Round Robin. After approximately 20 years the Commission has decided to put together another Quantitative Phase Analysis Round Robin, to assess the current state of this traditionally very important part of powder diffraction, particularly the impact that improved instrumentation, software and methodologies might have had on the field. The project will be coordinated by Dr Matthew Rowles from Curtin University in Australia. This is a considerable undertaking and will require the hiring of a temporary assistant. To cover this as well as the operational expenses, the CPD hopes to raise financial support from suppliers and other interested parties. Dr Rowles will put together a more detailed project plan and budget.

- PowderCIF project. It appears that this project has become dormant in the last triennium and it is necessary to reconsider an appropriate course of action once we have clarity of its current status.
- Commission publications: It is hoped that the Guidelines as well as the Call and subsequent results from the QPA Round Robin will all be published in IUCr Journals.

D. G. Billing, Chair

A8.19 Commission on Quantum Crystallography

This present triennial/quadrennial report presents highlights of activities already mentioned in the annual reports for individual years from 2017 to 2020.

This period has seen a significant change for the Commission and the whole community, as the Commission decided to increase its scope and, accordingly, change its name. Previously known as the Commission on Charge, Spin and Momentum Densities, we decided to clarify and broaden our spectrum by choosing the new name Commission on Quantum Crystallography, which was approved by the General Assembly at Hyderabad. The abbreviation QCr for quantum crystallography has also been adopted, and our regular conferences (among which are the Sagamore Conference, the International Charge Density Meeting and microsymposia at the IUCr Congress or at European Crystallography Meetings) now all feature the label QCr.

During the past four years, the Commission and the community have been very active in promoting quantum crystallography in journals and (upcoming) books and conferences. A Wikipedia page has been created (P. Macchi's initiative), a first CECAM discussion meeting was organized in Nancy (A. Genoni and S. Grabowsky) to better define the QCr area and a very successful Summer School was held in Erice (2018, hosted by D. Jayatilaka and P. Macchi), to name but a few activities.

The Commission is aware of the technical difficulties in attracting newcomers to a discipline at the crossroads of already complex science branches such as crystallography, quantum chemistry, solid-state physics, molecular physics or large instruments. Therefore, a collaborative online dictionary was recently initiated.

The success of the Erice Summer School motivated P. Dominiak and J. Contreras to propose a second edition (2022-2023). Another CECAM meeting is expected to take place soon in Milan, organized by P. Macchi.

The Commission is particularly eager to attract young researchers, and has decided on several actions to aid this. Most of our international meetings (QCr-specific, or microsymposia at the ECMs or IUCr Congresses) now have best poster presentation awards. We also have a Young Scientist Award and a Distinguished Scientist Award. However, the recent (and still ongoing) pandemic has been an impediment to awarding these in 2020.

The pandemic was a major obstacle to the usual Commission dynamics, since many meetings were either cancelled or postponed. Luckily, scientific exchanges were not totally suspended during summer 2020, since the Commission decided to organize a free online meeting, QCrOM2020 (Quantum Crystallography Online Meeting 2020), with an emphasis on discussion and poster sessions. The three-day conference was widely open, and we enjoyed the presence of 120 registered participants. Special attention was paid to newcomers with a satellite first day entirely dedicated to introductory talks to explain the past and present of quantum crystallography. A special issue of *Acta Crystallographica Section B* will feature a selection of the topics that were addressed during this meeting.

Everyone is now ready to meet up face-to-face with colleagues and friends, possibly during the next Congress (where there will be several QCr-related microsymposia and keynotes), and most certainly in the coming year.

J.-M. Gillet, Chair

A8.20 Commission on Small-Angle Scattering

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

Detailed reports for the years 2017-2019 can be found at https://www.iucr.org/iucr/commissions/small-angle-scattering.

For 2020, the business of the SAS Commission (CSAS) was conducted totally via e-mail, as personal meetings at national and international conferences were not possible because of the COVID-19 pandemic. The pandemic resulted in the postponement of the 2020 IUCr Congress (and the planned SAS 2021 conference) by a full year, and extension of the usual IUCr triennium to 4 years. The pandemic restricted many activities for all CSAS members and consultants. Nevertheless, what follows is a summary of activities for 2020.

Commission activities, meetings and communication

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

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

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

Educational activities

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

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

Eleonora Shtykova, with the help of Maxim Petoukhov, has been running a weekly online seminar on processing and interpretation of small-angle X-ray scattering data for students, postgraduates and young scientists at educational and scientific institutions in Moscow. Eleonora was also involved, with Vladimir Volkov, in a summer workshop on small-angle X-ray scattering methods for 4th and 5th year students of the Physics Faculty of Moscow State University, and gave a lecture for students of the Faculty of Bioengineering and Bioinformatics of Moscow State University on the use of small-angle scattering in the study of biological objects and modern nanomaterials as part of the course `Selected Physicochemical Methods in Biology'. For an online seminar jointly conducted by the Department of Physicochemical Methods of Research and the Center for Collective Use `SKIF' of the Institute of Catalysis of the Siberian Branch of the Russian Academy of Sciences Eleonora gave an invited talk Introduction to Small Angle Scattering and Structural Nanodiagnostics.

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

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

Community-building activities

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

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

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

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

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

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

Consultant activities

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

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

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

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

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

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

Daniel Clemens is a member of the Scientific and Technical Advisory Panel of the European Spallation Sources for the future instrumentation for neutron reflectometry and small-angle neutron scattering, and also serves as a member of the Neutron Science Advisory Council of The Pennsylvania State University.

Organizational activities

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

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

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

International activity

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

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

Technical activities

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

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

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

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

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

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

D. Svergun was also involved in collaborative research at the beamline P12 in Hamburg with the biotechnology company BioNTech to support development of anti-COVID mRNA vaccines (https://www.embl.org/news/science/biontech-uni-mainz-embl-hamburg/). Three collaborative papers were published with this company in 2020. In another COVID-related collaborative project, SAXS at P12 was used for screening and characterization of synthetic mini-antibodies called sybodies, which are able to bind to SARS-CoV-2 and prevent it from infecting human cells, see https://www.embl.org/news/science/sybody-against-sars-cov-2/.

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

Jill Trewhella is continuing as the lead coordinator (as Chair of the PDB SASvtf) for the initiative that aims to generate a set of SAS data sets that can be used to benchmark different approaches to predicting SAS profiles from atomic coordinates (see https://sas.wwpdb.org/?q=node/25 for full details and participants). The effort included CSAS consultants Javier Pérez and Dmitri Svergun, and has grown to include 41 structural biology and SAS experts from across Europe, Asia and the Americas. During 2020, data analysis has been progressing for the 150 SAXS data sets and more than 70 SANS data sets submitted from 12 SAXS facilities and 4 SANS facilities, including SEC-SAXS and batch SAXS, SEC-SANS and batch SANS in H_2O and D_2O. The analysis so far shows a strong consensus in the results obtained in terms of overall conformational parameters as well as in the detailed shapes of the scattering profiles. A draft paper is in progress for submission to *Acta Cryst. Section D* and work is proceeding toward deposition of a set of data as suitable for benchmarking methods for SAS profile prediction.

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

Masaaki Sugiyama developed a laboratory-based Size Exclusion Chromatography SAXS system in Kumatori, Japan.

Social activities

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

U-Ser Jeng, Chair

A8.21 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 on Crystallographic Teaching, as well as with important external bodies such as the Cambridge Crystallographic Data Centre (CCDC).

The Commission last met in person at the 2017 Hyderabad Congress and there agreed to focus on:
(i) support for appropriate crystallographic conferences and schools, in particular those that aim to expand crystallography to under-represented regions such as South America and Africa;
(ii) support for IUCr Journals, through encouraging submission of excellent scientific results to *IUCrJ* and other journals; and
(iii) building relations with other Commissions and external bodies such as IUPAC and the CCDC. In considering the future composition of the Commission, it could also be of value to include a member or consultant to represent relevant industries.

The membership of the Commission on Structural Chemistry was updated extensively at the 2017 IUCr Congress in Hyderabad. The members of the Commission for this period are: Rahul Banerjee (India), Susan Bourne (South Africa, Chair), Alison Edwards (Australia), Javier Ellena (Brazil), Katherina Fromm (Switzerland), Jun Harada (Japan), Christian Lehmann (Germany), Len MacGillivray (USA), Shie-Ming Peng (Taipei) and Giuseppe Resnati (Italy).

Stuart Batten (Australia) stood down as Chair, but remains a consultant to help ensure continuity. Other consultants are Pete Woods (UK), Petra Bombicz (Hungary), Ilia Guzei (USA), Agata Bialonska (Poland), Nadezhda Bolotina (Russia), Christer Aakeroy (USA), Alessia Bacchi (Italy) and Patrick Mercier (Canada). Pance Naumov (UAE) joined as a consultant in 2020. The members and consultants of the Commission provide liaison with other Commissions and important bodies, *e.g.* Patrick Mercier (Commission on Inorganic and Mineral Structures), Pete Wood (CCDC) and Len MacGillivray (Co-editor for *IUCrJ*).

Over the past four years, the Commission has supported a range of meetings, details of which are given below. The Commission members and consultants take seriously the task of interrogating the applications submitted, focusing specifically on (*a*) the centrality of structural chemistry to the aims of the conference or school, (*b*) support for students and early-career researchers and (*c*) diversity in terms of gender and geographic distribution of speakers and participants. Unfortunately, the COVID-19 pandemic has meant that organizing committees have had to make difficult decisions about whether to continue with planned events or not. Most meetings supported by the Commission which were planned between March 2020 and June 2021 have had to be cancelled, postponed or moved to an online or hybrid format.

Supported meetings, schools and workshops

1st Latinoamerican Crystallographic Association School on Small Molecule Crystallography, Montevideo, Uruguay, February 2018.
Indaba 9, Kruger Park, South Africa, September 2018.
Gordon Research Conference on Crystal Engineering, USA, June 2018.
American Crystallographic Association Annual Meeting, Toronto, Canada, July 2018.
2nd Porous Molecular Materials (POMOS) conference, Vietri sul Mare, Italy, June 2018.
5th European Crystallography School, Stellenbosch, South Africa, July 2018.
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.
3rd LACA School on Small Molecule Crystallography, Mexico City, Mexico, March 2020. (Postponed to November 2020 and held online. Reports are that this was very successful, with lectures hosted on the Zoom platform and Google Classroom. Problem-solving questions were also addressed through WhatsApp in English, Spanish and Portuguese.)
4th International Symposium on Halogen Bonding (ISXB-4), Stellenbosch, South Africa, March 2020. (Postponed to November 2020 and held online. Reports are that this was very successful, being hosted on a proprietary conference service. Pre-recorded lectures and panel discussion sessions allowed participation from around the world, with participants in over 12 time zones.)
6th European Crystallography School (ECS), Budapest, Hungary, July 2020. (Postponed to July 2021.)
AICS Italy Crystallography School, Parma, Italy, September 2020. (Postponed to September 2021.)
Gordon Research Conference on Crystal Engineering, USA, June 2020. (Postponed to July 2022.)
SARX, Puebla, Mexico, November 2020. (Cancelled.)
3rd Pan-African Crystallography Conference, Nairobi, Kenya, January 2021. (Postponed to January 2023, with an online e-PCCr planned for January 2022.)
Zurich Crystallography School, Zurich, Switzerland, June 2021. (Postponed to July 2022.)
ICCOSS XXV, Ohrid, Macedonia, June 2021. (Postponed to July 2022.)
6th Conference of the Bangladesh Crystallographic Association, Dhaka, Bangladesh, January 2021. (Successfully held online.)
International School of Crystallography on Molecular Crystal Engineering, Erice, Italy, May 2021. (To be held online.)
International School on Advanced Porous Materials 2, Como, Italy, June 2021. (To be held online.)

Activities of Commission members

Javier Ellena has been active in organizing crystallographic schools in Latin America, serving on the organizing committees and as a lecturer on the 1st and 3rd LACA Schools on Small Molecule Crystallography, held in Uruguay in 2018 and in Mexico in 2020. Susan Bourne chairs the Scientific Programme Committee of the 3rd Pan-African Crystallography Conference, and Alessia Bacchi is a member of the International Advisory Board for the same conference.

Looking forward to the Congress in Prague in 2021, we note the excellent work done by the Commission representatives Marijana Dakovic, Masaki Kawano and Catharine Esterhuysen, which has ensured a strong chemical crystallography programme. The Commission will meet during the Congress, though it is likely that this meeting will need to be virtual, as not all members and consultants will be able to attend in person.

S. Bourne, Chair

A8.22 Commission on Synchrotron and XFEL Radiation

The Commission (CSXR) organized several sessions at the IUCr Congress in Hyderabad and sponsored three keynote speakers: Janet Smith, Sakura Pascarelli and Henry Chapman.

Supported meetings

Italian Synchrotron Radiation 14th School on Synchrotron Radiation (18-29 September 2017), organized by the Italian Society (SILS) and held in Muggia.
RapiData course on automated data collection (supporting participation of Latin American students). The CSXR has endorsed this annual event for the last three years (https://www-ssrl.slac.stanford.edu/rapidata/rapidata-2020/about.html).
International School of Crystallography 49th Course: Integrative Structural Biology (2-11 June 2017), held in Erice (http://www.ccsem.infn.it/ef/emfcsc2017/posters/pdf/Cristallografia2017.pdf).
The Croatian Association of Crystallographers workshop, Hot Topics in Contemporary Crystallography (HTCC) has been supported for the last three years (http://htcc4.org/).

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

Meetings organized by members of the Commission

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

- Miguel A. G. Aranda is Chair of the ESRF Council (2018-2020), a member of the SRI 2018 Scientific Programme Committee, a Spanish observer at the European XFEL Council and a member of strategic group-1 of LEAPS.
- 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 organized a one-day workshop Advanced Light Sources in the Asia Oceania Region as part of the 14th Asia-Pacific Physics Conference in Kuching, Malaysia.
- Pawel Grochulski represented CSXR on the International Programme Committee of the 2017 IUCr Congress; co-organized and lectured at the Annual CLS Mx Data Collection Schools, Saskatoon; is a member of the SOLARIS SAC; and was a member of the International Programme Committee of the 14th International School and Symposium on Synchrotron Radiation in Natural Science, Zakopane (Poland), 9-14 June 2019.
- Eduardo Granado was Chair of the Organizing Committee of the LNLS 27th Annual Users' Meeting (RAU), 22-24 November 2017, in Campinas; Co-chair of the microsymposium Total Scattering in Hyderabad; a member of the organizing committee of the São Paulo School on Light, Neutrons and X-Rays, São Paulo, 17–21 July 2017; a member of the organizing committee of the Brazilian Synchrotron (LNLS) Users Meeting; a member of the Advisory Committee of the Latin American Crystallographic Association (LACA); was a founding member and the first Chair of the Brazilian Synchrotron Users Group (LNLSUG), starting November 2019; a member of the Scientific Committee of the 29th LNLS Annual Users Meeting (5-7 November 2019); and President of the Brazilian Crystallographic Association (ABCr), 2018-2020.
- Janet Smith is Scientific Director of the GM/CA@APS macromolecular crystallography facility at the Advanced Photon Source, Argonne National Lab, USA; is on the Science Advisory Committees of the Advanced Light Source, Lawrence Berkeley National Lab, USA, and the National Synchrotron Light Source II, Brookhaven National Lab, USA; and is on the Editorial Board of *IUCrJ*.
- Sakura Pascarelli co-organized two workshops at the ESRF (2nd Workshop on Studies of Dynamically Compressed Matter with X-rays, 29-30 March 2017, aimed at bringing together the community of future users of the High Power Laser Facility, and 2nd EUCALL Annual Meeting, 7-9 June 2017); is Chair of the upcoming Gordon Conference on Research on High Pressure, Holderness, NH, USA, July 2020; is on the Scientific Organizing Committee of the LEAPS Meets Quantum Technology Conference, Elba, Italy, May 2020; and worked within the International Programme Committee (IPC) for the IUCr Congress in Prague.

- Maciej Kozak was Chair of the 14th International School and Symposium on Synchrotron Radiation in Natural Science (ISSRNS'2019), Zakopane, Poland, 9-14 June 2019; was a member of the Organizing Committee of the 17th International Conference on X-ray Absorption Fine Structure, 2018, Krakow, Poland; was Project Leader of the SOLCRYS beamline at the SOLARIS National Synchrotron Radiation Centre (Krakow, Poland); was a member of the XIPS 2019 International Advisory Board; and was a member of the Programme Advisory Committee for Condensed Matter Physics, Joint Institute for Nuclear Research (Dubna, Russia).
- Thomas Tschentscher organized sessions on scientific applications and instrumentation of FEL facilities at the SPIE OPTICS conference in Prague (April 2017) and at the CLEO optics conference in Munich (July 2017); was Chair of the EUCALL (European Cluster of Advanced Laser Light Sources) project, funded by the European Commission, and grouping accelerator and laser-driven X-ray user facilities; organized practicals for 16 school participants at the European XFEL and DESY during March 2018; executed several science, technology and industrial liaison workshops in the framework of the Horizon 2020 project EUCALL; co-organized the HP4 international workshop (DLR, Berlin, Germany); and served on the programme and scientific committees of PhotonDiag-2018 (DESY, Germany), PNP-18 (St Malo, France) and RPDHM (DESY, Germany).
- Milan Sanyal organized the Winter School on Synchrotron Techniques in Materials Science at the S. N. Bose National Centre for Basics Science, Kolkata, India (25-31 October 2018), and executed three projects that provide preferred access to Indian scientists in internationally known facilities for carrying out diffraction and scattering experiments (at the Photon Factory Synchrotron, KEK, Japan, and at PETRA-III, DESY, Germany, for synchrotron X-ray and at the Rutherford Appleton Laboratory, UK, for neutron experiments).
- Nadia Zatsepin chaired the BioXFEL 6th Annual International Conference (February 2019) and was an advisor for the Workshop on Macromolecular Serial Crystallography using the LCP Jet Injector at the NSLS-II & CFN Users' Meeting.

Asia Oceania Forum for Synchrotron Radiation Research

The Asia Oceania Forum for Synchrotron Radiation Research (AOFSRR) is an international network of synchrotron and XFEL light source facilities and user organizations in the Asia Oceania region. One of the core activities of the AOFSRR has been the Cheiron School, a two-week international synchrotron school, which has been held annually at SPring-8 since 2007. A one-day workshop Advanced Light Sources in the AOFSRR Countries was held by the AOFSRR as a satellite to SRI2018 (10 June 2018); CSXR consultant Richard Garrett is Secretary-Treasurer of the forum, and CSXR member Youichi Murakami was AOFSRR President in 2015-16; the third annual AOF Synchrotron Radiation School was held in early November 2019, in Hsinchu, Taiwan.

P. Grochulski, Chair

A8.23 Commission on XAFS

(1) *Members and duties*
In the Commission on XAFS (CXAFS) we assign each member a 'portfolio' of responsibility, which aids our division of labour and hopefully productivity. During the 24th IUCr Congress and General Assembly (August 2017) in Hyderabad, India, the following members and consultants of CXAFS were approved: Christopher T. Chantler (Australia) (initially appointed to Commission in 2008), Chair 2014-2020; Valérie Briois (France) (2017) Secretary; Sofia Diaz-Moreno (UK) (2014) Secretary, website; Guiliana Aquilanti (Italy) (2014), liaison with the International Programme Committee; Dibyendu Bhattacharyya (India) (2017), coordinator of funding support including from the IUCr Congress and the IUCr for critical missions (IUCr Congress, workshops, satellite meetings, IXAS, Q2XAFS and others); Yasuhiro Inada (Japan) (2017), working group on databases and coordinator of summary from the Japan XAFS Society; Narcizo M. Souza-Neto (Brazil) (2017), IUCr dictionary of XAFS terminology; Steve M. Heald (USA) (2014), liaison with *International Tables for Crystallography* and IUCr Journals; Krystyna Lawniczak-Jablonska (Poland) (2011), coordinator for Q2XAFS workshop (Poland), IXAS liaison; and Carlo Lamberti (Italy) (2017-2019) IUCr Congress Workshop, liaison to *International Tables for Crystallography*.
Consultants: Federico Boscherini (Italy), Farideh Jalilehvand (Canada), Hiroyuki Oyanagi (2014-2019) (Japan), Peter Glatzel (France) and Richard Strange (UK).

(2) *24th IUCr Congress*
Tutorial Workshop at the 24th IUCr Congress (21 August 2017, with 80 attendees). The scope of this one-day, free tutorial workshop was to provide an overview of the physics and chemistry of X-ray absorption spectroscopy with a particular emphasis on its complementarity with diffraction techniques. The curriculum included introductions to beamline instrumentation, measurement methods, methods of data processing and analysis, and proposal writing. A software panel discussion discussed a wide variety of software packages.

Microsymposia. A record number of eight microsymposia were organized or co-organized by CXAFS:
MS-090 Spectroscopy Applications in Biological Systems; Co-chairs: Sofia Diaz-Moreno (UK), Bhoopesh Mishra (USA). Shared with the Commission on Biological Macromolecules.
MS-051 Recent Developments in XAFS Spectroscopy: Theory, Instrumentation and Data Analysis; Co-chairs: Hiroyuki Oyanagi (Japan), Konstantin Klementiev (Sweden).
MS-107 Synchrotron Measurement in Conservation and Cultural Heritage; Co-chairs: Bruce Ravel (USA), Eric Dooryhèe (USA). Shared with the Commission on Crystallography in Art and Cultural Heritage. (Chair: Gilberto Artioli, Italy.)

MS-060 XAS at Extreme Conditions: Co-chairs: Giuliana Aquilanti (Italy), Daniel Haskel (USA). Shared with the Commission on High Pressure. (Chair: Andrzej Katrusiak, Poland.)
MS-096 XAFS of Materials for Clean Energy: Co-chairs: Pieter Glatzer (France), Steve M. Heald (USA). Shared with the Commission on Crystallography of Materials (Chair: Artem Oganov, USA.)
MS-121 Synchrotron-Based X-ray Techniques and the Environment: Co-chairs: Richard Garrett (Australia), Hugh Harris (Australia). Shared with the Commission on Synchrotron and XFEL Radiation. (Chair: Richard Garrett, Australia.)
MS-042 High-Resolution Spectroscopy: Co-chairs: Dimosthenis Sokaras (USA), Hamid Reza Khavasi (Iran).
MS-074 Porous Frameworks for Catalysis and Renewable Energy: Co-chairs: Christian Doonan (Australia), Gustav Van Tendeloo (Belgium).

A keynote lecture entitled `Science at high pressure: the emerging role of X-ray absorption spectroscopies' was given by Sakura Pascarelli (France). Another keynote entitled `X-ray absorption spectroscopy and chemical speciation: from archaeology to biology' was given by Farideh Jalilehvand (Canada). A third excellent keynote was given by Vittal Yachandra (USA, India) on `Taking snapshots of photosynthetic water oxidation with an X-ray laser'.

We take a modest pride in noting both that our Commission representation of female speakers, presenters and keynotes (indeed also members) was particularly high and that no affirmative action was involved – we voted consultatively on all recommendations from the field of candidates as to merit. Perhaps X-ray absorption spectroscopy is particularly blessed or fortunate in this regard, or perhaps this should be more generally valid.

(3) *International Tables for Crystallography Volume I and editorial activities*
All three Editors have been working diligently towards the volume, and good progress has been made. The Editorial Office plan to post major sections online as they become available and proofed, and we hope that 2-3 main sections might get to that point in 2021. Some contributors have been patient with their accepted or revised manuscripts and a series of acceptances *etc*. should be going out within the next few months. The quality of the articles is in general excellent and the volume will make a major contribution to the literature, reference works and field.

2020 update: the first 14 chapters of around 160 have been edited and are now available online at https://it.iucr.org/I, with all Editors working towards critical and missing sections and chapters. The quality of the formatting and typesetting is excellent as expected.

(4) *IXAS Newsletter and links to IUCr Journals*
The Commission members have published a Special Issue in the *Journal of Synchrotron Radiation*, with ten articles related to the Diamond Q2XAFS meeting [*J. Synchrotron Rad*. (2018). **25**, Part 4], which was a satellite of the 24th IUCr Congress in Hyderabad.

(5) *XAFS 2018 conference*
At the XAFS 2018 Conference in Krakow, Poland, July 2018, two events shared by the IXAS and CXAFS were co-organized. A one-day workshop on Advances in XAFS Experimental Techniques with a special emphasis on the advent of fourth-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 XAFS 2018 conference was also organized with four lectures given by Farideh Jalilehvand, Peter Krüger, Hidekazu Ikeno and Ryan Trevorah on `Reactivity of antitumoral Rh complexes', `New developments within the ligand field multiplet theory for *L* edge absorption', `RIXS and RIXS-XMCD (resonant inelastic X-ray scattering – X-ray magnetic circular dichroism) spectra calculations' and `Robust self-absorption correction method for fluorescence data'.

A meeting of CXAFS was also held to discuss the preparation for the next IUCr Congress, which will be held in Prague, Czech Republic.

(6) *Preparation for the 25th IUCr Congress in Prague*
Thanks to efforts from all of the Commission, and especially our liaison Guiliana and Chairs and Co-chairs, a new record number of microsymposia organized/co-organized by CXAFS in Prague have been accepted for the Congress:
One unshared microsymposium:
MS60 Catalysis: Functionalized Materials Studied by XRD and XAFS. Co-chairs: V. Briois (France), A. Roodt (South Africa).
Shared microsymposia:
MS61 XAS and Crystallography Allied for Geomaterials and Environmental Problems. Shared with the Commission on Inorganic and Mineral Structures. Co-chairs: F. Mosselmans (France), A. Martucci (Italy).
MS57 Advanced Methods for Analysis of XAFS and Crystallographic Data. Shared with the Committee on Data (CommDat). Co-chairs: M. Girogetti (Italy), M. Milanesio (Italy).
MS59 Disordered Materials: Spectroscopic and Scattering Techniques. Shared with the Commission on Neutron Diffraction. Co-chairs: A. Trapananti (Italy), J. Simon (USA).
MS58 Spectroscopy Applied to Electrochemistry: Operando Studies. Shared with the Commission on NMR Crystallography and Related Methods. Co-chairs: D. Btattacharyya (India), J. Plaisier (Italy).
MS37 Matter at Extreme Conditions at SR and XFEL: Complementarity of Spectroscopy and Diffraction. Shared with the Commission on High Pressure and the Commission on Synchrotron and XFEL Radiation. Co-chairs: U. Zastrau (Germany), A. Rosa (France).

MS54 X-ray Spectrometry and X-ray Diffraction in Art and Archaeology. Shared with the Commission on Crystallography in Art and Cultural Heritage. Co-chairs: G. Cibin (UK), P. Bezdicka (Czech Republic).
MS138 The Mineral/Life Interface – Prebiotic Chemistry, Biomineralization, Advanced Biomimetic Materials. Shared with the Commission on Crystal Growth and Characterization of Materials. Co-chairs: J. M. Garcia-Ruiz (Spain), G. Falini (Italy).
MS181 4th Generation SR and XFEL Facilities. Shared with the Commission on Synchrotron and XFEL Radiation. Co-chairs: M. Thunissen (Sweden), M. Yabashi (Japan), S. Diaz-Moreno (UK).
MS52 Combining X-ray Diffraction and Spectroscopy to Characterize Materials. Shared with the Commission on Powder Diffraction. Co-chairs: C. Meneghini (Italy), S. Schmid (Australia).

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

2020 update: We still intend to run all of these and are excited by the prospect of the Congress; but of course there may be adjustments as to presentation modes and attendance under the circumstances.

(7) *IUCr XAFS Workshop*
The next workshop dedicated to XAFS for crystallographers was intended to be held the day before the Congress. This one-day, almost free (EUR 10) tutorial workshop would have provided an overview of the physics and chemistry of X-ray absorption spectroscopy with a particular emphasis on its complementarity with diffraction techniques. The curriculum would have included introductions to beamline instrumentation, measurement methods, and methods of data processing and analysis. Details can be found at https://www.xray.cz/iucr/workshops/xafs/. However, owing to the COVID pandemic this might be postponed to the next Congress.

(8) *Presentation by CXAFS*
At the request of the IUCr Executive Committee, an article co-authored by C. T. Chantler, G. Aquilanti, S. Diaz-Moreno and V. Briois reporting the roadmap and 2018 activities of CXAFS was prepared [*Materials Structure* (2019), **26**, 108].

(9) *2020 COVID update*
Naturally, efforts during this 'bonus year' have been directed towards preparation for the Congress, preparing for the handover to new Commission members and also work towards the workshop and Q2XAFS activity. Other areas have been postponed in part because of difficulties in getting together. We are confident that the incoming Commission will be effective and able to continue many of the key works of the current Commission, and that in the next cycle *International Tables* Volume I will be fully published. Some Commission initiatives may work together with IXAS on Journal Club activity and additional workshops, which can help us keep in contact more as we prepare to emerge from our COVID cocoons.

C. T Chantler, Chair, and V. Briois and S. Diaz Moreno, Secretaries

A9. Committee for the Maintenance of the CIF Standard (COMCIFS)

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

Dictionaries
A key aspect of the CIF project over the last two decades has been codification of crystallographic knowledge into machine-readable dictionaries. The current period has seen the addition of a small dictionary providing topological descriptors for crystallographic structures, and ongoing discussions towards codification of a high-pressure dictionary. A handful of new datanames were added to the core dictionary.

Macromolecular developments
In this quadrennium, submission to the wwPDB in CIF format was made mandatory, marking the end of a decades-long process in moving away from the previous legacy format. The wwPDB has continued rapid development of new definitions as new techniques appear.

Workshops and meetings
Several hours of lectures on the CIF standards were included in the data-focused 2019 International Crystallography School run by the Italian Crystallographic Association. The CIF standards were also briefly outlined to representatives of other scientific unions at the 2019 CODATA meeting in Beijing.

International Tables Volume G
The second edition of *International Tables for Crystallography* Volume G, covering crystallographic data standards, made solid progress during the quadrennium. Chapters covering all of the new fundamental standards for syntax and dictionaries have been written and reviewed, during which those standards were finalized and formalized.

Interaction with other data standards initiatives
COMCIFS has continued to maintain links with the NeXus International Advisory Committee (NIAC), which primarily develops raw data standards for large facilities. As a result, various NeXus standards for describing single-crystal crystallography experiments have been harmonized with CIF standards. More recently, various European efforts around materials modelling (EMMO and OPTIMADE) have also made contact with COMCIFS and are well advanced in plans to use CIF dictionaries to automatically populate the relevant parts of their ontologies.

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

Future concerns
A key concern for COMCIFS, in common with committees of similar International Scientific Unions, is accessing sufficient volunteer time to adequately support and develop standards. As the current generation of CIF experts move into retirement replacements will need to be found. There is a growing danger that the pace of scientific development will leave CIF dictionaries behind, resulting in *ad hoc* solutions for data description that, once embodied in software, are difficult to undo.

Membership
COMCIFS consists of five voting members and a broad collection of advisers and observers. The voting members, who remained unchanged in this period, are James Hester (Chair), John Bollinger (Co-Secretary), Brian McMahon (Co-Secretary), Herbert Bernstein and John Westbrook. A further notional voting position remains unfilled. No decisions in the last quadrennium have required a vote.

J. Hester, Chair

A10. *IUCr Newsletter*

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

This quadrennial report covers 14 issues: Volume 24 Numbers 3 and 4 and Volume 25 Numbers 1 and 2 (published in 2017), Volume 26 Numbers 1 and 2 (2018), Volume 27 Numbers 1–4 (2019), and Volume 28 Numbers 1–4 (2020). Volumes 24 and 25 were edited by Bill Duax and Volumes 26–28 by Mike Glazer. A President's column has appeared in all issues, the first three by Marvin Hackert and those following by Sven Lidin.

The issues published in 2017 devoted several pages – and covers – to promoting and reporting on the Hyderabad Congress. Other meeting/workshop reports included one on the First Pan-African Conference on Crystallography in Cameroon. Each issue also included articles related to IUCr publications and outreach activities, such as reports on OpenLabs in Albania, Bolivia and Senegal, and news of the IUCr crystal growing competition for schoolchildren. Important announcements included the retirement/appointment of the IUCr Executive Secretary, the publication of the 6th edition of *International Tables for Crystallography* Volume A, and the launch of the IUCr Associates Programme and the IUCr–IUPAP Lightsources for Africa, the Americas and Middle East Project (LAAMP).

Each 24-page issue was distributed electronically to approximately 13 000 people. Print copies went to an average of 555 libraries and individuals and were distributed at several meetings, including the Hyderabad Congress. In addition, 1000 reprints of the Crystallography in India section of Volume 15 Number 4 were made available at the Congress.

Volume 25 Number 2 marked Bill Duax and Patti Potter's retirement from their roles as Editor and Production Manager, respectively, and we are deeply appreciative of their dedicated work in disseminating news to the crystallographic community for 25 years.

At the IUCr Congress in Hyderabad in 2017, the IUCr Finance and Executive Committees decided that print production should be discontinued, and the *Newsletter* relaunched in 2018 in a new digital web format with an accompanying e-mail edition. As this coincided with Bill Duax's retirement as Editor, it was also decided to move the operation of the *Newsletter* from the USA to Chester. Mike Glazer was invited to act as Editor, and one of their first tasks was to appoint an international board of Regional Editors: Ted Baker (Asia including Australia, New Zealand and Pacific Island territories), Delia Haynes (Africa), Abel Moreno (Latin America), Amy Sarjeant followed by Tiffany Kinnibrugh and Andrey Yakovenko (USA and Canada) and Serena C. Tarantino (Europe including Russia and the Middle East). Chester staff took on the roles of Managing Editor (Andrea Sharpe) and Technical Editors (Mark Bates, Sarah Froggatt and Jennifer Skade). The first two issues of the new-format *Newsletter* (https://www.iucr.org/news/newsletter), designed by Brian McMahon and Michele Zema, appeared in the second half of 2018; since then, the *Newsletter* has reverted to quarterly publication.

The *Newsletter* is useful in providing extra publicity for IUCr Journals content, such as editorials and commentaries, and news of special issues, new Editors *etc*. It is also an attractive repository for meeting reports, and a special section provides information about the forthcoming IUCr Congress.

Other IUCr activities covered since the relaunch included the formation of the Gender Equity and Diversity Committee, a call for new contributing authors for the *Online Dictionary of Crystallography*, the publication of *International Tables for Crystallography* Volume H, *Powder Diffraction*, and a survey on archiving and using raw data. In addition, readers were brought up to date with the IUCr's outreach activities, for example, the Crystallography in Africa initiative. The People and History section included several articles of an international nature on the history of crystallography and celebrated recent awards, such as the 12th Ewald Prize, the inaugural W.H. and W.L. Bragg Prize for early-career crystallographers, and the 2020 Gjønnes Medal in Electron Crystallography, and the lives of crystallographers no longer with us.

Articles with educational content were also published, for example, a guide to using the terms crystal structure and lattice correctly and an article by the Editor on Bragg's balls and the demonstration of crystal packing. The *Newsletter* does not just aim to inform and educate but also entertain, and articles on topics such as crystallography in the movies, quartz and the use of Beevers–Lipson strips filled the `Editor's postbag'. Moreover, the role of crystallography in helping to solve global challenges is always at the forefront. In the first issue of 2020, we were pleased to publish a Letter to the Editor from Marvin Hackert describing the determination of the first molecular structure of the coronavirus spike protein, and the following issue included a COVID-19 section, containing articles describing crystallographic research on SARS-CoV-2 at synchrotrons around the world.

An average of 32 items was published in each issue. The e-mail editions were circulated to 13 500 crystallographers and structural scientists worldwide, and social-media channels provided additional exposure. The removal of the constraints imposed by print production has resulted in a publication that is cheaper to produce and able to publish articles in a timely manner. The attractive design includes prominent `buttons' to allow easy article submission, subscription and access to advertising information. A modest amount of full-page and banner advertising was achieved over the quadrennium, but it is hoped this can be increased to help cover costs. Two new low-cost advertising opportunities – New Products and Press Releases (for company news) – were introduced in 2020.

From the response of the international community, it seems that the new format of the *Newsletter* has been well received.

The current editor wishes to express their full appreciation of the work carried out by the Chester staff, especially Andrea Sharpe, in helping to make the *Newsletter* a success.

A.M. Glazer, Newsletter Editor

A11. Committee on Data (CommDat)

The Committee on Data was established by the IUCr Executive Committee at its meeting in Denver in July 2016. The specific terms of reference are `CommDat will advise the IUCr Executive Committee on all aspects of data with respect to policy and actions to be taken.' Details, including membership and consultants, can be found at https://www.iucr.org/iucr/governance/advisory-committees/committee-on-data.

Since CommDat's launch at the Hyderabad 2017 IUCr Congress, where we held our first meeting, there are the following matters to report.

(1) The IUCr Forum for CommDat (https://forums.iucr.org/viewforum.php?f=39&sid=8a6a0bda39ba305f88c05261b3bd7b82) has been very actively used.

(2) CommDat has participated fully in the work of the Prague IUCr Congress Programme Committee and the workshop immediately preceding it. Full details are given at http://www.xray.cz/ms/bul2019-2.htm, and CommDat's published contribution is at http://www.xray.cz/ms/bul2019-2/commdat.pdf.

(3) The top recommendation from the IUCr Diffraction Data Deposition Working Group (DDDWG) final report (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 was March 2019. The questionnaire can be found at https://docs.google.com/forms/d/e/1FAIpQLSdD-jIhcVIai1YcL8R-g35SMCtlTqcZl3aOANAOcfrQmOrTUw/viewform. Secondly, this top recommendation from the DDDWG was taken forward by the IUCr Commission on Biological Macromolecules (CBM) as a proposal to the IUCr Executive Committee, following the support of those present at its Open Commission meeting in Hyderabad. As discussed in Hyderabad, CommDat had endorsed this CBM proposal. CommDat worked with the CBM in the publishing of FAIR Diffraction Data Policy details for macromolecular crystallography papers in *Acta Cryst. Section D*, *IUCrJ*, *Acta Cryst. Section F* and *J. Appl. Cryst*. [see *e.g*. *Acta Cryst.* (2019). D**75**, 455-457, https://doi.org/10.1107/S2059798319004844].

(4) 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 version of checkCIF for raw data to automate the reusability is under development. Collaboration with COMCIFS is progressing towards this goal.

(5) CommDat has been active in the organization of workshops at ECM32 in Vienna in 2019 on Data Science Skills in Publishing: For Authors, Editors and Referees (see https://ecm2019.org/satellites/data-science-skills-in-publishing/) and at the upcoming Prague Congress on When Should Small Molecule Crystallographers Publish Raw Diffraction Data? (see https://www.iucr.org/resources/data/commdat/prague-workshop-cx) and on MX Raw Image Data Formats, Metadata and Validation, see https://www.iucr.org/resources/data/commdat/prague-workshop-mx-raw-data). CommDat assisted, along with COMCIFS, in the Italian Crystallographic Association CIFiesta in Naples in 2019 (see http://www.cristallografia.org/aicschool2019/eng/detail.asp?idn=3256).

(6) CommDat lecturers spoke at sessions dedicated to crystallographic data at the AsCA 2018/CRYSTAL 32 meeting in Auckland, New Zealand (see https://forums.iucr.org/viewtopic.php?f=39&t=411) and the ACA 2019 meeting in Covington, Kentucky (see https://forums.iucr.org/viewtopic.php?f=39&t=421) as well as at the very general symposium on data organized by PaNOSC (Photon and Neutron Open Science Cloud) in Trieste in late 2019 (see https://forums.iucr.org/viewtopic.php?f=39&t=426).

J.R. Helliwell, Chair

A12. Committee for Gender Equity and Diversity (GEDC)

This is a new committee of the IUCr, approved at the 2018 Executive Committee Meeting in Oviedo (August 2018). The committee was formally established in 2019, after a call for expressions of interest of membership. The IUCr approved 12 members (seven women, five men; five from Europe, four from Asia and three from the Americas).

The committee was very active in 2019, drafting an IUCr code of conduct, and an IUCr Gender Equity and Diversity Statement. These were submitted to the IUCr Executive Committee in 2019 at their meeting in Covington, Kentucky, and adopted with minor changes.

An IUCr web page for the GEDC has been established at https://www.iucr.org/iucr/governance/advisory-committees/gedc. The web page hosts the GEDC diversity statement and code of conduct.

The application form for IUCr funding of conferences and meetings now includes a link to these statements and these are considered as part of the process of recommending funding support from the Sub-committee on the Union Calendar.

The GEDC also recommended that the IUCr:
• Develop an updated mission, vision, values, statement that reflects diversity and inclusivity and the UN sustainable development goals, so that these can inform all policies.
• Develop a rights and responsibilities document, see https://sciencepolicy.agu.org/files/2013/07/AGU-Responsibilities-and-Rights-of-Scientists-Position-Statement-Adopted-2017-1.pdf.
• Sign up to the Hague ethical guidelines: https://www.opcw.org/hague-ethical-guidelines.
• Curate a list of crystallographers willing to be gender equity and diversity advisors for conference committees.

The COVID-19 pandemic in 2020 meant that the planned workshop to refresh the IUCr vision, mission, values at the 2020 Congress has been put on hold. Nevertheless, the committee addressed issues virtually during 2020 including: completing two surveys on efforts to promote women and gender diversity [one from the International Organization for Standardization (ISO) and one from the International Science Council (ISC)]; recommending that the IUCr sign up to the memorandum of understanding (MoU) created by the standing committee for gender equality in science; and approving an update to the IUCr diversity statement to better encompass race and ethnicity.

The IUCr GEDC recommended that the diversity of journal Editors and Commissions, as well as IUCr supported conferences and workshops, be reported at each General Assembly.

We are pleased that the IUCr Executive Committee now considers equity and diversity, routinely, when considering the impact of its decisions.

J. L. Martin, Chair

A13. Africa Initiative on Crystallography

The Africa Initiative focused on three general projects: equipment; OpenLabs and Schools; and networking and the African Crystallography Association (AfCA).

Equipment
Cote d'Ivoire: in March 2018 one single-crystal Apex diffractometer (with a low-temperature device) and one powder D5000 Bruker diffractometer were installed at Houphoet Boigny University, Cotonou, Cote d'Ivoire (Dierctor: Professor J. Tenon). The diffractometers were donated by Bruker, the shipping was paid by the IUCr and the low-temperature device by Ministere de l'education nationale de Cote d'Ivoire. The inauguration (22-23 March, with Professor Shechtman invited) was followed by an OpenLab with 40 participants (25 March - 3 April). This equipment is now used by colleagues from Cote d'Ivoire (Master and PhD students), Burkina Faso and Congo-Brazzaville.

Cameroon: New negotiations took place with Bruker, who gave an Apex licence and a low-temperature device for free. The IUCr, the University of Dschang and UNESCO Yaoundé contributed USD 7500, 8836 and 6000, respectively. This equipment will be inaugurated in 2021. One consequence of the installation of this equipment is that Dschang University has hired two lecturers in crystallography (Dr P. Kenfack, Department of Chemistry, and Dr B. Voufack, Department of Physics) as proposed by the Chair of the Africa Initiative.

Benin, Seme City: Negotiations with Bruker by Claude Lecomte and Michele Zema led to the provision of a D8 Quest Eco equipped with a low-temperature device at a significantly reduced cost. This D8 was installed in 2020. Two members of staff (Drs M. Agbahongbata and S. Bonou) have been hired to run the diffractometer.

OpenLabs and Schools
IUCr–UNESCO OpenLabs were organized in Ziguinchor (2017, in collaboration with the ICTP), Abidjan (2018) (see above), Accra (2019, parallel to the Pan African Conference on Crystallography, PCCr2) and Cotonou (2019, using a Bruker D8 Quest lent by Bruker). Other were planned for Congo-Brazzaville and Ethiopia in 2020 but were cancelled because of the Coronavirus pandemic.

Where no diffractometer was available, schools were organized (Franceville, Gabon, November 2018). One school in Lome in 2020 was cancelled, again because of the Coronavirus pandemic. The Chair notes that it is now almost impossible to organize OpenLabs with diffractometers lent by companies. Therefore in the future OpenLabs will be held in universities that have diffractometers (Cotonou, Dschang, Benin, North Africa and South Africa) or during PCCrs.

Networking, PCCrs, AfCA
The Pan African Crystallography meetings (PCCrs) contribute to crystallography networking in Africa. Following the first PCCr in Dschang (2016), the joint 2nd Pan African International Conference on Crystallography and African Light Sources was successfully hosted at the University of Ghana, 28 January – 2 February 2019, in partnership with the Ministry of Environment, Science, Technology and Innovation (MESTI) and the Ghana National Petroleum Company (GNPC). The conference was under the auspices of the IUCr; the United Nations Education, Scientific and Cultural Organization (UNESCO); the International Atomic Energy Agency (IAEA); the Light Sources for Africa, Asia, Americas and the Middle East project (LAAAMP); and the African Academy of Sciences (AAS). It was chaired by Professors B. Agyei-Tuffour and Kingsford, and there were 350 participants from over 35 countries. The Chair of the Africa Initiative was responsible for the bursaries (funding research and attribution) and was also a member of the Local Programme Committee (chaired by Professor G. Artioli).

It had been planned to hold PCCr3 in Nairobi, Kenya, in January 2021, but it has been rescheduled for 2022.

The PCCrs are extremely important in helping our African colleagues to follow crystallography news. The Chair feels that whatever the pandemic situation, PCCrs in the future must be organized on site and also remotely to allow many Africans to attend, and the IUCr should help in the organization of the remote conferences.

During PCCr2, an AfCA steering committee was created, chaired by Professor Delia Haynes (Stellenbosch University) and Dr P. Kenfack (Dschang University) as General Secretary. AfCA is subdivided into five regions with one representative for each region on the steering committee. This steering committee has already proposed rules for the PCCrs and developed the statutes for AfCA. AfCA should be launched during the opening ceremony for PCCr3 and become a Regional Associate of the IUCr in the coming years.

The next action should be to help Sub-Saharan African colleagues to create further national associations, as only Cameroon, Cote d'Ivoire and Congo Brazzaville have their own associations. Only the Cameroon Crystallographic Association is an IUCr member. The Chair notes, however, that becoming a member of the IUCr is almost impossible for African national associations, as it is too expensive for such emerging young associations.

C. Lecomte, Chair

A14. IUCr/Oxford University Press Book Series Committee

In 2017 our highly esteemed Chair Davide Viterbo passed away whilst in office. In 2017, in consultation with the IUCr President and the IUCr Executive Secretary, a diverse, highly experienced membership was assembled as follows: J.R. Helliwell (Chair, UK), G. Chapuis (Switzerland), J. Gulbis (Australia), R. Herbst-Irmer (Germany), H. Maynard-Casely (Australia), P. Mueller (USA), M. Nespolo (France), N. Yagi (Japan), X. Zou (Sweden), K.A. Kantardjieff (USA; *ex officio* as Chair of Commission on Crystallographic Teaching) and S. Adlung (*ex officio* representative of Oxford University Press).

The books published within the book series stretch back about 20 years and are now commissioned in two categories: Monographs on Crystallography and Texts on Crystallography.

We thank the members who retired from the Committee: Christian Baerlocher (Switzerland), Peter Colman (Australia), Yuji Ohashi (Japan), Thomas Mak (Hong Kong China) and Adam Pietraszko (Poland).

A visit was made to Oxford University Press (OUP) in April 2018 by the IUCr Executive Secretary, the IUCr Executive Managing Editor and the Chair of the Book Series Committee. The meeting there discussed current book titles under contract with authors within the Book Series. Also, following the meeting, OUP confirmed that an increase of revenues to the IUCr from sales of the books would be made.

Poster presentations were made about the Book Series titles by the Chair at the British Crystallographic Association 2018 Conference and at the European Crystallographic Meeting (ECM31) in Oviedo, Spain, in 2018.

The IUCr has very nicely restyled the books sections of the IUCr website, see https://www.iucr.org/publications/iucr-oup.

In both 2018 and 2019 the Book Series Committee members individually provided assessments of two book proposals, which were brought together as a Chair's report in each case. These four reports were first provided to the IUCr Executive Committee, which endorsed them, and then they were submitted to OUP. Another book, in full draft form, was requested by OUP to be commented on by the Book Series Committee, although outside the monographs or teaching books. This report was first provided to the IUCr Executive Committee, which endorsed it, and then it was submitted to OUP. Likewise a second, *i.e.* duly revised full draft, was received, a report was again provided to the IUCr Executive Committee, which endorsed it, and then it was again submitted to OUP.

In 2018 two IUCr Monographs on Crystallography were published. These were *Biological Small Angle Scattering Theory and Practice* by Eaton E. Lattman, Thomas D. Grant and Edward H. Snell (https://global.oup.com/academic/product/biological-small-angle-scattering-9780199670871?cc=gb&lang=en&) and *Aperiodic Crystals From Modulated Phases to Quasicrystals: Structure and Properties*, Second Edition, by Ted Janssen, Gervais Chapuis and Marc de Boissieu (https://global.oup.com/academic/product/aperiodic-crystals-9780198824442?cc=gb&lang=en&).

In order to ensure consistency with IUCr nomenclature policies, and to reduce the chance of errors, we have affirmed to OUP the need for us to assign volunteer(s) with requisite subject expertise, ideally from our Committee, so as to review a full draft of a new text in our Book Series before publication by OUP in the IUCr's name. This new approach was identified at the start of the current Chair's tenure when members were invited in 2017.

A meeting of the Committee and with the OUP Exhibition Delegate will be held at the IUCr Congress in Prague.

J. R. Helliwell, Chair

A15. Regional and Scientific Associates

A15.1 American Crystallographic Association (ACA)

This triennial report of the activities of the ACA (http://www.amercrystalassn.org/) as a Regional Associate of the IUCr is an overview of the more detailed annual reports presented each year since the Hyderabad Congress in 2017, as well as an outline of future activities announced by the ACA.

Serving as ACA Presidents during the period 2017-2019 were: Amy Sarjeant (2017), Lisa Keefe (2018) and Joseph Ferrara (2019). Diana Tomchick continued as the Secretary and Ilia Guzei relieved Sue Byram in 2019 as the Treasurer. S. N. Rao is the Chief Financial Officer (CFO) and Bill Duax served as Chief Executive Officer (CEO) until the end of 2019. Tomislav Friscic served as the Canadian National Committee for Crystallography Representative. Brian Toby is the ACA President for 2020. Kristin Stevens is the Director of Administrative Services and Kristina Vitale the Membership Secretary.

ACA activities are primarily focused on its Annual Meetings, support for the excellent Summer Schools, and the publication of the Newsletter *ACA RefleXions* (Editors Paul Swepston and Edwin D. Stevens), which is a meaningful source of information about all ACA activities (https://www.amercrystalassn.org/aca-reflexions).

The ACA Council works very efficiently to achieve a balanced budget, the main income coming from the Annual Meetings and from the members' dues. The membership of the ACA was steady in this triennium, with just over 1000 members. Most ACA members are from the USA and Canada, although there are some from other countries around the world.

The ACA 67th Annual Meeting in 2017 (an IUCr Congress year) was held from 26 to 30 May in New Orleans. At this meeting of 544 participants 27% were female. Twenty-six vendors participated in the Exhibit Show. The Programme Chairs were Yulia Sevryugina and Ilia Guzei.

Four outstanding scientists were honoured with the ACA's major awards at this meeting: Zbigniew Dauter (Patterson Award), Christine Durham (Etter Early Career Award), Helen M. Berman (David Rognlie Award) and James O'Brien (Elizabeth Wood Science Writing Award).

The ACA 68th Annual Meeting in 2018 was held from 20 to 24 July in Toronto, Ontario, Canada. The Chairs were Gerald Audette and Tiffany Kinninbrugh.

The 2018 Award Winners were Simon Billinge (Warren Award), Frank Hawthorne (Buerger Award) and Jason McLellan (Elizabeth Wood Science Writing Award). The Poster Session was named after the late Judy Flippen-Anderson, the 1991 ACA President. There were 663 attendees at this meeting.

The 69th Annual Meeting in 2019 was held from 20 to 24 July in Covington, Kentucky. Stephan Ginell and Vivien Yee co-chaired this meeting. Poster Chairs were Louise Dawe and David Rose. There were 519 attendees, the meeting was supported by 25 sponsors (including the IUCr) and a moderate financial profit was achieved. The 2019 ACA Award Winners were Brian Toby & Robert Von Dreele (Trueblood Award), Eaton (Ed) Lattman (Fankuchen Award), Bryan Chakoumakos (Bau Award) and Efrain Rodriguez (Etter Early Career Award).

The 2020 (70th) Annual ACA Meeting will be held in San Diego, California, from 2 to 6 August. The 2021 (71st) ACA Meeting will be held in Baltimore, Maryland, from 31 July to 3 August, and the 2022 (72nd) in Portland, Oregon, from 30 July to 2 August.

Meeting statistics and details about programmes and adjacent workshops are available at https://www.amercrystalassn.org/past-meetings.

The ACA Summer Courses for Chemical Crystallography were organized either in Notre Dame or in Northwestern Universities (info@acasummercourse.net) by Charlotte Stern, Allen Oliver, Christos Malliakas and Amy Sarjeant. They are very high level and very popular.

The ACA/AIP journal *Structural Dynamics* achieved an impact factor of 2.99 in 2019 (https://www.researchgate.net/journal/2329-7778_Structural_Dynamics). The journal is not bringing any profit to the ACA yet. Recently Majed Chergui stepped down as the Editor-in-Chief of the journal.

The ACA Fellows Program was created to recognize a high level of excellence in scientific research, teaching and professional duties as well as service, leadership and personal engagement in the ACA and the broader world of crystallography and science. During the past three years Marilyn Olmstead, Brian Toby, Andrew Allen, James Britten, Majed Chergui, Wladek Minor, Thomas Proffen, Janet Smith, Robert Von Dreele, Craig M. Brown, Susan K. Byram, Charles W. Carter Jr, Elspeth F. Garman and Xiaoping Wang joined the rank of ACA Fellows.

For the ACA History Fund, Virginia Pett has compiled a series of Living History articles that have been published in *RefleXions*. The full documents with references have been archived in the AIP History Center Niels Bohr Library & Archives (NBLANDA).

The Canadian National Committee for Crystallography (CNCC) (http://xtallography.ca/) is chaired by Tomislav Friscic, the Vice Chair is Louise Dawe, the Secretary is Michel Fodje and the Treasurer is Brian Patrick. The CNCC organized many excellent, crystallography-oriented courses and schools in the last triennium.

As the National Science Foundation (NSF) recently de-funded the US National Committee on Crystallography (USNC/Cr), it remains to be decided which organization will be the adhering body for the USA to the IUCr after 2020.

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

H.A. Dabkowska, IUCr Representative

A15.2 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, albeit last year's activities were impacted by the COVID-19 pandemic.

AsCA Executive Officers

In the period 2017–2019 the office bearers of AsCA (elected in Hanoi in December 2016) were Jennifer Martin (President, Australia), Xiao-Dong Su (Vice-President, China), Edward R.T. Tiekink (Secretary/Treasurer, Malaysia) and Pinak Chakrabarti (Immediate Past President, India). The current Executive Officers for the term 2020–2022 were elected in Singapore and are Xiao-Dong Su (President, China), Genji Kurisu (Vice-President, Japan), Siegbert Schmid (Secretary/Treasurer, Australia) and Jennifer Martin (Immediate Past President, Australia).

AsCA scientific meetings

AsCA 2018. The 15th Conference of AsCA (AsCA 2018/Crystal 32) was held at The University of Auckland, New Zealand, 2-5 December 2018. Profsessors Chris Squire and Kurt Krause were Co-chairs of the Local Organizing Committee and Professors 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 and Vietnam 1. Gender: 131 female, 295 male; 31%:69% (51 undisclosed). Local Organizing Committee (LOC) members (total

10): 3 female, 7 male. International Programme Committee members (total 14): 6 female, 8 male. Plenary and keynote lecturers (total 10): 6 female, 4 male. The Plenary Lectures were given by David Eisenberg (USA), Susan Lea (UK), Cameron Kepert (Australia) and Amy Rosenzweig (USA), and the Keynote speakers were Yanli Wang (China), Hiroshi Kitagawa (Japan), Richard Neutze (Sweden), Catherine Day (New Zealand), Deanna D'Alessandro (Australia) and Ayana Sato-Tomita (Japan). Speakers in microsymposia (total 107): 33 female, 74 male. Chairs of microsymposia (total 38): 18 female, 20 male. Chairs of plenary and keynote lectures (total 10): 4 female, 6 male.

AsCA 2019. The 16th AsCA scientific meeting (AsCA 2019) was held at the National University of Singapore in December 2019, with Professor J. J. Vittal as the Local Chair. The conference attracted 526 participants from 29 countries: Japan (93), India (68), Korea (64), Singapore (55), China (46) and Taiwan (35) were represented by the largest number of participants. The conference adopted the IUCr's gender equity statement and aimed for gender balance where possible. The International Programme Committee comprised 11 female and 10 male members including Co-chairs Jenny Martin, Sara Sandin and Edward Tiekink. The LOC comprised 1 female and 8 male members (11% women). During the conference 22/66 (33%) symposia Chairs, 68/172 (39%) oral presenters and 19/46 (41%) younger participants were female. Overall 161 attendees were women (31%).

The AsCA conference goal is to strive for gender balance in plenary/keynote speakers, invited microsymposia speakers, selected microsymposia speakers and Co-chairs. We know this will take time, so we are collecting and reporting data to provide a baseline with the aim to move towards gender balance at each successive conference (*i.e.* no less than 40% delegates/speakers of one gender).

The financial report for the conference was not yet available at the time of writing this report. It is understood that a substantial surplus was achieved. Distribution of this surplus is still being negotiated.

AsCA 2020 and beyond. At the Council meeting held in Hanoi on 6 December 2016, a proposal was received from the Malaysian representative to host the 17th AsCA Conference at Sunway University, Petaling Jaya, Malaysia, during December 2021. Unfortunately, this conference had to be postponed to 2024 because of COVID-19 travel restrictions. The next AsCA conference therefore is to be held in the Republic of Korea in October 2022 on Jeju Island (also subject to favourable global development regarding the pandemic as well as travel funds). The AsCA Executive Committee is in conversation with the local organizers regarding establishment of the Local Organizing Committee as well as the Programme Committee.

AsCA Regional Committee membership

As Singapore and Bangladesh have become full members of the IUCr, it is planned to include Cambodia and Sri Lanka in their place as members of the AsCA Regional Committee of the IUCr (along with Indonesia, Malaysia, Thailand and Vietnam).

An application was received from the crystallographic community in the United Arab Emirates in 2020 for membership of AsCA. This was favourably considered by the Executive Committee and will be put to the AsCA Council for approval at the upcoming business meeting during the 2021 IUCr Congress.

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.

S. Schmid, Secretary/Treasurer of AsCA

A15.3 European Crystallographic Association (ECA)

The ECA is a scientific association with national and individual members, and corporate affiliates. It has 13 SIGs (Special Interest Groups) and three GIGs (General Interest Groups). The ECA main events – the ECMs (European Crystallographic Meetings) – were held in Oviedo, Spain, 22-27 August 2018 (conference Chair: Santiago Garcia Granda) and in Vienna, Austria, 18-23 August 2019 with several satellite meetings and workshops usually preceding the conferences (the three conference Chairs were Klaudia Hradil, Kristina Djinovic-Carugo and Ronald Miletich).

Some statistics for ECM-32 (with ECM-31 in parentheses) are 193 (222) ECA individual members participating, 468 (316) other regular participants, 247 (204) students or retired people, 76 (75) exhibitors, 36 (39) accompanying persons and 40 (61) children. Overall, there were 1061 (983) registered participants. The proportion of women was nearly 35 (39)%.

The numbers of abstracts in different focus areas were 165 (179 at ECM-31) in Biological and Macromolecular Crystallography, 103 (158) in Materials and Minerals, 117 (119) in Physics and Fundamental Crystallography, 142 (157) in Chemical Crystallography, 64 (116) in Experimental and Computational Techniques and 17 (59) in General Interest sessions.

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

As usual, two sessions of the ECA council meeting also took place during the ECMs.

The main ECA prizes were awarded as follows. In 2018 the Max Perutz Prize was awarded to Sine Larsen (a former IUCr President) in recognition of their multi-faceted contributions to crystallography, including crystal structure analyses of organic molecules and proteins, charge-density studies, and the development of synchrotron-radiation facilities. In 2019, it was awarded to Professor Elspeth Garman from the Department of Biochemistry, University of Oxford, UK, in recognition of their invaluable contribution to the field of macromolecular crystallographic methods by developing tools and methods for improving the quality of diffraction data. The ninth Erwin Felix Lewy Bertaut Prize, awarded to young scientists, was given to Matthias Zschornak from Technical University Bergakademie Freiberg in 2018, in recognition of their outstanding contributions to the the development of resonant X-ray diffraction, their structural studies of perovskites, and their extensive electronic calculations providing a thorough physical understanding of the properties of important materials.

A new prize was introduced. The International Kálmán Prize preserves the memory of the late Alajos Kálmán, an eminent scientist in the field of chemical crystallography. The prize was established by the Hungarian Chemical Society and was endorsed by the ECA. The first prize was awarded to Professor Luigi Nassimbeni from University of Cape Town, South Africa.

There was quite significant renewal of the ECA Executive Committee (EC) in 2018. The new committee was elected as follows: *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). Names in italics indicate the four persons from the previous committee who remained in office.

The EC regular winter meetings, which are always very efficient, were held in February 2017 in Asturias, Spain, in 2018, in Vienna in February 2019 in Berlin (at the office of the current ECA President, Udo Heinemann) and in February 2019 in St Aubin, France, close to the location of ECM-33. More online ECA EC meetings were organized on the changes of the statutes, with new candidates for national membership and with the bidders for the ECM in 2025. There are two new candidates for national membership – Romania and United Arab Emirates.

The ECA schools - European Schools of Crystallography (ECS) - are already regular and are organized under detailed ECA guidelines. The fifth European Crystallographic School (ECS5) was held 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 6th ECS in Budapest was postponed from July 2020 to July 2021 and will be purely online. The 7th ECS will be in Lisbon, Portugal, and preliminary interest for ECS8 was shown by Manfred Weiss from Berlin.

The African Crystallography Steering Committee has been established and defined six African regions. It is chaired by Delia Haynes and it is expected that it will lead to the foundation of the African Crystallographic Association (AfCA). The 3rd PanAfrican Crystallographic Conference (PCCr3), initially scheduled for January 2022 in Kenya, will now be online (e-PCCr3) but still in January 2022, with the aim of consolidating the network of African crystallographers, followed by a physical PCCr3 in 2023, which will serve as a platform for the launch of the African Crystallographic Association.

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

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

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

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

R. Kuzel, IUCr Representative

A15.4 Latin-American Crystallographic Association (LACA)

LACA has experienced rapid growth since it was approved as a Regional Associate (RA) at the 23rd IUCr Congress and General Assembly in 2014 in Montreal. LACA had a strong presence at the Hyderabad 2017 Congress and has shown that it is a productive and vibrant RA. Detailed activities of our region can be found at https://www.iucr.org/iucr/ab.html/regional-associates/latin-american-crystallographic-association. Highlights of activities and achievements in this quadrennium are as follows.

Meetings organized by LACA

LACA successfully celebrated its III and IV Regional Meetings and conducted three very successful schools and an OpenLab:

1. The IUCr-UNESCO-LAAMP OpenLab was held in Costa Rica, 4-9 December 2017, at LANOTEC-CeNAT-CONARE, Escuela de Química of Universidad de Costa Rica, and Escuela de Ciencias e Ingeniería de Materiales of Tecnológico de Costa Rica. Intensive lectures and practical sessions in single-crystal and powder diffraction took place. Many students and young researchers from most Central American countries were able to participate.

2. A very successful 1st LACA School on Small Molecule Crystallography took place at Facultad de Química, Universidad de la República, in Montevideo, Uruguay, 19–25 February 2018.

3. Pontificia Universidad Católica de Valparaíso (PUCV), Valparaíso, Chile, hosted the III-LACA Meeting on 10-12 October 2018, along with the I Meeting of the Chilean Crystallographic Association (AChCr). An Olex2 workshop (OlexSys) at PUCV and a PDF-4 Database (ICDD) workshop at Universidad Federico Santa María (UFSM) preceded the meeting. New LACA authorities were elected and the proposal from Colombia to host the IV-LACA Meeting and II-LACA School in 2019 was approved. Requests to hold the III-LACA School in Mexico (March 2020) and the IV-LACA School in Chile (December 2020) were also approved.

4. The II-LACA School: Structure Solution from Single Crystal and Powder Diffraction Data took place on 1-6 October 2019 at Parque Tecnológico Guatiguará of Universidad Industrial de Santander (UIS), Bucaramanga, Colombia.

5. The IV-LACA Meeting followed the II-LACA School, at UIS in Bucaramanga, on 7-10 October 2019. The I Meeting of the Colombian Crystallographic Association was also held. A group of crystallographers from different Colombian institutions will work on reviving the Colombian Crystallographic Society and applying for membership of the IUCr. The LACA General Assembly (GA) ratified the LACA authorities elected at the III-LACA Meeting in Chile. Possible venues for the 2021 and 2022 meetings were considered, since 2020 was a Congress year. Costa Rica and Uruguay are the possible sites, although the meetings will now be in 2022 and 2024.

6. The III-LACA School, focused on small molecule crystallography, was held as a virtual event on 23-27 November and 7-11 December 2020. The feedback on the virtual format for this school was very positive.

Other meetings organized in the region

1. Universidad de San Carlos de Guatemala (founded in 1676) was the venue of the Crystallography and X-ray Diffraction Seminar in May 2018. The Asociación Guatemalteca de Cristalografía was formed.

2. Professor Ada Yonath, winner of the Nobel Prize in Chemistry in 2009, was the Invited Speaker at the International Chemistry Congress at ESPOCH in Riobamba, Ecuador, 31 July - 2 August 2018. Professor Yonath gave an inspiring lecture to an auditorium of more than 500 students, professors and researchers from Ecuadorian universities and neighboring countries. A three-day pre-Congress course Introduction to Crystallographic Techniques was also organized.

3. Several workshops were organized by the Commission on Crystallography in Art and Cultural Heritage (CrysAC) (in Mexico and Chile), the Commission on Mathematical and Theoretical Crystallography (MaThCryst) (in Colombia), Macromolecular Crystallography Schools were held in Brazil and Uruguay, and the Commission on Small-Angle Scattering held a To.Sca.Lat School in Brazil. IUCr Commissions have supported all events in the LACA region.

Involvement of LACA in IUCr activities

The Latin American presence in IUCr Commissions has increased significantly, indicating that the research interests of our community cover most of the areas represented by the IUCr Commissions. This is also due to the receptive nature of the Union.

Our region is represented on the International Committee (IPC) of the 25th IUCr Congress. Professors José Miguel Delgado (Venezuela), Diego Lamas (Argentina), and Abel Moreno (Mexico) actively participated in the discussions of the IPC.

Several teams from Latin America have had the opportunity to get training and carry out experiments at synchrotron sources around the world through the LAAAMP initiative. The participation of IUCr, LAAAMP, and LACA representatives in the II Latin America and the Caribbean Open Science Forum (CiLAC) in Panamá City in October 2018 provided an opportunity to reach scientists and policy makers to establish collaborations that can have a positive impact on the scientific, economic, and social development of our region. The participation of the IUCr and LACA in future events should continue.

Three new Co-editors from Latin America joined the Editorial Board of *Acta Crystallographica Section E* in 2017-2020. Professor Javier Ellena (IFSC, Brazil) joined in 2017, and Professor Vojtech Jancick (UNAM, Mexico) and Dr Alexander Briceño (IVIC, Venezuela) joined in 2020.

Large-scale facilities

The new state-of-the-art Brazilian Synchrotron facility, Sirius, started operation of the first beamline in 2020. The first experiments carried out allowed researchers from University of São Paulo (USP) to study proteins from the SARS-Cov-2 virus. It is expected that 14 beamlines will be set up and will be operative in the next few years. Two other large-scale facilities are planned for the region. The Mexican Society of Synchrotron Light (SMLS) was founded in December 2019 to promote the construction of the Mexican Synchrotron Light Source in the state of Hidalgo. The National Commission for Atomic Energy (CNEA) in Argentina is planning the construction of Laboratorio Argentino de Haces de Neutrones.

Activities of Latin American Crystallographic Societies and Associations

The Argentinian Association (AACr), the Brazilian Association (ABCr), and the Mexican Society (SMCr) have held their regular meetings and courses. Argentina, Chile (AChCr), and Uruguay (RUCr) have been particularly active in national Crystal

Growth Competitions. Participants from these countries have received awards in the IUCr competition. The mineral exhibit continues to be an attraction at Encuentro con la Física, Química, Matemática y Biología organized every year at Universidad de Los Andes in Mérida, Venezuela. In 2020, most of the activities took advantage of online meeting platforms.

G. C. Díaz de Delgado, IUCr Representative

A15.5 Worldwide Protein Data Bank (wwPDB)

The past four years, and particularly the current COVID-19 pandemic, have emphasized ever more emphatically the critical importance of the Protein Data Bank (PDB) as an international resource for science and society. The IUCr can take great pride in the role played by crystallographers in its establishment and development.

The four original partners in the Worldwide PDB (wwPDB), the RCSB-PDB in the USA, PDBe in Europe, PDBj in Japan and BMRB (NMR database), have now been joined by the EMDB (Electron Microscopy Database), giving five core partners. The centres collaborate intimately and share the load, maintaining a single, freely-accessible curated archive of three-dimensional structures of biological macromolecules. The wwPDB was formally designated a Scientific Associate of the IUCr in 2015, and the IUCr provides a representative on the wwPDB Advisory Committee (wwPDB-AC).

The wwPDB partners focus on fast and accurate processing and annotation of new entries, together with remediation of older entries where necessary. Most of the development work is done in the background, by expert Task Forces drawn from the relevant communities, but implementation of new policies and release of new tools must be ratified by the wwPDB-AC.

Highlights from the past 4 years, focusing on those of greatest relevance to the IUCr, are as follows:

• As of April 2021, the archive comprises over 176,000 macromolecular structures, the majority (88%) determined by crystallography, and smaller numbers by NMR or cryo-EM. Some 14,000 structures were deposited in 2019 at a rate that, together with the growing size and complexity of entries, places increasing demands on the efficiency of annotation, checking and validation.

• The wwPDB has been of critical value in the fight against COVID-19. The first SARS-CoV-2 protein structure was deposited and released in February 2020 and since then over 1000 more have been determined and released immediately after processing, as crucial data towards new COVID therapies. Both drug and vaccine development continue to be informed by this molecular knowledge base. • The number of structures determined by cryo-EM is increasing rapidly as new detectors and more powerful processing protocols are applied. The total number is now almost 7000, with 2400 new structures deposited in the past year. Many of these are also very large and complex.

• Robust validation procedures are critical for maintaining the quality of the archive. An important advance in the past four years has been the implementation of robust validation of ligands associated with protein structures, using BUSTER software. Validation reports now analyse ligand geometry and their fit to bias-removed electron density.

• The size and complexity of deposited structures continues to increase; the number with molecular weight > 500,000 is growing significantly, as is the number with many chains and more than 100,000 atoms. To cope with this, the old `card image' format has been superseded to allow extremely large structures, such as ribosomes, to be presented in a single file. This change has been well accepted by users of the archive.

• Validation reports have now been implemented for both NMR and cryo-EM depositions, following the pattern developed for crystallographic structures, but with method-specific variations. These continue to be enhanced by the relevant Task Forces.

• In response to requests from the IUCr Commission on Biological Macromolecules, the wwPDB will now make the e-mail contact addresses of lead depositors available to users. This is necessary because of the growing number of structures that are never published in the primary literature.

• The wwPDB has also agreed with an IUCr initiative seeking proper, curated deposition of the raw data underpinning structures deposited to the PDB. As an initial step, depositors will be directed towards existing curated depositories while the PDB will seek further funding to expand on this initiative.

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

• Work continues 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 raw data sets and the SASB database that is being developed, led by Professor Jill Trewhella, for archiving biological SAXS data.

• Plans to establish a Chinese partner site (PDBc) for the wwPDB, led by Drs Wenqing Xu and Zhijie Liu, are now well advanced. Funding for the initiative has been obtained and although recruitment and training of key personnel has been disrupted by COVID-19 it is now proceeding well. This new partner site will be of great importance for dealing with the continuing flood of depositions. A similar initiative in India is also planned.

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

The wwPDB archive is of enormous importance to the life sciences community, and the IUCr can be proud of the contribution made by the crystallographic community. 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

A15.6 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

A15.7 International Organization of Crystal Growth (IOCG)

The most important event concerning the IOCG (http://www.iocg.org/) in 2019 was the official meeting of the association, the 19th International Conference on Crystal Growth and Epitaxy, ICCGE-19, 28 July – 2 August 2019, in Keystone, Colorado, USA. 24 general sessions were organized. The conference was successful and well organized, even if the number of participants was lower than in the previous edition. The week before the conference, from 21 to 27 July, the 17th International Summer School on Crystal Growth, ISSCG-17, was held, with about 100 students. Both the conference and the school were supported by the IUCr. Many members and consultants of the IUCr's Commission on Crystal Growth and Characterization of Materials (CCGCM) were involved in the organization of the conference and the school, but I would like to mention in particular the contribution of Thomas F. Kuech, Chair of ISSCG-17 and member of the CCGCM.

The IOCG is also the chance to consolidate the officers and Executive Committee members of the organization. Koichi Kakimoto (Japan) was confirmed as President (also a consultant of the CCGCM). Co-Vice-Presidents are H. Dabkowska (Canada) and E. Vlieg (Netherlands) (member of the CCGCM), the Secretary is S. Krukowski (Poland), and the Treasurer is J. Derby (USA). The members of the Executive Committee are Abel Moreno (Mexico), J. Y. Wang (China), both consultants of the CCGCM, Y. Mori (Japan), D. Maes (Belgium), A. Voloshin (Russia), C. Frank-Rotsch (Germany), J. De Yoreo (USA) and P. Muller (France). As IUCr representative, I had the chance to take part in the meetings of the Executive Committee of the IOCG in Keystone, and also to take part in the Executive Committee's discussions by e-mail during the triennium.

The next International Conference on Crystal Growth and Epitaxy, ICCGE-20 and ISSCG-18, will be held in Naples, Italy, in 2022. Antonio Vecchione and I will be the Co-chairs of the conference. The International Summer School on Crystal Growth ISSCG-18 will be in Parma, Italy, and will be co-chaired by Roberto Fornari, Past President of the IOCG and also a past Chair of the CCGCM.

The IOCG General Assembly also evaluated the proposals for ICCGE-21 and ISSCG-19, and it was decided that these events in 2025 will be organized in China.

At the end of 2010 the European Network of Crystal Growth (ENCG) was formed. One of the scopes of the ENCG is the organization of the European Conference on Crystal Growth (ECCG). After ECCG4, which was held in Glasgow in 2012, and ECCG5 in Bologna in 2015, the Sixth European Conference on Crystal Growth was organized in Varna, Bulgaria, together with the Second European School on Crystal Growth. Many members and consultants of the Commission on Crystal Growth and Characterization of Materials were involved in the organization of these events. Both events were very successful. It had already been decided that in 2021 the Seventh European Conference on Crystal Growth together with the Third European School of Crystal Growth will be held in Paris, France. These events are quite important for keeping the crystal-growth tradition alive in Europe.

I would also like to mention that since IYCr some national associations have started campaigns to promote crystal growth among young students and scholars. They have offered visits to crystal-growth laboratories and organized crystal-growth contests. Initiatives have been organized in several countries such as Spain, Italy, Poland and Germany.

In conclusion I would like to report that the IOCG is very active in promoting crystal-growth conferences and schools, and that cooperation in this field with the CCGM is very strong.

A. Zappettini, IUCr Representative

A16. Bodies not belonging to the Union

A16.1 Interdivisional Committee on Terminology, Nomenclature and Symbols of the International Union of Pure and Applied Chemistry (IUPAC ICTNS)

The Chair of the Commission on Crystallographic Nomenclature is a member of the ICTNS.

Members of the ICTNS receive regular requests to referee papers and reports submitted to the IUPAC. Most submissions are in specialized areas unrelated to crystallography but reviews were written for three manuscripts on general topics (the definition of the mole and Avogadro's number, uncertainty of standard atomic weights, and end-of-line hyphenation).

In January 2017 an IUPAC project started titled: BACKUP, MAINTENANCE, AND REDEVELOPMENT OF THE IUPAC GOLD BOOK WEBSITE (see https://iupac.org/projects/project-details/?project_nr=2016-046-1-024). The first e-mail to the ICTNS about this project was sent in January 2018; there were no further communications until 2019. During the last year the ICTNS has been circulating documents and meeting electronically to set up procedures for adding new definitions to the Gold Book. Considerable time is being contributed to this effort by some of the other ICTNS members but progress has been slow.

C.P. Brock, IUCr Representative

A16.2 International Science Council (ISC)

The International Science Council (ISC) was created in 2018 from a merger of the International Council for Science (ICSU; founded in 1931) and the International Social Science Council (ISSC; founded in 1952). I attended their joint General Assembly in Taipei in October 2017, when members of ICSU and ISSC made the decision to merge the two organizations to become the International Science Council (ISC). The ISC represents 40 international scientific unions (including the IUCr) and associations, and more than 140 national and regional scientific organizations, and has the stated aim to be `a global voice for science'.

Key Meetings (2017–2021)

October 2017, Taipei: Vote to merge ISCU and ISSC into ISC.

July 2018, Paris: 1st General Assembly meeting: The first General Assembly meeting of ISC was held in July 2018 in Paris to finalize the merger, work on governance issues, and elect a Governing Board. The Governing Board consists of 16 members, including the President (Daya Reddy, South Africa), the President-elect (Peter Gluckman, New Zealand), as well as four further officers and ten additional ordinary members. Heide Hackmann serves as the Chief Executive Officer of ISC, which is headquartered in Brussels.

October 2018, ISC Governing Board: An Action Plan was initiated at the October 2018 meeting of the ISC Governing Board. The Action Plan is intended to be a living document, allowing the ISC the flexibility to respond to new and emerging opportunities, and to adapt as needed. At that meeting, members of the Board identified four domains of critical importance for contemporary science – see below.

1-4 February 2021, Virtual (using Hopin) Extraordinary General Assembly meeting: The purpose of this meeting was to elect members of the Elections Committee, and discuss and vote on a number of proposed changes to the ISC Statutes and Rules of Procedure. Items discussed included membership categories, Governing Board composition, voting procedures, *etc*.

11-15 October 2021, Virtual 2nd ISC General Assembly (GA): At the 2nd GA meeting the proposed changes to the ISC Statutes and Rules of Procedure will be finalized, a membership dues proposal is expected, and reports on various ISC activities will be presented. Dues are currently paid as before the merger by organization. Questions remain: if dues are to be paid by country, how will this be allocated across different organizations from each country?

ISC Action Plan

The Action Plan (https://council.science/actionplan/) was initiated at the October 2018 meeting of the ISC Governing Board. At that meeting, members of the Board identified four domains of critical importance for contemporary science to frame the Council's scientific work in the coming years that require action from the ISC as the global voice for science. The domains are:

Domain One: The 2030 Agenda for Sustainable Development

Domain Two: The Digital Revolution

Domain Three: Science in Policy and Public Discourse

Domain Four: The Evolution of Science and Science Systems

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

• Freedom of movement

• Freedom of association

• Freedom of expression and communication

• Freedom of access to data and information.

Other activities

International Years (IYs): IYs are organized to educate the public and celebrate important aspects of how science impacts life and the world in which we live. ISC works to have science recognized by the United Nations via International Year proclamations - just as the UN designated 2014 as the International Year of Crystallography (IYCr). Recent and future International Years include

2019: International Year of the Periodic Table of Chemical Elements

2020: International Year of Plant Health

2020/2021: International Year of Sound

2021/2022: International Year of Caves and Karst

2022: International Year of Basic Sciences for Sustainable Development

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

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

M.L. Hackert, IUCr Representative

A16.3 ISC Committee on Data for Science and Technology (CODATA)

CODATA is the interdisciplinary Committee on Data for Science and Technology of the International Science Council (ISC). It is a worldwide network whose mission is `to strengthen international science for the benefit of society by promoting improved scientific and technical data management and use'. Specific projects are addressed by Task Groups answerable to the CODATA General Assembly, by Working Groups, by themed workshops or conferences, and by publications on specific aspects of data handling or data compilation. Full details of CODATA activities are available from its website at http://www.codata.org.

CODATA organized two workshops in 2017 on the theme of interoperability of scientific data in which the IUCr took part, making oral presentations at each, firstly in Paris by John R. Helliwell and then in London by Simon Coles (as JRH alternate). The IUCr is regarded as one of the disciplinary groups that have made considerable advances in exploiting modern data resources and thereby can provide examples and advice, which we did at both workshops.

In 2018, as IUCr Representative I attended CODATA's biannual conference and General Assembly held in November in Gaborone, Botswana. This was part of an `International Data Week', *i.e*. organized jointly by CODATA, the Research Data Alliance and the ISC World Data System (see 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'. 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. From the CODATA General Assembly I highlight 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.

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 initiative on Data Integration has led to further workshops and the identification of three important themes for CODATA and the International Science Council to focus on: (i) infectious diseases, (ii) resilient cities and (iii) disaster risks reduction. See http://www.dataintegration.codata.org.

My detailed report on IDW 2018 and the CODATA General Assembly is available at http://forums.iucr.org/viewtopic.php?f=39&t=409.

In September 2019 CODATA organized a meeting in Beijing entitled Towards Next-Generation Data-Driven Science: Policies, Practices and Platforms (https://codata.org/events/conferences/codata-2019-beijing/). This included a session entitled The Key Role of the Scientific Unions in Enabling Transdisciplinary Data-Intensive Science in Support of Global Challenges. This was within the Data Integration initiative of CODATA (http://dataintegration.codata.org/). James Hester (COMCIFS Chair) attended as the representative of the IUCr. The other unions taking part were the International Union on Geodesy and Geophysics (IUGG), the International Union of Geological Sciences (IUGS), and the International Astronomical Union (IAU), from the outside perspective of the International Virtual Observatory Alliance (IVOA). We note that `data integration' can be shown to work in specific cases such as the Ocean Data Interoperability Platform, http://www.odip.org/. Between the more diverse International Unions little progress was documented at this event in Beijing. We think that a more specific focus on interoperability could yield more progress for CODATA. Indeed data interoperability was effectively explored at the International Data Week in Botswana in November 2018 as cited above.

We are very grateful to Dr Simon Hodson, Executive Director of CODATA, who gave the opening lecture at the CIFiesta Naples School in August/September 2019, an information-, metadata- and data-centric school organized by the Italian Crystallographic Association with participation from members of COMCIFS and CommDat.

J.R. Helliwell, IUCr Representative

A16.4 ISC Committee on Space Research (COSPAR)

COSPAR's (http://cosparhq.cnes.fr/) main objective is to promote international collaboration in scientific research in space, with an emphasis on the exchange of results, information and opinions. Developing world standards for the space environment and its protection requires perpetual creation of national and international organizations and specialist working groups.

The President of COSPAR 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, July 2018. The 43rd COSPAR Assembly will take place in Sydney, Australia, 15-23 August 2020 (https://www.cospar-assembly.org/admin/congress.php?congress=8). The 44th COSPAR Assembly will be in Athens, Greece, in 2022.

Most COSPAR activities are related to space topics (astronomy, astrobiology, geophysics, atmosphere studies, investigation of natural and artificial ecosystems, as well as space travel). For the IUCr, the most interesting division of COSPAR is the Scientific Commission on Materials Science in Space (MSS Commission G), chaired by M. Avila (Germany). This Commission coordinates fundamental experiments in materials and fluid sciences performed in space, utilizing reduced gravity for their objectives, and recommends future research pathways.

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

Advances in Space Research (*ASR*, http://ees.elsevier.com/asr/, impact factor 0.98 in 2018) is the official journal of COSPAR. It covers all areas of space research including - but not limited to - space studies of earth surface, climate, meteorology, fundamental physics and materials physics in space, space debris, weather and earth observation of space phenomena. *ASR* also encloses COSPAR's information bulletin, *Space Research Today*, and *Life Sciences in Space Research*, a quarterly peer-reviewed scientific journal covering astrobiology, origins of life, life in extreme environments, habitability, effects of spaceflight on the human body, radiation risks, and other aspects of life sciences relevant in space research.

In 2017-2019 COSPAR co-sponsored 10 different Capacity Building Workshops.

To find out more about other COSPAR activities please go to http://cosparhq.cnes.fr/events.

H.A. Dabkowska, IUCr Representative (2005-2019), and Y. Kimura IUCr Representative (2019-)

A16.5 International Organization for Standards (ISO)

The Chair of the Commission on Crystallographic Nomenclature is a member of the ISO.

There were no activities in 2019 related to crystallography. (This group sends numerous e-mails but as far as I could tell none of the subjects listed in those messages involved crystallography. I do log onto their website and read documents there from time to time so that they will know I am still monitoring the organization's activities.)

C.P. Brock, IUCr Representative

A17. Sponsorship of meetings: Sub-committee on the Union Calendar

The present membership of the Sub-committee comprises: W. Depmeier (Germany), H.A. Dabkowska (Canada), A. Serquis (Argentina), D. Billing (South Africa), L. Dawe (Canada), A. Guerri (Italy), K. Shankland (UK), A. Nakagawa (Japan) and O. Asojo (USA; *ex officio* as Interim Chair of the Commission on Crystallographic Teaching), being chaired by G. Diaz de Delgado (Venezuela). The Sub-committee members, including the Chair, for the next triennium will be decided in Prague.

During the past three years, the Sub-committee has considered and analyzed many requests for sponsorship and financial support by the IUCr, and subsequently has made recommendations to the Executive Committee. The main policy consists of giving financial support to help young scientists, meaning graduate students, post-graduate students or post-doctoral fellows, with a maximum age of 30 (exceptionally 35). Additional financial support for organizational expenses was considered by the Executive Committee whenever necessary and justified. Special attention was given to applications from regions where crystallography is less developed. The entire procedure, from the submission of proposals to the final decision by the Executive Committee, was carried out by e-mail. The evaluation process was very efficiently conducted by e-mail discussions involving all members of the Sub-committee.

The total amount used for sponsoring the participation of young scientists in meetings was USD 133,853 in 2017, USD 134,536 in 2018, USD 111,772 in 2019 and USD 17,517 in 2020. The much lower figure in 2020 was due to the cancellation or postponement of many schools and workshops due to the pandemic.

The following meetings received support during this four-year period:

XVI Intensive Teaching School in X-ray Structure Analysis, Durham, UK, 25 March – 2 April 2017.

4th School on Crystal Structure Determination from Diffraction Data. Application on Powder Samples, Hammamet, Tunisia, 7–9 April 2017.

RapiData 2017, Stanford, USA, 16–21 April 2017.

Macromolecular Crystallography School 2017; Structural Biology to Enhance High Impact Research in Health and Disease, Montevideo, Uruguay, 13–23 November 2017.

Understanding Biology Through Structure, Santa Fe, USA, 13–17 May 2017.

Modern Trends in Mathematical Crystallography – 2nd Manila International Workshop on Mathematical Crystallography, Manila, Philippines, 20–24 May 2017.

6th International School on Biological Crystallization, Granada, Spain, 29 May – 2 June 2017.

To.Sca.Lake 2017: Total Scattering for Nanotechnology on the Como Lake, Como, Italy, 29 May – 2 June 2017.

6th ALMA Conference 'Painting as a Story' and 2nd CrysAC Workshop, Brno, Czech Republic, 31 May – 3 June 2017.

Integrative Structural Biology (50th Erice School), Erice, Italy, 2–11 June 2017.

Shanghai International Crystallographic School Working with Bilbao Crystallographic Server, Shanghai, People's Republic of China, 11–17 June 2017.

Zürich School of Crystallography 2017: Bring Your Own Crystals, Zürich, Switzerland, 11–23 June 2017.

School on Charge Density and MoPro, Mexico City, Mexico, 12–15 June 2017.

Mineral Fibres: Crystal Chemistry, Chemical-Physical Properties, Biological Interaction and Toxicity, Modena, Italy, 17–21 June 2017.

4th European Crystallogrpahy School (ECS4): High-Throughput Structure Analysis – From Routine Chemical Problems to Advanced Applications, Warsaw, Poland, 2–7 July 2017.

International School on Fundamental Crystallography and Workshop on Structural Phase Transitions: Satellite School of the 24th IUCr Congress 2017, Odisha, India, 30 August – 4 September 2017.

Macromolecular Crystallography School 2017: Structural Biology to Enhance High Impact Research in Health and Disease, Montevideo, Uruguay, 13–23 November 2017.

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 4D 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, Jordan Hotel at Sunday River, Newry, Maine, USA, 24–29 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.

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

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.

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

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

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 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, Kola Peninsula, 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.

19th International Conference on Crystal Growth and Epitaxy (Crystal Growth 2019), Keystone, Colorado, 28 July – 2 August 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 (ECM32 Vienna), Vienna, Austria, 18–23 August 2019.

AICS2019 – Crystallographic Information Fiesta, Naples, Italy, 30 August – 3 September 2019.

ECSSC 17: 17th European Conference on Solid State Chemistry, Lille, France, 1–4 September 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.

EXPO&more International Workshop, Bari, Italy, 30 September – 3 October 2019.

Hot Topics in Contemporary Crystallography 4, Mlini, Dubrovnik, Croatia, 1–6 October 2019.

II LACA School 2019: Crystal Structure Determination by Powder and Single Crystal X-ray Diffraction, Bucaramanga, Colombia, 1–6 October 2019.

IV Meeting of the Latin American Crystallographic Association, Bucaramanga, Colombia, 7–10 October 2019.

XI School of Asociación Argentina de Cristalografía, San Carlos de Bariloche, Argentina, 18–22 November 2019.

16th Conference of the Asian Crystallographic Association, Singapore, 17–20 December 2019.

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

4th International Symposium on Halogen Bonding (ISXB4), Stellenbosch, South Africa, 23–27 March 2020. Moved to virtual, 2-5 November 2020.

3rd LACA School on Small Molecule Crystallography, Universidad Nacional Autónoma de México, Mexico, 26–29 March 2020. Moved to virtual, 23-27 November 2020 and 7-11 December 2020.

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

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

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

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

Annual Meeting of the American Crystallographic Association (ACA 2020), virtual, 2-7 August 2020.

6th Conference (Virtual) of the Bangladesh Crystallographic Association, 15-16 January 2021.

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

A18. Budget estimates for period to Twenty-Sixth General Assembly: determination of unit contribution

A18.1 Budget estimates

The estimated budget excluding income from and expenditure on IUCr publications is set out below for the period until the next General Assembly. Since the budget estimates had to be prepared at a time when the decisions on many activities were still to be made, these estimates should be considered with due reserve. With this *proviso*, and in accordance with Statute 9.3, the Executive Committee presents to the General Assembly the following estimates for the three-year period 1 January 2020 – 31 December 2022.

	USD	USD
INCOME		
Subscriptions from Adhering Bodies	540,000	
Yield from investments and banking accounts	150,000	
Associates Programme	30,000	
		720,000

EXPENDITURE		
Administration	680,000	
Subscriptions to ISC and bodies of ISC	14,000	
Administrative meetings	236,000	
Outreach and Education	680,000	
		1,610,000
ESTIMATED PROFIT/(DEFICIT)		(890,000)

A18.2 Unit Contribution

According to Statute 5.10(*k*), the General Assembly has to determine the Unit Contribution to be paid by the Adhering Bodies for the period to the next General Assembly. The Executive Committee recommends to the General Assembly that the Unit Contribution should remain at its present level of CHF 1,000 (set at the Beijing Congress in 1993) for the years 2022–2023.