

INTERNATIONAL UNION OF CRYSTALLOGRAPHY**TWENTY-SIXTH GENERAL ASSEMBLY****Appendix 1 to Agenda****Approval of Agenda**

By-Law 1.7 requires that, unless decided otherwise by the General Assembly, matters concerning adherence to the Union shall take precedence over all other business at the first business session of the General Assembly.

Appendix 2 to Agenda**Amendments to Statutes and By-Laws affecting adherence to the Union**

There are no proposals to amend the Statutes and By-Laws in matters affecting adherence to the Union.

Appendix 3 to Agenda**Applications for membership of the Union***African Crystallographic Association*

The African Crystallographic Association (AfCA) has applied to become a Regional Associate of the International Union of Crystallography (IUCr).

The members of the AfCA Executive Committee at the time of establishment are as follows:

President:	Professor Delia HAYNES
Vice-President:	Dr. Patrice KENFACK TSOBNANG
Secretary:	Dr. Gift MEHLANA
Treasurer:	Dr. Rim BENALI-CHERIF
Member:	Professor Seham KAMAL ABDEL-AAL
Member:	Dr. Adam BOURAIMA
Member:	Dr. Marielle AGBAHOUNGBATA
Member:	Dr. Dickson ANDALA
Member:	Dr. Mamoudou DIALLO

The Executive Committee invites representatives of AfCA to present their application at the General Assembly for approval.

Appendix 4 to Agenda**Withdrawal of Adhering Bodies***Algeria*

The subscriptions due from the Adhering Body in Algeria, the Algerian Association of Crystallography had not been paid for the years 2019, 2020, 2021 and 2022. Accordingly, the membership of the Adhering Body for Algeria had been automatically suspended in February 2023, in accordance with Statute 9.6. If there are no further developments, the General Assembly will be asked to confirm the withdrawal of the Adhering Body for Algeria.

Chile

The subscriptions due from the Adhering Body in Chile, the Asociacion Chilena de Cristalografia, had not been paid for the years 2019, 2020, 2021 and 2022. Accordingly, the membership of the Adhering Body for Chile had been automatically suspended in February 2023, in accordance with Statute 9.6. If there are no further developments, the General Assembly will be asked to confirm the withdrawal of the Adhering Body for Chile

Russia

A motion to suspend the IUCr adhering body for Russia, Russian Academy of Sciences, from the IUCr has been received by the Polish adhering body (Committee for Crystallography, Polish Academy of Sciences) and co-signed by the adhering body for France (French Crystallographic Association). The motion will be presented for discussion.

Appendix 5 to Agenda**Changes in names of Adhering Bodies***Norway*

The Adhering Body for Norway is now the Norwegian Chemical Society Division for Crystallography and Structural Chemistry, (formerly Norwegian Academies of Science).

Appendix 6 to Agenda

Changes in Category of Adherence of Adhering Bodies

Poland

A request from Committee for the Crystallography, Polish Academy of Sciences to change the adherence of Poland from Category I to II has been received. The Executive Committee has considered the application and recommends to the General Assembly that the application be approved.

Appendix 7 to Agenda

Approval of Minutes of Twenty-Fifth General Assembly

The Minutes of the Assembly are contained in the Report of the Twenty-Fifth General Assembly and International Congress of Crystallography published in *Acta Crystallographica* Section A [*Acta Cryst.* (2023), A79, 220-228] (2023). Copies of this Report were sent to the Secretaries of all National Committees for Crystallography.

Appendix 8 to Agenda

Amendments to Statutes and By-Laws not affecting adherence to the Union

There are two proposals to amend the By-Laws in matters not affecting adherence to the Union.

The first proposes that the term 'Executive Secretary' should be substituted for 'Chief Executive Officer (CEO)' to acknowledge the change in the job title of this role. The titular change to CEO has been enacted by the Executive Committee to identify that the work carried out by the Executive Secretary is not only secretarial but also responsible for leading the day-to-day IUCr team activities, namely journal publishing, marketing, and balancing activities from a financial aspect. The role of Executive Secretary/CEO does not bring with it changes to the running of the IUCr or variation in duties which include aligning the mission, values, and vision of the union in collaboration with the Executive Committee and General Assembly, whilst maintaining financial viability. In addition, omitting the term 'Secretary' from the above title reduces the confusion between the General Assembly appointed 'General Secretary' and improves the clarity of the functions of the two roles.

The title of 'Executive Secretary' is referred to three times in By-Law 4.4 of the IUCr Statutes and By-Laws, and should the proposal be approved, the following amendments would be required:

By-Law 4.4 (current)

The General Secretary may appoint a permanent Executive Secretary to assist with the running of the Union. In the event that an Executive Secretary is appointed the posts of General Secretary and Treasurer will be combined. In these Statutes and By-Laws administrative tasks assigned to the General Secretary will be considered to have been fulfilled if carried out by the Executive Secretary.

By-Law 4.4 (proposed)

The General Secretary may appoint a permanent Chief Executive Officer to assist with the running of the Union. In the event that a Chief Executive Officer is appointed the posts of General Secretary and Treasurer will be combined. In these Statutes and By-Laws administrative tasks assigned to the General Secretary will be considered to have been fulfilled if carried out by the Chief Executive Officer.

The second proposal for changes to the By-Laws are as follows. In the Annual Report of the IUCr, the section entitled Sub-Committee on the Union Calendar lists the meetings, workshops, symposia and schools that the IUCr support as part of their ongoing education and outreach remit. It has been suggested that the activities of this committee could be made clearer to readers of the annual report, who may not be intimately involved with the organization, by changing the name of this sub-committee to Meeting Support Committee. In doing so, the new name would serve to better advertise the support IUCr provides for such endeavours and make it clearer to those wishing to apply for funding, who to contact. The name change will not affect duties or roles performed by the sub-committee.

If the proposal is accepted it will require a change to By-Law 6.2, where both the Sub-committee on the Union Calendar and the alternative name of Calendar Sub-committee are referred to a single time, with the following amendment required:

By-Law 6.2 (current)

6.2. The Sub-committee on the Union Calendar is appointed by the Executive Committee to advise on the sponsorship of the Union for meetings, symposia and schools. The Chair of the Calendar Sub-committee should be a member of the Executive Committee.

By-Law 6.2 (proposed)

6.2. The Meeting Support Committee is appointed by the Executive Committee to advise on the sponsorship of the Union for meetings, symposia and schools. The Chair of the Meeting Support Committee should be a member of the Executive Committee.

Appendix 9 to Agenda**Report of Executive Committee***Executive Committee and Finance Committee meetings*

The Executive Committee met in Prague, Czech Republic, in August 2021 both virtually and in-person before and during the General Assembly and in Versailles, France, in August 2022 at the time of the European Crystallographic Meeting. The Finance Committee met in March 2022, August 2022, March 2023, 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 biennium at these meetings, and in e-mail ballots between meetings, were:

appointment of a new Chief Executive Officer, 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;

review of contract with Wiley;

approval of audited accounts;

review of applications for membership of the IUCr;

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,

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

IUCr Newsletter, *World Database of Crystallographers*;

marketing and promotional activities;

Outreach and Education;

LAAAMP and other activities;

OpenLabs and other activities;

appointment of the Selection Committee for thirteenth Ewald Prize;

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

sponsorship of other prizes;

discussion of arrangements for Melbourne Congress;

approval of membership of Programme Committee for Melbourne Congress, approval of Programme for Melbourne Congress;

level of financial support for Melbourne Congress;

consideration of progress with arrangements for 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.

IUCr web site;

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;

relations with other Scientific Unions;

Items concerning the Chester office were:

staffing requirements in the IUCr office in Chester;

risk analysis;

Closure of premises and dilapidations;

Publications

The open-access charge for *Acta C* and *Acta F* was unchanged, while the charges for *Acta A*, *Acta B*, *Acta D* and *Journal of Applied Crystallography* were increased. In 2022, *JSR* moved to become fully open-access.

The total annual number of pages published in 2020, 2021 and 2022 were:

	2020	2021	2022
<i>Acta Crystallographica</i> Section A	783	638	519
<i>Acta Crystallographica</i> Section B	1,147	1,054	892
<i>Acta Crystallographica</i> Section C	1,107	815	759
<i>Acta Crystallographica</i> Section D	1,279	1,623	1,473
<i>Acta Crystallographica</i> Section E	1,879	1,329	1,288
<i>Acta Crystallographica</i> Section F	623	483	422
<i>Journal of Applied Crystallography</i> ^{1,631}	1,902	1,706	
<i>Journal of Synchrotron Radiation</i>	1,754	2,002	1,503
<i>IUCrj</i>	1,215	1,034	791
<i>IUCrData</i>	407	293	286
Total	11,825	11,173	9,639

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*, *JSR*, *Acta E* and *IUCrData* are fully open access.

The IUCr home page on the web (<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 Annual Report of this Commission (Appendix 17 to the Agenda).

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 Chester office. A report on the *IUCr Newsletter* is given in Appendix 19 to the Agenda.

The IUCr/Oxford University Press Book Series continues to be successful. Details are given in Appendix 23 to the Agenda.

Sponsorship of meetings

The Sub-committee on the Union Calendar (newly proposed Meeting Support Committee), considers and advises the Executive Committee on requests for IUCr sponsorship and financial support of meetings. The Chair of the Sub-committee is M. Weiss. A list of IUCr-sponsored meetings is given in Appendix 30 to the Agenda.

Details of how to apply for financial support, along with guidelines are available on the IUCr website.

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. Support from at least one IUCr Commission is required. Applications will be considered by the Sub-committee on the Union Calendar.

Commissions of the IUCr

Each Commission Chair is required to provide a written annual report to the General Assembly. These reports are included as Appendix 24 to the Agenda. Financial assistance has again been offered to the Commission Chairs, to enable them to attend the General Assembly for the presentation and discussion of their reports and to meet the Executive Committee prior to the General Assembly.

Regional Associates, Scientific Associates, and other bodies

The reports of the Representatives on these bodies are given as separate Appendices 27 and 28 to the Agenda.

IUCr staff

The present members of staff in the IUCr offices in Chester are: A. Stanley, (Chief Executive Officer), C. Jones (Administrative Assistant to the Chief Executive Officer), P.R. Strickland (Executive Managing Editor), D. Holden (Head of R. & D.), 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 Developer), C. Cook (Administrative Assistant), E. Morgan (Digital Marketing Apprentice).

Acknowledgements

On behalf of the IUCr, the Executive Committee wishes to express its deep gratitude to the Society of Crystallographers in Australia and New Zealand for the invitation to hold the Twenty-Sixth General Assembly and International Congress of Crystallography in Melbourne.

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.

Appendix 10 to Agenda

Financial Report

Extracts from the full financial statements for the two years 2021 and 2022 are summarized in Tables 1–2. 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.

General financial development

Table 1 shows a comparison of the balance sheets at the beginning and the end of the biennium. The total assets have decreased by USD 739,959 from USD 4,697,664 to USD 3,957,705, or 15.7%, over the biennium in line with the global economic state. The great majority of the amounts under debtors and creditors have been settled since year-end. The total holding of investments on 31 December 2022 was USD 2,642,928 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 in 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. This declaration was not required by the Swiss Tax Authorities in 2021 or 2022. 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.

Income and expenditure

The academic publishing market faces difficult challenges, with business models in flux and increased financial and regulatory pressure from funders and politicians. There has also been an increase in general running costs, inline with the global economic state. It is also becoming increasingly expensive to maintain business insurances as a Swiss registered organisation, wholly operating from the UK as there are very few insurance companies willing to underwrite our activities, meaning that the insurance market is not

competitive. In addition, Wiley is now taking a larger share of the proceeds from IUCr Journals in the future, so the losses were not un-expected for this biennium.

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

	<u>31 December 2021</u>	<u>31 December 2022</u>
FIXED ASSETS		
Tangible fixed assets	39,735	37,617
Investments at market value	<u>2,501,896</u>	<u>2,605,311</u>
	2,541,631	2,642,928
CURRENT ASSETS		
Stock	43,590	8,488
Debtors	554,020	438,560
Cash at bank and in hand	<u>2,716,577</u>	<u>2,004,167</u>
	3,314,187	2,451,215
Creditors: amounts falling due within one year	-1,158,154	-1,136,438
NET CURRENT ASSETS	2,156,033	1,314,777
TOTAL ASSETS	4,697,664	3,957,705

TABLE 2. INCOME AND EXPENDITURE. US Dollars

	<u>2021</u>	<u>2022</u>
I. INCOME		
Membership income	194,232	168,197
Journals, back numbers and single issues	2,362,331	1,762,898
Open access income	1,005,119	1,172,325
Books	155,661	67,043
Donations Received		1,684
	3,523,111	3,003,950
Income from investments	21,633	28,393
Bank interest	102	2,116
	21,735	30,509
Royalties and copyright fees	33,029	35,050
Advertising income	16,406	16,363
Checking services	13,492	34,740
Associates programme	16,142	25,535
	79,069	111,688
TOTAL INCOME	3,818,147	3,314,344
II. EXPENDITURE		
Journals		
Publication costs	(731,435)	(690,320)
Editorial expenses	(128,855)	(55,684)
Technical editing	(1,247,469)	(1,153,341)
Subscription administration	(40,500)	(63,099)
Journal development costs	(599,149)	(472,416)
Checking services	(58,665)	(35,861)
	(2,806,073)	(2,470,721)
Books		
Editorial expenses	(6,375)	(5,801)
Technical editing	(102,326)	(61,500)
	(108,701)	(67,301)
Outreach and education		
Outreach	(147,367)	(95,976)
President's Fund and other grants		
Young scientists' support	(10,763)	(120,656)
Visiting professorship programme	(337)	(2,503)
	(158,467)	(219,135)
General Assembly costs	(5,534)	0
Ewald Prize		
Promotion, advertising and marketing costs	(56,812)	(62,187)
Newsletter costs	(7,421)	(6,646)

Administrative expenses			
Committee meetings and expenses	(4,084)	(97,531)	
Subscriptions	(4,845)	(4,478)	
Audit and accountancy fees	(22,567)	(20,763)	
Legal and professional fees	(18,984)	(11,878)	
Bank charges	(34,416)	(22,368)	
Travel expenses	0	(12,242)	
Executive office salaries	(143,799)	(166,293)	
		(228,695)	(335,553)
Chester office expenses			
Office costs	(248,182)	(307,738)	
Staff overheads	(43,098)	(56,383)	
		(291,280)	(364,121)
Depreciation		(18,758)	(15,758)
TOTAL EXPENDITURE	(3,681,741)		(3,541,422)
SURPLUS OF INCOME OVER EXPENDITURE	136,406		(227,078)
Other gains and losses			
MOVEMENT IN MARKET VALUE OF INVESTMENTS	162,783	(389,125)	
EXCHANGE MOVEMENTS ON TRADING ACTIVITIES	(124,479)	(86,108)	
EXCHANGE DIFFERENCES ON INVESTMENT ACTIVITIES	(10,996)	(201,284)	
	27,308		(676,517)
TOTAL RECOGNISED GAINS RELATING TO THE YEAR			
	163,714		(903,595)
ACCUMULATED BALANCE AT 1 JANUARY	4,759,487		4,923,201
ACCUMULATED BALANCE AT 31 DECEMBER	4,923,201		4,019,606

Appendix 11 to Agenda

Proposal to Research the IUCr Country of Domicile

The IUCr Executive Committee propose to investigate a significant change for our charitable organization, the International Union of Crystallography, regarding its country of domicile and financial reporting currency. After evaluation of various factors, the Executive Committee believe it is in the best interest of the organization to research the relocation of its domicile from Switzerland to the United Kingdom (UK) and change its financial reporting currency from United States Dollar (USD) to Great British Pound (GBP).

I. Rationale and Benefits:

1. Domicile Change:

- Tax Implications: Like Switzerland, the UK offers a favourable tax environment for charitable organizations. By relocating our domicile, we can take advantage of the UK's tax incentives, including tax exemptions on donations and potential Gift Aid benefits. This will enable us to maximize the impact of our funds and increase our ability to carry out our mission effectively.
- Enhanced Insurance Coverage: Relocating to the UK will allow the IUCr to access a wider range of insurance options tailored specifically for charitable organizations. This will enable us to secure comprehensive coverage at competitive rates, ensuring better protection for our organization, assets, and stakeholders.
- Streamlined Account Reporting: By moving our domicile to the UK, we will align ourselves with the accounting and reporting standards recognized globally. This will simplify our financial reporting processes and ensure compliance with international standards, making it easier for us to communicate and collaborate with other organizations, partners, and stakeholders worldwide.

2. Financial Reporting Currency Change:

- Consistency and Transparency: Changing our financial reporting currency from USD to GBP will bring consistency and transparency to our financial statements. It will align our reporting with the currency in which most of our operations and transactions take place, enhancing the clarity and comparability of our financial information.

- International Recognition: GBP is widely recognized and used as a global currency. Reporting our financials in GBP will make it easier for international stakeholders, including donors, grant organizations, and partners, to understand our financial position and performance, facilitating stronger relationships and potential collaborations. A large proportion of income and expenditure is transacted in GBP and reporting in this currency means that the reporting is not exposed to currency fluctuations such as those observed in 2022.

3. Investment Opportunity Change:

- By changing our domicile to the UK, it should no longer be necessary to limit our sterling investments to funds available off-shore, thereby offering us a greater variety of investment opportunities in GBP

II. Proposed Implementation Plan:

Before making a move to make this change, the following evaluations should be thoroughly investigated to ensure that there would be no financial or operational repercussions.

1. Legal Considerations:

- We would plan to engage legal professionals specialized in international nonprofit law to guide us through the process of changing our domicile and updating our organizational documents accordingly. They will help us understand and fulfil all the legal requirements involved in both the domicile change and currency conversion aspects.

2. Tax Consultation:

- We would consult with tax experts specializing in nonprofit tax regulations in both Switzerland and the UK. They will assist us in understanding the specific tax implications of the relocation and guide us through any necessary steps to ensure a smooth transition. This will include assessing potential tax liabilities, establishing tax-efficient structures, and applying for relevant tax exemptions and reliefs.

3. Insurance Assessment:

- We would conduct a comprehensive review of our current insurance policies and engage insurance brokers specializing in the nonprofit sector to assess our coverage needs in the UK. They will help us identify suitable insurance providers and negotiate favourable terms for our organization, ensuring that our insurance policies align with our new domicile.

4. Financial and Reporting Transition:

- We would work closely with our financial team and auditors to facilitate the transition of our financial records and reporting systems to comply with UK standards. This will involve updating our accounting practices, chart of accounts, and financial statements to meet the requirements of UK regulatory bodies and stakeholders. Additionally, we will convert our financial figures from USD to GBP using the prevailing exchange rates and implement robust currency conversion procedures for future reporting.

5. Executive and Financial Committee Structure:

The relocation of our domicile from Switzerland to the UK may have implications for the structure of our Executive and Financial Committees. As part of the implementation plan, we will research the following:

Review and Revise Committee Composition:

We plan to assess the current composition of our Executive and Financial Committees to ensure that it aligns with the requirements and best practices in the UK. This may involve revising the committee roles, and responsibilities of the committees to reflect the needs and expectations of our new domicile.

Legal and Governance Compliance:

We plan to collaborate with legal professionals and governance experts to ensure that our Executive and Financial Committees comply with the relevant laws, regulations, and governance frameworks in the UK. This will involve updating our statutes and by-laws, and internal guidelines to reflect the new jurisdiction, whilst preserving the operational ethos of the organisation.

Training and Education:

We plan to provide necessary training and education to the committee members to familiarize them with the legal, regulatory, and governance requirements in the UK. This will equip them with the knowledge and skills needed to effectively fulfil their roles and responsibilities in the new domicile.

III. Timeline:

It is anticipated that the process of researching the change the domicile of our charitable organization, financial reporting currency, and adapting the Executive and Financial Committee structure will take approximately 6 months. However, the exact duration will depend on various factors, including legal and regulatory requirements, coordination with external stakeholders, and the complexity of the transition process. After this period, and if there are no discovered barriers to the move, the Executive Committee may request an extraordinary meeting of the General Assembly to approve the decision to proceed with the change of domicile.

IV. Conclusion:

Relocating the charitable organization's domicile from Switzerland to the UK represents a strategic move that aligns with our long-term goals and will significantly benefit the organization. We are confident that this proposal, when executed effectively, will en-

hance our operations, strengthen our financial standing, and ultimately enable us to make an even greater impact in fulfilling our mission.

The Executive Committee kindly request your thoughts for this proposal for discussion during the General Assembly 2023 and after comments have been evaluated, we may move to take a vote on whether the activity of researching the change of domicile is approved by the membership.

Alex Stanley, CEO, IUCr

on behalf of Bo Brummerstedt Iversen, GST, IUCr Executive Committee

Appendix 12 to Agenda

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 his 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, his 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 thirteenth Ewald Prize has been awarded to

Professor Wayne A. Hendrickson

for his exceptional contribution to structural biology including the development of MAD/SAD methods and crystallographic theory. No-one else is so singularly and formatively identified with the explosive growth in biological crystallography and the consequent benefits to chemistry and biology.

Wayne Hendrickson transformed structural biology when he discovered and perfected resonant diffraction methods for determining the atomic-level structures of biological molecules, namely the methods of MAD (multiwavelength anomalous diffraction) and its single-wavelength variation SAD, which are now "household" terms in the field of crystallography. MAD and SAD derive from a marriage of chemistry with physics and biology and are the methods of choice for de novo X-ray determinations where there is no structural precedent. The ease with which macromolecular structures are determined by these methods served in founding the field of structural genomics, and has led to a flood of atomic-level molecular hypotheses, including many from Hendrickson himself, to inform biochemistry, physiology and genomics.

Like the late Professor Ewald, Hendrickson advanced the foundations of crystallography; his essential contributions include not only MAD and SAD but also his phase-encoding coefficients (Hendrickson-Lattman coefficients) and stereochemically restrained refinement.

Professor Hendrickson will deliver the Ewald Prize Lecture during the Opening Ceremony of the 26th IUCr Congress on 22 August 2023.

Appendix 13 to Agenda

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 2023 W. H. and W. L. Bragg Prize for outstanding early-career crystallographers has been awarded to **Professor Arkadiy Simonov** (ETH Zürich, Switzerland) for his development of the three-dimensional difference pair distribution function (3D- Δ PDF) approach and its transformative effect on the field of materials.

Over the past decade, Arkadiy has established himself as the single most talented young researcher in the interpretation of diffuse scattering from single crystals. Not only is he the author of the foremost codes for data reduction (MEERKAT) and 3D- Δ PDF refinement (YELL) but also he is applying his 3D- Δ PDF methods to solve crucially important problems in materials science.

Professor Simonov started his academic career under the tutelage of Dr Thomas Weber and Professor Walter Steurer at ETH Zürich. The YELL code was a key outcome of his Doctorate; this software enabled the fitting of the 3D- Δ PDF in terms of pairwise correlation parameters. In this way, Arkadiy established the first general approach for refinement of the diffuse scattering contribution to single-crystal diffraction patterns. He applied his methodology to a range of systems, and in doing so both established a series of proofs-of-concept and solved a number of important outstanding problems in the field of complex materials.

Professor Simonov will present a Keynote Lecture during the 26th IUCr Congress in Melbourne, Australia, in August 2023.

Appendix 14 to Agenda

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. He was 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. He served as a member of the Executive Committee of the IUCr in 1990-1993 and was elected the Vice-President of the IUCr at the XVI General Assembly in Beijing in 1993. He did not finish his term as a VP, as he passed away in August 1995. In order to commemorate the life achievements of Prof. Struchkov, his friends and former colleagues established the Struchkov Prize in 1997. Between 1997 and 2020, the Prize was awarded annually to a young (<35 years) 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 held 24 annual competitions, awarded almost 30 top and more than 50 secondary prizes. Since 2000, the Prize was funded by former colleagues and students of Prof. Struchkov, researchers who used to know him personally or were closely familiar and appreciative of his scientific achievements as well as his 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.

Dr Robert R. Fayzullin (Laboratory of Diffraction Research Methods, Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russian Academy of Sciences, Kazan, Russia) has won the 2023 Struchkov Prize for his work on real-space interpretation of chemical bonding by combining one-electron potentials and associated force fields derived from high-resolution X-ray diffraction data.

Dr Fayzullin is a specialist in the field of high-resolution X-ray diffraction crystal structure determination, and experimental and theoretical charge-density studies, co-author of about 100 publications. He managed to successfully describe chemical bonding, interatomic charge transfer, electron exchange effects in crystals using novel physically grounded descriptors based on electronic potentials and corresponding vector fields measurable by diffraction techniques. The selection committee appreciated his quite general scientific contribution and its novelty.

Appendix 15 to Agenda

Outreach and Education

The IUCr is actively engaged in a number of outreach and education initiatives, targeting emerging countries worldwide and students of all ages, from schoolchildren to early career researchers and established crystallographers. 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; extend further the public understanding of science in general and crystallography in particular.

To increase the scope of the outreach programme and boost its impact, the IUCr is partnering with several other societies and organizations. Thanks to the great achievements reached since IYCr2014, the IUCr has reinforced its high reputation in the contexts of the global science diplomacy and advocacy debate, and of science capacity building assessment through the implementation of actions towards developing scientific research, education and infrastructure worldwide. The IUCr is therefore playing a crucial and strategic role, while targeting the scientific community at large.

The pandemic has imposed a re-organisation of the IUCr outreach efforts for about a couple of years. Of course, many in-person events were cancelled or postponed, but new formats and modalities allowed the crystallographic community to gather together, so

that the momentum was not lost. Since 2022, a gradual resumption of in-person activities has allowed outreach initiatives to be revitalised and new actions are being implemented.

The present report highlights outreach and education activities implemented since the last General Assembly meeting held in Prague in 2021. Some activities are presently held within the framework of the IUPAP-IUCr-ICTP LAAAMP initiative (<https://laaamp.iucr.org>), hereafter referred to as LAAAMP, which stands for Lightsources for Africa, the Americas, Asia, Middle East and Pacific. The initiative was originally funded with a € 300K grant by the International Science Council (ISC) in 2016. The IUCr Executive Outreach Officer has acted as Chair of the LAAAMP Executive Committee in the triennium 2020-2022.

Reaching out to schoolchildren and schoolteachers

After being suspended from 2020 to 2022, the IUCr crystal growing competition (<https://www.iucr.org/outreach/crystal-growing-competition>) has been re-launched in 2023. The competition, coordinated by Luc Van Meervelt, is open to all schoolchildren (three categories: “under 11”; “high school middle forms”; “high school upper forms”) and aims to introduce students to the exciting, challenging and sometimes frustrating world of growing crystals. It has generated great enthusiasm among schoolchildren from several parts of the worlds in the six editions run from 2014 to 2019, and efforts are being done to reach a wider audience. A new series of online workshops dedicated to schoolteachers has been initiated in 2021 within the framework of LAAAMP to facilitate connections between science curricula and inquiry-based learning, with synchrotron research stories as a focus. The goal of the LAAAMP High-school Teachers Workshops (<https://laaamp.iucr.org/events/high-school-teachers-workshops-list>) is to introduce high school teachers to science research, STEM, inquiry, and indigenous connections and how they could connect these concepts to their classroom. Three editions have already been held in 2021 (in collaboration with the Canadian Light Source, CLS), 2022 (in collaboration with SESAME) and 2023 (in collaboration with Synchrotron Light Research Institute, SLRI, Thailand).

Reaching out to early-career researchers and young professors

Several actions are in place targeting early-career researchers and young professors, particularly from emerging countries worldwide. Such actions are aimed at expanding the scope of crystallography worldwide by offering new research and education opportunities and developing research infrastructure.

A LAAAMP mobility programme allows teams composed by a faculty member and a Ph.D. student from any of the targeted regions of LAAAMP (Africa, Mexico, the Caribbean, South America, Central and Southeast Asia, Middle East and the Pacific Islands) to spend a period of two months at a LAAAMP-participating synchrotron facility to get trained about the use of SR-based techniques (LAAAMP FAST Teams; <https://laaamp.iucr.org/calls>). Over a hundred individuals have been trained by this programme since 2017. The programme was re-launched in 2022, some FAST Teams are presently at synchrotrons for their training, and a new call is presently active with deadline 27 October 2023 for training visits to be completed within 2024.

The LAAAMP SPARC (Synchronizing Partners to Advance Research Characterization) initiative, a mail-in access programme to AdLS for researchers from targeted areas of the project, was launched while the mobility programme was suspended in 2020 to 2022 because of COVID-19. This initiative is still active although priority is given to in-presence visits to synchrotron facilities. The IUCr-UNESCO OpenLab initiative (<https://www.iucr.org/outreach/openlabs>), launched during IYCr2014, is still in full swing. Over 30 editions have been implemented in 25+ countries, with different modalities and in partnership with several companies and organisations. Several hundred students have been reached by the programme. The essential need of reliable and up-to-date in-house equipment has arisen very clearly. This has brought to design a new concept idea, developed by the IUCr Executive Outreach Officer within the framework of LAAAMP and in collaboration with the government of Benin, UNESCO and instrumentation manufacturers. The X-TechLab (<https://www.xtechlab.co/>) was founded in 2019. It is the first X-ray techniques facility established in Benin and acting as a hub for Central and Western Africa. The X-TechLab is funded by the government of Benin and is one of the flagship laboratories of Sèmè City (<https://semecity.bj/en/>), the International City of Innovation and Knowledge. It is equipped with new instrumentation including a Bruker AXS Quest Eco single crystal diffractometer with an Oxford Cryosystems cryostat; a Malvern Panalytical Empyrean powder diffractometer and a Bruker X-ray micro-tomograph, the latter to be installed later during the present year. In addition, the facility has access to the CSD through the CCDC FAIRE programme, and to IUCr Journals and International Tables for Crystallography. Staff has been appointed on a permanent basis. The facility is devoted to education, research and service to local industry. Two OpenLabs of two weeks each are organised every year, and they already reached over a hundred students from across Africa. A grand inauguration event of the powder diffraction lab is scheduled on 18 September 2023 and will be followed by an OpenLab. During the years of the pandemic, when travelling to Benin from abroad was not allowed, a training programme on crystal symmetry was offered by the X-TechLab staff, coordinated by the IUCr Executive Outreach Officer, to students from the Faculty of Science and Technology, U. of Abomey-Calavi, reaching over a thousand participants.

The X-TechLab model is now being implemented in another region of the world, namely, the Caribbean. Work is in progress towards the establishment of crXstal (Caribbean Regional X-ray Science Toward Advancement Laboratory) at the University of West Indies, Jamaica. The project is developed by the IUCr Executive Outreach Officer within the framework of LAAAMP, and in collaboration with UNESCO, ISC-LAC and Bruker AXS. More partners are expected to join soon. Negotiation and fund raising are ongoing for acquiring a new single-crystal diffractometer and the first OpenLab Jamaica is expected to be organised in early 2024.

In addition to the educational programme offered through the OpenLab and the other initiatives reported above, several other schools and workshops are regularly organised as part of the outreach programme of the IUCr, and participation in congresses and conferences ensures visibility to the programme itself. Schools and workshops organised include: two editions of the LAAAMP-ICTP School on Synchrotron Light Sources and their Applications in Dec 2021 (107 participants) and Feb 2023 (180 participants); SESAME-Africa Online Workshop (July 2022); LAAAMP-AfLS Africa Workshop (Sept 2022). Invited talks delivered by the IUCr Executive

Outreach Officer include: AfLS-AfPS-ePCCr conference (Nov 2021); IMA conference (July 2022); "The Glory of International Cooperation" workshop (International Conference on Research Infrastructure; Oct 2022); AfLS conference (Nov 2022); Inaugural meeting of the Synchrotron for the Greater Caribbean steering committee (Jan 2023); PCCr3 conference (Jan 2023); IUCr Journal Management Board meeting (Mar 2023); IUCr Congress (Aug 2023); AIC Congress (Sept 2023).

Initiatives for new large-scale facilities

Around 50 synchrotron facilities are operational in the world and none of these is located in Africa, while Sirius in Brazil (which has recently become partner of LAAAMP) is the only facility operating in Latin America.

Two major initiatives are presently active for an African Light Source (AfLS) and for a Synchrotron for the Greater Caribbean, LAMISTAD (the latter embedding the original initiative for a Mexican synchrotron), respectively. The IUCr is playing a fundamental political-diplomatic as well as scientific role in the whole process towards the establishment of these facilities. The IUCr Executive Outreach Officer is member of the Executive Committee of the AfLS Foundation and has participated in all the preliminary meetings for setting up a steering committee for LAMISTAD. Moreover, LAAAMP has signed an MOU with the AfLS Foundation and is leading in capacity building for the African Light Source project. In line with the generally agreed motto that "we need to build the users before building the facilities", the X-TechLab and crXstal facilities are considered by the international community as "feeders" of the two synchrotrons, and it is expected that future users of the synchrotrons will be trained in crystallography at these facilities, thus generating great enthusiasm and expectations around these initiatives.

Reaching out to the wider community and the general public

The IUCr is partnering with several other institutions for the organisation and implementation of the activities for the UN International Year of Basic Sciences for Sustainable Development (chaired by IUPAP and partnered by over 50 associations; <https://www.iybssd2022.org/en/home/>) and the Year of Mineralogy (declared by the International Mineralogical Association, IMA), to be celebrated across 2022 and 2023. The IUCr Executive Outreach Officer is member of the Steering Committees of both events. He was honoured to deliver the official opening speech of the Year of Mineralogy at the IMA 2022 Conference in Lyon, France. Reaching out to new countries and regions

Since the first appeal signed at the IYCr2014 Summit meeting in Bloemfontein in 2014, envisaging the formation of an African Crystallographic Association (AfCA), and the inception of the first Steering Committee (chaired by Andreas Roodt) at the Hyderabad Congress in 2017, through all the Panafrican Conferences on Crystallography (PCCr), and to the formal foundation of the African Crystallographic Association (AfCA) under the leadership of Delia Haynes, the IUCr Executive Outreach Officer has participated in all the activities that have brought AfCA to apply for becoming the fifth Regional Associate of the IUCr (as a member of the Steering Committee first and as Advisor to the Executive Committee after its foundation). Of course, the capacity building effort for reaching such a milestone has started several years ago (perhaps, formally, with the launch of the IUCr Initiative in Africa back in 1999) and involved many people and several initiatives that cannot be all mentioned here. In a relatively short period, AfCA represents today a large and growing community of crystallographers, it has already gained strong credibility in the context of science, science education and science policy within the African continent, and has established excellent relationships with several organizations, like AfLS, LAAAMP, AfPS and many others. Several of the actions described in the present report are contributing to the development of the community and of the association as such, and continuous support will certainly be ensured through the outreach and education programme of the IUCr.

Other activities

The IUCr Executive Outreach Officer has been working with other members of the Chester staff on several aspects of general IUCr business, including promotion of activities, transfer of the outcomes of the outreach programme into the development of IUCr Journals, maintenance of some sections of the IUCr website the IUCr Newsletter (both redesigned by the IUCr Executive Outreach Officer in collaboration with Brian McMahon in 2020 and 2018, respectively). He has also been contributing to the work of other bodies, including:

- IUCr Commission on Crystallographic Teaching (consultant);
- IUCr Gender Equity and Diversity Committee (member);
- IUCr2023 Congress (member of the IPC);
- IUCr Journals Management Board (guest);
- IUCr Journals (proposer and Guest Editor of the virtual special collection celebrating the foundation of AfCA);
- LAAAMP (co-founder and member of the Executive Committee; chair from 2020 to 2022);
- X-TechLab (co-founder and chair of the International Scientific Committee);
- African Crystallographic Association (advisor to the Executive Committee and previously, ex-officio member of the Steering Committee);
- International Mineralogical Association (member of the Executive Committee);
- African Light Source Foundation (member of the Executive Committee);

He regularly maintains liaison with several institutions and associations.

M. Zema, IUCr Executive Outreach Officer

Appendix 16 to Agenda

IUCr Associates Programme

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, Bruker and Eldico Scientific for joining in Category 1, ThermoFisher Scientific for joining in Category 2 and Stoe and Anton Paar for joining in Category 3.

Appendix 17 to Agenda

Commission on Journals

Overview

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

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

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

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

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

for *Journal of Synchrotron Radiation (JSR)*. This has gone well with high-quality papers published and an initial decrease in submissions within projections.

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

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

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

Reports by Commissioning Editors

Biology

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

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

R. Steiner, Commissioning Editor, Biology

Chemistry

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

E. Boldyreva, Commissioning Editor, Chemistry

Materials, Methods and Instrumentation

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

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

Acta Crystallographica Section A

	2017	2018	2019	2020	2021	2022
No. of submissions	93	150	115	94	90	81
Rejection rate (%)	40	29	38	35	34	38
No. of published papers	62	76	88	79	65	57
Research papers – Foundations	34 5	45 9	59 15	50 5	42 8	36 6
Short communications	5	2	0	4	2 (1 advances)	5 (1 advance)
Lead articles	0	0	0	2 (1 advances)	1	0
Feature articles	0	1 (advances)	0	0	1	0
Topical reviews	0	1	0	1 (advances)	0	0

Editorials	0	1 (advances)	1	0	1	0
Commentaries	3	0	1	2 (1 advances)	2	0
Abstracts	1864	1124	1217	227	1566	328
Other	15	0	12	15	9	10
No. of open-access papers	5	13	28	20	20	16
No. of pages	488	713	918	783	638	519
Average length (pages)	9.9	11.1	11.3	11.4	11.8	10.4
Average publication time (months)	5.6	5.7	6.1	6.2	5.8	6.0
Impact factor	7.9	1.9	2.0	2.3	2.3	
5 year impact factor	4.2	4.6	3.1	3.3	2.7	
Cited half life (years)	>10.0	>10.0	>10.0	>10.0	8.2	

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

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

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

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

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

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

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

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

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

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

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

Like many of the other IUCr journals, the number of open-access papers we publish has been increasing over the last few years. We have found that open-access articles are around 4 times as likely to be viewed, and almost twice as likely to be cited, as articles that are not open-access. Other things that can help to boost readership and citations are featuring the article in a scientific commentary

(which can be particularly beneficial for the more theoretical or mathematical papers), highlighting it on the cover or the home page of the journal, tweeting about it from the journal's account @ActaCrystA, and featuring it in the *IUCr Newsletter* (<https://www.iucr.org/news/newsletter>).

An Editorial published in January 2021 (*Acta Cryst.* A77, 1) outlined some simple steps that authors could take to help maintain the relevancy, vibrancy and broader impact of the journal. These include making sure that the crystallographic context of the work is emphasized early on in the article (*e.g.* in the title, synopsis, keywords or abstract), thus making it clear who in the materials or structural communities will use it and what they will use it for. Throughout 2022 all our Co-editors and the staff in the Editorial Office have been encouraging authors to emphasize the broader context of their work, if necessary by requesting that this is done before an article is sent out for review.

We were very pleased to welcome two new Co-editors to the Editorial Board in 2022: Louise De Las Peñas from Ateneo de Manila University, Philippines, and Tatiana Gorelik from the Helmholtz Centre for Infection Research in Braunschweig, Germany. In addition, Vitaliy Kurlin (University of Liverpool, UK) has been acting as a Guest Editor, alongside Mois Aroyo, for a Special Issue on crystal lattices, which is now well under way. A Special Issue on machine learning (joint with the *Journal of Applied Crystallography*) is also still planned.

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

Acta Crystallographica Section B

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

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

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

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

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

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

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

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

Acta Crystallographica Section C

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

Cited half life (years)	9.2	3.9	4.8	5.8	6.8	
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In 2022 *Acta C* continued its push towards being a journal with appeal not only to the broad range of structural chemists but also synthetic, computational and biological chemists. The page length has been maintained at just over eight pages per article, a result of the increased non-crystallography content.

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

A Special Issue was commissioned in 2022 entitled 'Halogen, Chalcogen, Pnictogen and Tetrel bonds: Structural Chemistry and Beyond' with Guest Editors Lee Brammer, Anssi Peuronen and Thomas Rosaveare (University of Sheffield). The submissions are essentially complete (10) and the issue is expected to be officially launched in early 2023 with a Lead Article to take the form of a short Topical Review by the Editors. The ten papers have a healthy number of downloads with two being promoted as front covers. The team of Co-editors have done an excellent job reviewing submitted manuscripts, selecting referees, accepting or rejecting the submissions and carrying out careful editing of the chemistry and crystallography. Co-editor retirements were Tong-Bu Lu, Chris Frampton and Eugene Cheung. Two new Co-editors have been appointed: Carol Hua (recently appointed at University of Melbourne, Australia) and Xiaoping Wang (Oakridge National Laboratory, US) who bring a combined expertise in synchrotron radiation and neutron diffraction.

Amy Sarjeant and Alan Kennedy have been appointed as *Acta C* Section Editors, overlapping for one year with Paul Raithby and Larry Falvello, who retire in August 2023.

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

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

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

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

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

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

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

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

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

Acta Crystallographica Section D

	2017	2018	2019	2020	2021	2022
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No. of submissions	153	152	160	194	186	153
Rejection rate (%)	24	19	29	15	20	24
No. of published papers	105	120	112	129	146	129
Research papers	95	110	98	115	133	122
Feature articles	0	0	2	2	1	1
Topical reviews	1	0	1	1	3	2
Editorials	0	1	2	3	2	1
Commentaries	0	1	1	1	2	0
Other	9	7	8	7	5	3
No. of open-access papers	56	66	60	69	93	83
No. of pages	1030	1244	1147	1279	1623	1473
Average length (pages)	10.5	10.9	10.9	10.5	11.7	11.6
Average publication time (months)	4.9	5.6	4.9	4.7	5.4	4.9
Impact factor	3.1	3.2	5.3	7.7	5.7	
5 year impact factor	3.4	3.0	3.2	5.0	6.0	
Cited half life (years)	7.7	8.7	9.6	>10.0	>10.0	

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

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

Special Issues continue to play a positive role for the journal, particularly those from the recurring series of annual CCP4 Study Weekends and CCP-EM symposia. As instituted last year, the timeliness of the papers is emphasised by publication in regular issues as soon as they are accepted and typeset, rather than waiting until all the papers in preparation are ready. Once all papers for a Special Issue are available they are also collected into a 'virtual Special Issue'. One paper on high-pressure crystallography was also published.

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

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

At the launch of *Acta D*, there were fewer than 1000 structures deposited in the Protein Data Bank (PDB). Many folds were unknown and protein structure prediction was primitive, so experimental phasing methods were essential. Since that date, 99.5% of currently

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

As ever, we sincerely thank the highly efficient and excellent work of Louise Jones and Simon Glynn in the Chester office, under the supervision of Executive Managing Editor Peter Strickland and Editor-in-chief Andrew Allen. We are very grateful for their hard work, attention to detail and dedication.

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

Acta Crystallographica Section E

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

In 2022, the number of submissions decreased by approximately 12% compared to 2021 (while the number of publications has remained stable). This reduction follows the general trend of the *Acta* chemistry journals, which shows an average decrease of ca 15%. The journal continues to attract papers from across the world, and authors from 55 countries have published in *Section E* in 2022. The top five countries were the USA (18.6%), Germany (12.1%), India (8%), Ukraine (6.3%) and Japan (5.7%). As could be expected, there was a decrease in the proportion of papers from Ukraine, which, however, remains in the top five contributors. *Acta E* remains the journal with the highest number of downloads among the IUCr journals (6.2 million out of a total of over 14.1 million; both these figures have increased compared with 2022).

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

Acta E is currently included in the Thomson Reuters Emerging Sources Citation Index and will receive an impact factor from summer 2023.

In September 2021, a tribute Special Issue in conjunction with the *Journal of Chemical Crystallography* was dedicated to the memory of Jerry Jasinski, a long-time Co-editor for *Acta E*. The virtual issue, which was edited by David Manke and Matthias Zeller, was published at the end of 2022 and contains 19 publications.

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

- (1) Fábry, J. (2018). *Acta Cryst.* E74, 1344–1357.
- (2) Tan, S. L., Jotani, M. M. & Tiekink, E. R. T. (2019). *Acta Cryst.* E75, 308–318.
- (3) Clegg, W. (2019). *Acta Cryst.* E75, 1812–1819.
- (4) Spek, A. L. (2020). *Acta Cryst.* E76, 1–11.
- (5) Linden, A. (2020). *Acta Cryst.* E76, 765–775.
- (6) Parkin, S. R. (2021). *Acta Cryst.* E77, 452–465.
- (7) Foxman, B. M. (2021). *Acta Cryst.* E77, 857–863.
- (8) Zheng, S.-L. & Campbell, M. G. (2021). *Acta Cryst.* E77, 864–866.
- (9) Wouters, J. & Van Meervelt, L. (2022). *Acta Cryst.* E78, 874–879.
- (10) van Terwingen, S. & Englert, U. (2022). *Acta Cryst.* E78, 966–970.
- (11) Milewski, M., Caminade, A.-M., Hey-Hawkins, E. & Lönnecke, P. (2022). *Acta Cryst.* E78, 1145–1150.
- (12) Vinaya, Basavaraju, Y. B., Srinivasa, G. R., Shreenivas, M. T., Yathirajan, H. S. & Parkin, S. (2023). *Acta Cryst.* E79, 54–59.

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

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

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

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

Acta Crystallographica Section F

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

5 year impact factor	0.7	0.8	0.9	1.1	1.1	
Cited half life (years)	5.4	6.2	6.5	7.5	8.1	

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

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

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

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

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

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

IUCrData

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

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

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

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

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

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

IUCrJ

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

Cited half life (years)	2.6	3.1	3.0	3.5	3.8	
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The number of submissions to *IUCr* was down in 2022. However, the journal continued to establish itself within the wider scientific communities that use results obtained from diffraction methods, and impressions from authors, readers, referees and commentators remain positive.

The impact factor of *IUCr* increased to 5.6 in 2022. All submissions undergo preliminary screening by a panel consisting of the Main Editors (Dimitri Argyriou, Ted Baker, Richard Catlow, Henry Chapman, Gautam Desiraju, Sriram Subramaniam and Xiaodong Zou) and the Editor-in-chief (Andrew Allen), and this has helped to provide a rapid and efficient preliminary review process. Articles that do not meet the journal's requirement for broad scientific significance are often transferred, with the agreement of the authors, to another IUCr journal. Such transfers are seamless and do not require any further work by the authors.

The six issues of *IUCr* published in 2022 have featured papers from a wide variety of areas including biology, chemistry, crystal engineering, cryo-EM, electron crystallography, materials, physics and FELs. The number of articles submitted to the journal was 105; a total of 89 papers were published with an average turnaround time of 18 weeks. Articles have been publicised in *IUCr*'s social media feeds and by other methods, with 12 articles highlighted *via* in-depth commentaries.

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

IUCr published 27 papers in the *Chemistry and Crystal Engineering* section in 2022 out of the total of 220 in this section since the inception of the journal in 2014. The contribution of this section has stabilized but we hope to encourage more papers in the MOF/COF area as well as papers in popular areas such as pharmaceutical cocrystals and polymorphs, including the events leading up to their crystallization.

Submissions to the *cryo-EM* section of *IUCr* were slightly higher than in 2021, with 8 articles published in 2022. Cryo-EM publications continue to feature in the list of most read articles in *IUCr*, and are well cited.

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

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

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

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

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

Journal of Applied Crystallography

	2017	2018	2019	2020	2021	2022
No. of submissions	330	299	284	297	282	275
Rejection rate (%)	37	33	32	33	33	26
No. of published papers	211	201	146	188	202	175
Research papers	165	152	121	132	145	131
Short communications	4	5	4	4	7	6
Feature articles	0	1	0	0	1	0
Computer programs	18	20	21	26	23	23

Editorials	1	2	1	0	1	0
Commentaries	1	0	0	2	1	0
Other	22	21	0	24	41	15
No. of open-access papers	55	38	33	55	83	99
No. of pages	1852	1776	1468	1631	1902	1706
Average length (pages)	9.8	9.7	9.7	9.8	10.5	10.2
Average publication time (months)	5.2	5.5	5.6	5.7	5.8	6.1
Impact factor	3.4	2.9	3.0	3.3	4.9	
5 year impact factor	4.3	3.4	3.4	4.2	4.5	
Cited half life (years)	>10.0	>10.0	>10.0	>10.0	>10.0	

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

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

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

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

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

Journal of Synchrotron Radiation

	2017	2018	2019	2020	2021	2022
No. of submissions	247	334	297	299	273	178
Rejection rate (%)	25	20	25	24	24	17

No. of published papers	156	222	249	209	215	169
Research papers	121	172	203	158	151	130
Short communications	6	6	10	14	9	4
Feature articles	0	4	0	0	0	0
Beamlines articles	13	17	27	23	39	19
Editorials	2	2	1	2	3	1
Commentaries	0	0	0	0	2	0
Other	14	21	6	12	11	15
No. of open-access papers	54	88	87	91	100	169
No. of pages	1300	1894	2096	1754	2002	1503
Average length (pages)	8.8	8.9	8.7	9.0	9.9	9.4
Average publication time (months)	5.6	5.6	5.7	5.3	5.3	5.3
Impact factor	3.2	2.5	2.3	2.6	2.6	
5 year impact factor	3.0	2.8	2.8	2.9	2.8	
Cited half life (years)	7.1	8.0	7.8	8.1	8.0	

The number of published papers was 169 – down from 215 in 2021 and 209 in 2020. The number of published pages was 1503 – down from 2002 in 2021 and 1754 in 2020. Submissions were down to 178 from 273 in 2021, and the rejection rate fell to 17% from 24%.

The virtual Special Issue on Actinide Physics and Chemistry with Synchrotron Radiation was finalised and the papers brought together in 2002, with the Foreword to the Special Issue published in the September issue of the journal. Proposed and developed by Main Editor Kristina Kvashnina, with help from Guest Editors Sergei Butorin, Shuao Wang and WeiQun Shi, the issue featured 20 Special Issue papers totalling almost 200 pages.

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

2022 was the year that JSR went fully open access. Thanks to all the groundwork put in during 2020 and 2021, the transition has been smooth on the whole. Submissions are down, but have been in line with Wiley's predictions for the first year of open access. There were increases in the proportion of papers from China, France and the USA, and decreases in the proportion of papers from Germany, Japan and Sweden. The top three countries for JSR were the USA (22%), France (14%) and Germany (13%). We thank the readers of JSR for their continued interest and support, the authors for publishing in our journal, and the Co-editors for their great services to the journal and to the community.

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

Appendix 18 to Agenda

Commission on International Tables

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

While *International Tables* has long been a collection of printed books it has been transformed into an electronic resource. Parts of it became available online starting in 2006. The transition is advantageous because it allows more material to be included, makes it easier to correct or add material, and because it has financial benefits. Printed copies of some volumes (e.g., Vols. A and E) are, how-

ever, expected to remain available because so many users prefer a version that they can page through and annotate. An online version of the *Teaching Edition* is being developed.

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

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

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

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

Descriptions of activities during 2022 for the individual volumes follow:

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

In 2022 the Executive Committee decided that the 17 plane-group tables in Vol. A should become freely available because they are so important for crystallographic education. The change has been implemented. An article for the *IUCr Newsletter* was written announcing that decision. The article also advertised for 2017 edition (the third) of Caroline MacGillavry's book *Symmetry Aspects of M. C. Escher's Periodic Drawings*, and for Danny Litvin's massive e-book compilation of magnetic (i.e., antisymmetry) groups.

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

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

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

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

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

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

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

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

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

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

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

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

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

Plans for the near future:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

C. P. Brock, Chair

Appendix 19 to Agenda

Committee for the Maintenance of the CIF Standard (COMCIFS)

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

COMCIFS currently has 4 voting members and a broad collection of advisers and observers. The voting members are James Hester (Chair), John Bollinger (Co-Secretary), Brian McMahon (Co-Secretary), and Herbert Bernstein. Ongoing COMCIFS business is conducted via the associated IUCr mailing lists.

Brian McMahon has now retired from the IUCr office in Chester, and has indicated that he will also be stepping down as Secretary.

Dictionary development

New categories and data names for more detailed descriptions of elemental composition analysis were added to the core dictionary. The powder dictionary also saw significant work related to detailed calibration specifications for intensities and angles, as well as ongoing work on preferred orientation data names.

International Tables Volume G

COMCIFS members are closely involved with the preparation of the second edition of *International Tables Volume G (Definition and exchange of crystallographic data)*. This year saw several more chapters become ready for technical editing, and the remainder of the applications chapters commissioned. Further information is available in the report of the Commission for *International Tables*.

Interactions with other groups

COMCIFS is represented on the NeXus International Advisory Committee (NIAC), which primarily develops the NeXus raw data standards for large facilities. J. Hester continues to participate in the crystallography domain of the European Materials and Modelling Ontology (EMMO) consortium, who are developing a semantic description of crystallographic knowledge and practice.

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

S. Grazulis represented COMCIFS on the IUCr 2023 Programme Committee.

Looking forward

As flagged in previous years, a small group of people is drawn upon to support CIF maintenance and development. This situation is not sustainable, particularly as the first generation of CIF experts move into retirement.

The original set of six voting members of COMCIFS has now shrunk to three. A slate of replacement candidates from stakeholder communities will be prepared for the 2023 IUCr General Assembly.

J. Hester, Chair

Appendix 20 to Agenda

IUCr Newsletter

The *IUCr Newsletter* (<https://www.iucr.org/news/newsletter>) has something for everyone. Not only does it report on the interests and activities of the IUCr and its Regional Associates and Commissions, but it also aims to inform, educate and entertain the global community of crystallographers and structural scientists.

This annual report covers four issues: Volume 30 Numbers 1–4 (2022). An average of 32 articles were published in each issue, leading with a Letter from the President, Hanna Dabkowska, and an Editorial from the Editor, Mike Glazer.

Still reeling from the effects of the COVID-19 pandemic, the world suffered another shock when Russia invaded Ukraine in February 2022. The IUCr was quick to condemn this action, and the *Newsletter* published statements denouncing the invasion and declaring the Union's solidarity with the international scientific community in calling for a peaceful end to the crisis. Later in the year, the *Newsletter* included a Letter highlighting the dire situation facing students and scientists in Iran.

In 2023, the IUCr celebrates its 75th anniversary and hosts its 26th Congress. In 2022, the *Newsletter* invited its readers to participate in a timely refresh of the IUCr's vision/purpose and values and kept them abreast of news from the Congress organisers.

In other IUCr business, the *Newsletter* advertised for Alex Ashcroft's successor and subsequently introduced the new CEO, Alex Stanley; called for nominations for the 2023 Ewald, W. H. and W. L. Bragg and Struchkov Prizes, and for members of the Executive Committee and Commissions; and introduced changes to the procedure for applying for meeting support.

Each issue republished scientific commentaries from IUCr Journals and included other journal news, such as information about Special Issues, the new electron crystallography section in *IUCrJ* and the launch of Raw Data Letters in *IUCrData*.

Reviving a feature of the old series, a report on Crystallography in France was included, just ahead of ECM33 in Versailles. In Regional Associate news, the ACA's new logo and the ECA's 25th anniversary were celebrated. The Crystallography in Africa section reported on the launch of the Senegalese Crystallographic Association, the African Crystallographic Association's outreach activities and the 2022 OpenLab in Brazzaville, Republic of Congo, which used remote diffraction facilities for the first time.

Topical issues such as the impact of machine learning and artificial intelligence on crystallography, protein structure prediction, and recent advances at the world's synchrotrons, including the use of augmented and virtual reality and solutions to the Big Data challenge, were covered in this volume. Another article described the use of synchrotron powder diffraction experiments to investigate the mineralogy of waste-to-energy ashes – an application of crystallography that is key to finding alternative feedstocks for energy-intensive industries and enhancing environmental sustainability.

But these developments would not be possible without the ingenuity of our forefathers, and articles describing their lives and work – a regular feature of the *Newsletter* – make for very interesting reading.

The e-mail editions of the *Newsletter* were circulated to 13,500 crystallographers and structural scientists worldwide, and social media channels provided additional exposure. The complete *Newsletter* archive is available at <https://www.iucr.org/news/newsletter/archive>.

During 2022, I was pleased to welcome Professor Nan Zhang from Xi'an Jiao Tong University as a Regional Editor to represent China; I look forward to hearing more about crystallography in their part of the world.

I am especially grateful for the staff at Chester for their support and especially the help from Andrea Sharpe.

A. M. Glazer, Newsletter Editor

Appendix 21 to Agenda

Committee on Data (CommDat)

For 2022 there are the following matters to report:

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

(ii) CommDat has participated fully in the work of the Melbourne IUCr 2023 Congress Programme Committee including a one-day workshop on raw diffraction data reuse, with a wide range of invited speakers; details are at <https://www.iucr.org/resources/data/comm-dat/melbourne-workshop>. Two microsymbiosia from CommDat were accepted, one on interoperability of data and one on raw diffraction data reuse.

(iii) *IUCrData* launched a new article category in September 2022 entitled Raw Data Letters, led by CommDat Member, as Main Editor, Dr Loes Kroon-Batenburg, see <https://iucrdata.iucr.org/x/issues/2022/09/00/me6192/index.html>. A checkcif for raw data to automate the reusability was developed in collaboration with COMCIFS, IUCr Journals staff and the Photon and Neutron Open Science Cloud EU project staff from ESRF and EuroXFEL.

(iv) CommDat members spoke at sessions dedicated to crystallographic data at the US National Academies Course on Crystallographic and Structural Databases, at the Stanford Linear Accelerator Center 2022 Users Meeting and at the German national project DAPHNE4NFDI (<https://www.daphne4nfdi.de/english/>), which focuses on data archiving and reuse for research with photons and neutrons at large-scale research facilities.

(v) Close ties remain strong with COMCIFS, the IUCr technical committee maintaining the CIF standard, which is chaired by James Hester. James has been a very active member of CommDat and is involved in the Raw Data Letters initiative [see point (iii) above].

J. R. Helliwell, Chair, and B. McMahon, Secretary

Appendix 22 to Agenda

Committee for Gender Equity and Diversity (GEDC)

The GEDC was very active in 2022, providing advice and recommendations to the IUCr Executive Committee (EC) on a number of issues.

During 2022, the GEDC members developed a toolkit for inclusive conference organisation and this is now on the IUCr GEDC web page.

The GEDC recommended to the EC that the IUCr vision be refreshed in line with the 75th anniversary of the Union in 2023. The recommendation was approved by the EC and subsequently an article was printed in the December 2022 issue of the *IUCr Newsletter* to advise crystallographers of a 2023 survey on this topic, and a workshop to be held at IUCr2023 in Melbourne.

The GEDC advised the IUCr that the following four (of ten) recommendations from the International Standing Committee for Gender Equality in Science be implemented as priorities for the IUCr in 2023:

- Actively promote the visibility of female scientists, in particular at conferences.
- Actively promote gender balance at every level of the organization, including its leadership, committees and institutional events.
- Welcome families in scientific activities.
- Encourage the diversification of scientific awards, actively encouraging the nomination of women.

Related to the last of the four priorities, the Executive Committee tasked the GEDC with developing guidelines for IUCr prizes.

J. L. Martin, Chair

Appendix 23 to Agenda

Africa Initiative on Crystallography

2022 Report on Africa initiative

Year 2022 was very fruitful for the Africa initiative - two openlabs one in Congo Brazzaville and the other in Mauritania both using remote facilities to collect data - Concept of remote laboratories together with CNRS (AFRAMED) - MoU between IUCr , UNESCO and CNRS - Openlab during PCCr3 (Main Tutor E. Bendeif) 1) The first OpenLab on Crystallography using remote diffraction facilities was held in Brazzaville, Republic of Congo, from 11 to 22 May 2022 at the Marien Ngouabi). This OpenLab was organized by the Congolese Association of Crystallography (ACCr) in partnership with Marien Ngouabi University, the Geological and Mining Research Center (CRGM) of Brazzaville, the CRM2 laboratory (CNRS/Université de Lorraine. This event was attended by 28 young academics and PhD students in Chemistry, After the opening ceremony, theoretical courses and tutorial sessions were carried out by CL. These courses focused on crystal lattices, crystallographic calculations, point groups, space groups, the International Tables of Crystallography, Fourier series and transforms, X-ray scattering by atoms and molecules and diffraction by crystals, introduction to single-crystal and powder diffraction, and resolution and refinements of crystal structures from single-crystal and powder diffraction data. After 3.5 days of lectures and tutorials, practical activities were carried out for 5 more days. These activities focused on the remote use in Brazzaville of the Bruker D8 Venture single-crystal and Panalytical X'pert PRO powder diffractometers (Drs Emmanuel Wenger , Florence Porcher , Pierrick Durand and El Eulmi Bendeif, CRM2 were the main tutors). WINGX was used for this purpose with a special emphasis on SHELXS, SHELXL, and Mercury and CIF software.. The powder analysis was performed using Qualx software (Rietveld refinement) and the Crystallographic Open Database (COD). 2) The first Mauritania Openlab on C in was held at the University of Nouakchott, from November 14th to 19th, 2022. This openlab was organized by the Mauritanian Chemical Society (Prof. A Barry) in partnership with the Faculty of Sciences and Technics of the University of Nouakchott, the CRM2 laboratory (CNRS/ Université de Lorraine) .Forty-three (43) young professor-researchers, postdoctoral researchers, PhD and master's students in Chemistry, Geology and Physics attended this openlab , mainly from Islamic Republic of Mauritania, Senegal and Guinea. The program was close to the Congo one ; one of the highlights of this event, was the remote visit of the French Synchrotron SOLEIL On this occasion, for more than 2 hours , Dr Jean Daillant , director of SOLEIL, offered a guided tour of Soleil followed by a discussion with the openlab participants . Practical activities were carried out during 3 days (day 3 to 5). For participants of group A (XRD single crystal), the activities were focused on the remote use of the Bruker D8 Venture single crystal diffractometer of the CRM2 laboratory. 3) Remote diffraction experiments : the AFRAMED network (Appui à la Formation Doctorale et à la Recherche en Afrique par des Mesures à Distance) The CNRS AFRAMED network is based on the possibility of connecting a diffractometer from the CRM2 laboratory remotely driven by an African colleague previously trained in the use of a CRM2 diffractometer during one full month. The

trained African colleague is thus able to use the diffractometer remotely for his own research and for his master's and doctoral teaching. The sample to be measured is centered by a CRM2 researcher (Dr E. Wenger) who then authorizes the African colleague to take control of the instrument for the duration of the experiment (about ten hours), via a secure internet connection.. The proof of concept was validated in December 2021 with a remote experiment between the "Plateforme de Mesures de Diffraction et Diffusion des Rayons X "of the CRM2 in Nancy and the University of Dschang in Cameroon and then by the openlab at the University Marien Nguabi in Brazzaville in May 2022. This project is supported by CNRS, IUCr and soon by UNESCO. During september 2022 , Drs Patrice Kenfack (Cameroon) , Adam Bouraima (Gabon) , Ayi Hounsi (Togo) and Seham Kamal (Egypt) were trained in Nancy and are now using remotely the CRM2 diffractometer. 4) A MoU between IUCr , CNRS and UNESCO has been signed; this is a result of CL work to organize Remote Experiments in Africa . Each participant sponsors the AFRAMED remote project with 10KE a year during 5 years starting 2022. 5) An Openlab in Nairobi , January 2023 , was organized by Dr E Bendeif who was supported by the Africa initiative . 6) 2023 projects already realized - Master course in Lomé March - Openlab in Franceville May - 7) 2023 projects to be realized - September AFRAMED training of the colleagues in Nancy (from Senegal, Congo , Algeria) - November Openlab in Guinea

Claude Lecomte , Chairman of the IUCr Africa Initiative

C. Lecomte, Chair

Appendix 24 to Agenda

IUCr/Oxford University Press Book Series Committee

The books published within the book series, which was launched in 1987 (<http://ww1.iucr.org/iucr-top/genasm/rep93/oup.htm>), are commissioned in two categories: Monographs on Crystallography and Texts on Crystallography.

The membership of the Committee has remained stable and very active. See <https://www.iucr.org/iucr/governance/advisory-committees/book-series>.

The Book Series Committee members individually provide assessments of book proposals, which I brought together as a Chair's report in each case. These reports were first provided to the IUCr Executive Committee, which endorsed them, and then they were submitted to OUP.

In 2022 Richard Welberry's book *Diffuse X-ray Scattering and Models of Disorder* (2nd edition) was published.

In order to ensure consistency to IUCr nomenclature policies, and to reduce the chance of errors, we continue to affirm 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 our, the IUCr's, name.

J. R. Helliwell, Chair

Appendix 25 to Agenda

Non-publishing Commissions

25.1 Commission on Aperiodic Crystals

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

The 5th International School on Aperiodic Crystals was held in Kutna Hora (Czech Republic), 23–27 May 2022. This International School is our central educational activity, with the objective of providing an overview of aperiodic order, of the basics of the mathematical description of both modulated structures and quasicrystals, and of the physical properties and chemical understanding of aperiodic crystals. The number of participants (66, an in-person meeting) is a measure of the success of this edition.

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

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

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

O. Perez, Chair

25.2 Commission on Biological Macromolecules

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

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

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

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

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

(5) The IUCr should advertise resources like Proteopedia as a great resource for undergraduate, graduate students, and biologists. The Proteopedia page on the lifecycle of SARS-CoV-2, created by Raimond Ravelli and Kèvin Knoops, provides a detailed description of the virus's lifecycle and the role of its proteins. This page can be a valuable resource for students and researchers studying the virus and its impact on human health (https://proteopedia.org/wiki/index.php/Lifecycle_of_SARS-CoV-2). A very nice animation was also put together by PDB.

Meetings, workshops, and other outreach activities

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

W. Minor, Chair

25.3 Commission on Crystal Growth and Characterization of Materials

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

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

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

MS 42: Quantum materials; and

MS43: Crystal growth and characterization of biominerals and biomimetics.

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

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

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

G. Balakrishnan, Chair

25.4 Commission on Crystallographic Computing

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

M. Lutz, Chair

25.5 Commission on Crystallographic Nomenclature

The members of this Commission (the CCN) are the Editors of the Union's journals, the Editors of the volumes of *International Tables*, the Chair of the IUCr/OUP Book Series Committee, the Chair of the Commission on Crystallographic Teaching, the Chair of the Committee for the Maintenance of the Crystallographic Information File Standard, and both the IUCr President and General Secretary. In 2022 the number of members was 51. There were also two appointed consultants.

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

Online Dictionary of Crystallography (the ODC); Editor Gervais Chapuis. The CCN is responsible for maintaining the ODC, which was established in 2006 as a wiki and continues to be run as such, i.e., as a website of definitions that qualified members of the crystallographic community can add to or modify.

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

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

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

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

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

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

C. P. Brock, Chair

25.6 Commission on Crystallographic Teaching

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

O. A. Asojo, Chair

25.7 Commission on Crystallography in Art and Cultural Heritage

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

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

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

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

33rd European Crystallographic Meeting (ECM33)

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

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

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

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

43rd International Symposium on Archaeometry

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

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

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

Molecular Transformations in Oil Paint

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

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

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

Exhibition: Rises and Falls of Portrait Miniature

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

School of XFEL and Synchrotron Radiation Users

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

Quasicrystals: State of the art and outlooks

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

The Historical Materials BAG event

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

ERASMUS+ project 'Building Power Skills through ART'

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

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

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

CrysAC website

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

*G. Artioli, Chair***25.8 Commission on Crystallography of Materials***Organizing conferences and symposia*

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

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

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

Disseminating knowledge and technical skills

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

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

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

*Changqing Jin, Chair***25.9 Commission on Diffraction Microstructure Imaging**

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

Also during 2022, the DMI Commission hosted a hybrid workshop on 25–26 June in Washington DC, USA. The workshop had in-person and virtual attendees from around the world. Over 50 attendees heard 8 invited talks (with focuses on machine learning, coherent techniques, and high-pressure) and 8 contributed talks, along with discussions of Commission business. The workshop also had a special session that provided young DMI practitioners with the opportunity to give invited talks that were selected by the outreach sub-committee.

Maintaining momentum is a goal of next year. A major Commission goal for the upcoming year is to develop a DMI 'taxonomy' giving a broad overview of DMI techniques and developing a standardized nomenclature.

D. Pagan, Chair

25.10 Commission on Electron Crystallography

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

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

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

Activity in workshops and schools for teaching electron crystallography

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

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

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

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

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

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

M. Gemmi, Chair

25.11 Commission on High Pressure

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

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

(2) The 56th Course of the International School of Crystallography was held in Erice, Italy, 3–11 June 2022, under the title "Crystallography under extreme conditions: the future is bright and very compressed". The CHP Chair was one of the co-directors of the School, while several CHP members (Stephen Moggach and Narcizo Marques Souza-Neto) and consultants (Agnès Dewaele, Andrzej

Katrusiak and Yongjae Lee) were among the lecturers and tutors. An extensive report of the School was published in the *IUCr Newsletter*, see https://www.iucr.org/news/newsletter/etc/articles?issue=155020&result_138339_result_page=19.

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

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

K. Dziubek, Chair

25.12 Commission on Inorganic and Mineral Structures

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

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

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

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

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

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

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

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

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

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

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

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

C. Ling, Chair

25.13 Commission on Magnetic Structures

Preparations for the 2023 IUCr Congress in Melbourne

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

scientists in parts of the world with less IUCr representation. We particularly thank Maxim Avdeev (ANSTO, Australia) for the extensive effort and patience required to represent the Commission on the Congress International Planning Committee.

Standard and data development

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

Meetings

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

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

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

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

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

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

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

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

25.14 Commission on Mathematical and Theoretical Crystallography

International schools and workshops organized by MaThCryst Commission members

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

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

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

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

International seminar series

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

Meetings

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

Editorial work

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

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

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

Software and educational material

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

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

Planning and sponsorship

Planing for activities during 2023 has been ongoing.

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

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

L. Suescun, Chair

25.15 Commission on Neutron Scattering

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

The major neutron facilities have continued operation.

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

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

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

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

The Australian Centre for Neutron Scattering (ACNS) is continuing with a number of upgrade projects. The new improved Koala Laue Diffraction instrument took its first diffraction pattern in early February 2023 and is expected to be returned to the user programme soon. A shutdown of the OPAL reactor is planned for 2024 during which the Cold Neutron Source will be replaced. The OPAL long

shutdown in 2024 will run from 18 March to 5 July 2024. Some ACNS instruments will also be unavailable for users in July 2024 as performance measurements for the new Cold Neutron Source are undertaken after the reactor returns to normal operations. As a consequence of the reduced days, the proposal rounds will be adjusted with the 2023-2 round running from 1 August 2023 to 17 March 2024 and the 2024-2 round running from 1 August 2024 to 31 January 2025.

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

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

T. Ishigaki, Chair

25.16 Commission on NMR Crystallography and Related Methods

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

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

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

D. Bryce, Chair

25.17 Commission on Powder Diffraction

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

The CPD did however support the following meetings:

ePCCr3 2023, Nairobi, Kenya;

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

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

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

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

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

D. G. Billing, Chair

25.18 Commission on Quantum Crystallography

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

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

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

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

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

P. Dominiak, Chair

25.19 Commission on Small-Angle Scattering

Commission activities, meetings, and communication

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

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

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

Educational activities

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

Community-building activities

Members serve as Editors and Co-editors of IUCr journals such as *Journal of Applied Crystallography (JAC)* and *Journal of Synchrotron Radiation (JSR)*. Dr Ilavsky and Dr Meneau are serving as Co-editors of open-access Special Issues of the *Journal of Applied Crystallography* associated with the SAS 2022 meeting in Campinas, Brazil. Dr Gilbert is Guest Co-editor for the Special Issue of *JAC* dedicated

to “Magnetic small-angle neutron scattering – from nanoscale magnetism to long-range magnetic structures”. Dr Allen (consultant) is Editor-in-chief of the IUCr journals. CSAS members in collaboration with the SAS2022 team have administered the Guinier prize and other prizes and competitions for SAS2022.

Consultant activities

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

Technical activities summary

Members of CSAS spearheaded round-robin experiments where small-angle X-ray scattering (SAXS) and small-angle neutron scattering (SANS) measurements of five standard proteins in solution using 12 SAXS and four SANS instruments demonstrate reproducibility and yield consensus scattering profiles that provide a foundation benchmarking set to evaluate approaches to scattering profile prediction from atomic coordinates [*Acta Cryst.* (2022). D7B, 1315–1336]. CSAS supported and members participated in a round-robin experiment in data analysis (“The human factor: results of a small-angle scattering data analysis round robin”, submitted to the IOP journal *Measurement Science and Technology*). Other standards are being developed or maintained: the existing NIST SRM 3600 (absolute intensity standard), a future SAXS q-calibration standard, and NIST Reference Materials RM8012 and RM8013, partially based on SAXS measurements.

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

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

J. Ilavsky, Chair

25.20 Commission on Structural Chemistry

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

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

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

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

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

MOF School 2023, Como, Italy, June 2023.

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

The CSC members interrogated the degree to which structural chemistry was represented as a science, rather than simply a tool, at each conference. Aspects such as support for students or early-career researchers were taken into account. The diversity (gender, geographical distribution) of speakers was also identified as an important criterion for consideration of future applications for support. These factors play a key role in the degree of support expressed to the Sub-committee on the Union Calendar.

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

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

S. Bourne, Chair

25.21 Commission on Synchrotron and XFEL Radiation

Synchrotron radiation and free electron laser facilities

Following the beginning of operations of the first “4th generation” storage ring, MAX IV in Sweden, many synchrotron facilities have been planning to upgrade or build new rings. For example, the ESRF completed a major upgrade of its accelerator in 2020 and beamlines have been upgraded since 2021. The APS upgrade was approved and user operation will cease in April 2023. Following in the footsteps of these two hard X-ray facilities, Spring-8 is also planning significant upgrade programmes based on these new designs. In addition, SIRIUS, the 4th generation Brazilian facility, has most of the beamlines under commissioning and the 6 GeV High Energy Photon Source (HEPS) is being built near Beijing, China. Many other facilities have plans to adapt the new high-brightness designs.

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

Supported meetings, schools and workshops

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

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

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

CSXR member and consultant activities

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

M. A. G. Aranda, Chair

25.22 Commission on XAFS

International Tables for Crystallography Volume I

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

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

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

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

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

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

Round-robin activities

Preparations for the planned first inter-laboratory round-robin test of XAFS results were finished in 2022. The exercise aims to test the reproducibility and comparability of XAFS spectra measured at different facilities, and to compile a catalogue of essential metadata needed to describe the experiments and understand possible differences between spectra. The first three samples, titanium, copper and molybdenum metal foils, have been sent to more than 20 (synchrotron) facilities worldwide. The XAFS beamlines involved in the tests use undulators, wigglers or bending magnets as X-ray sources, and are in operation in 3rd and 4th generation storage rings. Bench-top XAFS instruments have also been included in these tests. The first results will be presented and discussed during the Q2XAFS2023 satellite meeting to the IUCr Congress in Melbourne, Australia, in August 2023.

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

Appendix 26 to Agenda

Review of existing Commissions

The Executive Committee will meet the Commission Chairs prior to the Congress to review the work and structure of the Commissions and will present any recommendations it may have to the General Assembly.

Appendix 27 to Agenda

Determination of number of elected members of each Commission

Statutes 5.10(d) and 8.2 and By-Laws 7.3 and 7.4 of the Union prescribe the procedures relating to the election of members of the Union's Commissions. Statute 5.10(d) requires the General Assembly to determine the number of elected members of each Commission set up by the General Assembly.

The present number of **elected** members of each individual Commission is given in the following table. The Chairs are **not** included in the numbers given, nor are any *ex officio* members.

Present number

1. Commission on Journals 0
2. Commission on International Tables 0
3. Commission on Aperiodic Crystals 8
4. Commission on Biological Macromolecules 13
5. Commission on Crystal Growth and Characterization of Materials 8
6. Commission on Crystallographic Computing 8
7. Commission on Crystallographic of Materials 7
8. Commission on Crystallographic Nomenclature 0
9. Commission on Crystallographic Teaching 8
10. Commission on Crystallography in Art and Cultural Heritage 7
11. Commission on Diffraction Microstructure Imaging 8
12. Commission on Electron Crystallography 9
13. Commission on High Pressure 9
14. Commission on Inorganic and Mineral Structures 9
15. Commission on Magnetic Structures 9
16. Commission on Mathematical and Theoretical Crystallography 10
17. Commission on Neutron Scattering 8
18. Commission on NMR Crystallography and Related Methods 8
19. Commission on Powder Diffraction 9
20. Commission on Quantum Crystallography 9
21. Commission on Small-Angle Scattering 7
22. Commission on Structural Chemistry 9
23. Commission on Synchrotron and XFEL Radiation 9
24. Commission on XAFS 9

Appendix 28 to Agenda

Regional and Scientific Associates

28.1 American Crystallographic Association (ACA)

The American Crystallographic Association, Inc. (ACA) is a nonprofit, scientific organization of under 1,200 members. It was founded in 1949. The objective of the ACA is to promote interactions among scientists who study the structure of matter at atomic (or near atomic) resolution. For more details please visit the regularly updated, informative and easy to navigate ACA website (<http://www.amerystalassn.org>).

The 2022 ACA Council consisted of Diana Tomchick (President), Cora Lind-Kovacs (Vice-President), David Rose (Past-President), Stephan Ginell (Treasurer), Kushol Gupta (Secretary), and Chelsy Chesterman as the Young Scientists Special Interest Group (YSSIG) representative to the Council (*ex officio*). Gerald Audette continued to serve as the Canadian National Committee for Crystallography (CNCC) representative and Thomas Proffen as the IUCr representative (*ex officio*). Kristin Stevens continues as the ACA Executive Director and Kristina Vitale continues as the ACA Membership Coordinator. Membership of all committees and officers of all special interest groups are listed in the Spring 2022 edition of *RefleXions* (<https://www.amerystalassn.org/reflexions-archive>).

In 2022 the Council continued the highly successful once-a-month teleconferences started during the COVID-19 pandemic. The Council also met in person during the ACA Annual Meeting in Portland.

The 72nd Annual Meeting of the American Crystallographic Association was held in Portland, Oregon, 29 July – 2 August 2022. The meeting offered a hybrid option, allowing remote participants to attend a subset of sessions. One change that has occurred because of the COVID-19 pandemic is the pivot to holding Scientific Interest Group (SIG) meetings by Zoom prior to the Annual Meeting. Attendance at these meetings has been robust and diverse, including many new members. Brandon Mercado, Anna Gardberg, Carla Slebodnick and Samantha Powell co-chaired this meeting. The 2022 Transaction Symposium was *The Contributions of Structural Science to Tackling a Pandemic: COVID-19 As a Paradigm*. The meeting was well attended with 563 attendees; around 480 participated in person and 86 remotely. The programme included 8 workshops held the day before the meeting, attracting over 200 participants. Other meeting statistics are available at <https://www.amerystalassn.org/past-meetings>.

The 2022 ACA Award Winners (to be presented at the 2023 Annual Meeting) are Kristin M. Hutchins (Margaret C. Etter Early Career Award), Majed Chergui (David G. Rognlie Award), Tamir Gonen (A.L. Patterson Award) and Juan Manuel García-Ruiz (Elizabeth A. Wood Science Writing Award). The 2022 ACA Fellow titles were bestowed on Ian Wilson, Hyotcherl Ihee, Stephen Ginell, Lin Chen and Eddie Snell.

The 2023 (73rd) ACA:SSS Meeting will be held in Baltimore, Maryland, 7–11 July 2023. The meeting will be in-person only.

The ACA/AIP journal *Structural Dynamics* achieved an impact factor of 2.92 in 2022.

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

Th. Proffen, IUCr Representative

28.2 Asian Crystallographic Association (AsCA)

AsCA continues to grow in the Asia-Pacific region, with the most recent AsCA conference held on Jeju Island, Korea (Republic of), 30 October – 2 November 2022. The conference attracted in excess of 600 attendees (in person and online), and achieved good gender representation with a ratio of 65%:35% invited talks given by male:female speakers.

A business meeting was held at the conference at which the following items were discussed:

Conference support: A draft policy was presented for AsCA-badged conferences concerning conference support (seed money) from AsCA and distribution of any financial surplus/loss. There was general agreement that conference seed funding was needed; however, it was queried whether AUD 10,000 would be enough. The seed funding should be made available at an early stage of preparations. Members agreed to revisit the amount and details after the next AsCA conference.

AsCA MCR Award: A draft policy was presented to establish two mid-career researcher (MCR) awards. This will be developed further at the next Council meeting.

IUCr 2023 Melbourne, Australia: The organisation is well advanced and sponsorship income looks good. Registration and abstract submission are open. The next AsCA business meeting will be held at the Congress.

AsCA 2024 Malaysia: A brief update was provided, with arrangements to be confirmed in 2023.

AsCA 2025: The AsCA 2025 conference is proposed to be held jointly by Japan and Taiwan.

Elections: The 3-year positions of Vice-President and Secretary/Treasurer were open for election in 2022. Geoff Jameson (New Zealand) was elected Vice-President unopposed. Siegfried Schmidt (Australia) was elected unopposed as Secretary/Treasurer for a second term. Genji Kurisu (Japan) became President, and Xiao-Dong Su (China) became Past President. Jenny Martin (former Past President) stepped off the AsCA Council at the 2022 business meeting.

J. L. Martin, Past President

28.3 European Crystallographic Association (ECA)

The ECA Council meeting was held during the 33rd edition of the European Crystallography Meeting (ECM33), Versailles, 23–27 August 2022. The Council discussed scientific and organisational aspects of the ECA activities. Antonia Neels (EMPA/University of Friebourg) was elected Treasurer to the ECA Executive Committee.

ECM33 was successfully carried out, and attracted over 900 participants, from Europe and outside, with a large number of sponsors and quite good gender balance. The 25th anniversary of the ECA and the 50th anniversary of the European Crystallographic Committee were celebrated during ECM33 (<https://ecanews.org/blog/2022/04/03/gold-and-silver-treasures-of-european-crystallography/>). The Perutz Prize was awarded to William Clegg (UK), the Bertaut Prize to Lukáš Gajdos (France) and the Kalman Prize to Eric Collet (France). The organisers of ECM33 decided to donate a part of the financial profit of the conference to ECM35, expected to be held in Lviv, Ukraine, in 2025. The next ECM has been scheduled for Padua, Italy, 26–31 August 2024, in a synergistic combination with the 18th European Powder Diffraction Conference, EPDIC18, 30 August – 2 September 2024.

The 2022 European Crystallographic School, held in Lisbon, 10–15 July 2022, focused on X-ray crystallography of powders, small molecules and proteins, covering the fundamentals of diffraction to the latest developments, including theoretical and practical lectures, hands-on tutorials, and laboratory practical sessions. Lectures were also given on the application of cryo-EM to macromolecules, solid-state NMR, and PDF analysis. 47 students, among undergraduate, graduate, postgraduate and young scientists, and 25 teachers, predominantly from European countries, attended the school. Students showed keen interest and enthusiastic participation in all the sessions. The next school, ECS8, will take place in Berlin, 18–24 June 2023. The first steps towards the organisation of ECS9 in Nancy have been taken.

The ECA has organized a series of virtual lunchtime webinars (https://ecanews.org/education/eca-lunch-webinars_past-events/). Online Distinguished Lectures on Quantum Crystallography and Complementary Fields have been organized under the auspices of the Quantum Crystallography Commission of the IUCr and the ECA Special Interest Group SIG-02 on Quantum Crystallography with the support of the Department of Chemistry of the University of Warsaw (Poland).

The ECA Executive Committee is in contact with members of the ACA, AsCA, AfCA and LACA to share activities, in particular, to support the OpenLab on Crystallography project and develop crystallography over the continent of Africa.

The ECA General Interest Group devoted to promoting and spreading crystallography through education at different levels (GIG-03) is working on a special project on 'Women in Crystallography'. Initiatives will be presented at the 26th IUCr Congress in Melbourne.

Two new prizes have been proposed, the Sheldrick Prize (proposed by Professor Isabel Uson) and a prize for young crystallographers in memory of Professor Lodovico Riva di Sanseverino (proposed by GIG-03). The decision on the prizes will be made by the Council.

Owing to the relevant role of heritage science in crystallographic research, a new Special Interest Group (SIG-15) on 'Crystallography in Art and Cultural Heritage' has been proposed. It needs to be approved by the Council. This new SIG will be concerned with two main issues: crystallography and symmetry in art; and crystallographic analysis (based on diffraction, X-ray absorption spectroscopy, fluorescence etc.) of artworks and ancient materials.

The ECA's activities are effectively dedicated to supporting and promoting crystallography on a European and also on an international level.

The ECA Executive Committee winter meeting was held in Padua in February 2023 in hybrid form. The next ECA Council meeting has been planned (online) for the end of September 2023.

A. Altomare, IUCr Representative

28.4 Latin-American Crystallographic Association (LACA)

The gradual lifting of COVID-19 restrictions in 2022 allowed the members of LACA to organize in-person and hybrid meetings during this period. The main events for LACA in 2022 were as follows.

(1) The IV-LACA School "Phase identification and Microstructural Characterization of Materials using X-ray Powder Diffraction Techniques" was organized (in hybrid format) by Professor Claudio Aguilar at Universidad Técnica Federico Santa María (UTFSM) in Valparaíso, Chile, 24–28 January 2022. The school had as instructors Diego Lamas (Universidad Nacional General San Martín, Argentina), Claudio Aguilar (UTFSM, Chile), Raúl Cardoso-Gil (Max Planck Institute) and David Rafaja (Technical University of Freiberg, Germany), Tom Blanton (ICDD, USA), and Miguel Delgado and Graciela Díaz de Delgado (ULA, Venezuela). Participants on site (23) and online (35) were from Argentina, Bolivia, Brazil, Chile, Colombia, Ecuador, Guatemala, Mexico, Peru, Uruguay, Spain, and the USA. 43% were female and 57% male. Funding for the school was provided by UTFSM, the ICDD, and the IUCr.

(2) The V-Meeting of the Latin American Crystallographic Association (LACA) took place at Universidad de Costa Rica in San José, 28–30 November 2022, in conjunction with the Chemistry Congress CR2022. The meeting was organized by Unión Costarricense de Cristalografía (UCCR), with Dr Andrea Araya Sibaja as Chair of the organizing committee. The IUCr President, Hanna Dabkowska (McMaster University, Canada), attended in person and delivered opening remarks and a Plenary Lecture. Four other plenaries were given in person by Tom Blanton (ICDD, USA) and Jim Kaduk (North Central College & Illinois Institute of Technology, USA) and online by Jennifer Swift (Georgetown University, USA) and Abel Moreno-Cárcamo (UNAM, Mexico). The 40 participants (26 on site and 14 online) represented 13 countries. A total of 13 students and young scientists received travel and subsistence scholarships from IUCr funds to attend the Congress. The programme also included semi-plenaries, oral presentations, and short oral presentations (instead

of posters). IUCr prizes were awarded to Teresa García (México), Eduardo Gutiérrez (Argentina), and Analio Dugarte (Venezuela). An honorary mention was given to Cristian Albarracín (Colombia). The CCDC prize was awarded to Julián Ticona Chambi (Bolivia).

During the LACA General Assembly, the delegates decided the members of the new Executive Council for the 2022–2024 period. They are M. Delgado (President, Venezuela), J.R. Vega (Vice-President, Costa Rica). M. Fuentelba (Chile) and Natalia Álvarez (Uruguay) will share the General Secretary role, M. Saleta (Argentina) and Carla Godillo (Guatemala) will share the Adjunct Secretary role, Iris Torriani (Brazil) will be Treasurer, and J. Reyes-Gasga (Mexico) is the Past-President. For the same period, the Deliberative Council will be formed by S. Klinke (Argentina), Javier Ellena (Brazil), A. Araya (Costa Rica), L. Velásquez (Guatemala), J. Martínez-Juárez (México), L. Suescún (Uruguay), and A. Briceño (Venezuela). The new LACA Council will work towards completing the registration process of the association so elections can take place in 2024.

(3) The V-LACA School “Polymorphism: applications in industry” followed (1–3 December 2022) at the Costa Rica National Laboratory of Nanotechnology (LANOTEC-CeNAT-CONARE). Thirty participants from 13 countries attended on site and online and 13 attendees received support from IUCr funds. A CSD workshop was taught remotely by Suzanna Ward and Ilaria Gimondi from the CCDC, with the help of Natalia Álvarez (Universidad de la República, Uruguay) in person. T. Blanton (USA) and M. Delgado (Venezuela) ran a hands-on session on the ICDD’s PDF-4 Database. Other instructors participated on site (J. Kaduk) and virtually: J. Swift (USA), Serena Tarantino and Michele Zema (Italy), Alejandro Ayala and Fabio Furlan-Ferreira (Brazil), and Diego Lamas (Argentina).

The next LACA Congress and School will be organized by Red Uruguaya de Cristalografía (RUCr) in Uruguay in 2024. Natalia Álvarez will be the Chair of the organizing committee.

Latin American member countries also held their own national events. Argentina and Guatemala had very successful crystal growing competitions. It is also worth mentioning that the LACA region is well represented on almost all the Commissions and Committees of the IUCr, as well as on the International Programme Committee for the IUCr Congress in Melbourne, Australia. In addition, three members of the LACA region have proposed candidates for positions on the IUCr’s Executive Committee. The LACA region will continue to make efforts to promote crystallography and to promote the creation of new associations.

G. C. Díaz de Delgado, IUCr Representative

28.5 Worldwide Protein Data Bank (wwPDB)

The Protein Data Bank (PDB) has been a key resource for macromolecular crystallographers for 50 years, and its policies and development have been strongly influenced by the crystallographic community. Now known as the Worldwide PDB (wwPDB), it comprises five core entities: the RCSB-PDB in the USA, PDBe in Europe, PDBj in Japan, the BMRB (NMR database) and the Electron Microscopy Database (EMDB). The centres collaborate closely and share the load on deposition, maintaining a single open access archive that is freely accessible to anyone – researchers, educators and students – throughout the world.

The wwPDB was formally designated a Scientific Associate of the IUCr in 2015, and the IUCr provides a representative to the wwPDB Advisory Committee (wwPDB-AC). The wwPDB-AC also has representatives from the NMR and cryo-EM communities, as well as regional representation.

Professor Jennifer Martin (Australia) (IUCr Executive Committee member) was appointed IUCr representative in 2021. The wwPDB Principal Investigators invited Professor Martin to Chair the wwPDB-AC from 2022–2024.

The 2022 meeting of the wwPDB-AC was held virtually in October.

There were 14,285 new depositions released in 2022 and the archive was expected to reach >200,000 macromolecular structures in early 2023. This is impressive growth, noting that the 100,000 structure landmark was reached in 2014, the International Year of Crystallography. Numbers of structures in the data bank continue to grow, and the size and complexity of structures also continues to increase. About 87% of structures in the database have been determined by crystallography, though the number determined by cryo-EM is increasing rapidly (4112 by cryoEM in 2022, 9845 by crystallography in 2022). The number of NMR structures remains relatively low in comparison (304 in 2022).

The wwPDB accepted PDBc, China, as an Associate Member in 2022 and PDBi, India, is being considered for future Associate Membership.

J. L. Martin, IUCr Representative

28.6 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. G. Billing, IUCr Representative

28.7 International Organization for Crystal Growth (IOCG)

After a hiatus of a few years due to the COVID-19 pandemic, which slowed down events related to the IOCG considerably, we are all now eagerly looking forward to the next meeting of the IOCG. After meeting at the 19th International Conference on Crystal Growth and Epitaxy (ICCGE 19) at Keystone, USA, the IOCG is scheduled to meet again in Italy at the 20th International Conference on Crystal Growth and Epitaxy (ICCGE 20, <https://www.iccge20.org/>) to be held in Naples, Italy, 30 July – 4 August 2023. (This conference was moved from 2022 to 2023, again due to the uncertainties brought about by the pandemic situation.) During the meeting in Naples the election of new IOCG Executive Committee Members and Officers is intended to be convened.

Many members and consultants of the Commission on Crystal Growth and Characterization of Materials (CCGCM) are involved in the organization of the ICCGE 20, and I would like to highlight in particular the huge contribution being made by the two Co-Chairs of this conference, A. Vecchione and A. Zappettini. Several other members of the CCGCM are also involved in various capacities (Programme Chairs, International Advisory Board, session Chairs and of course as invited speakers) in putting together what is going to be a fantastic conference where fruitful exchange of new developments in research in the field, and a free and frank exchange of ideas will be possible in person again. The school preceding this conference, ISSCG18 to be held in Parma, Italy (<https://isscg-18.unipr.it/>), will bring together students and early career researchers in the community, which is crucial to ensure future success in the activities of both the CCGCM and the IOCG.

Some members of the CCGCM also had the opportunity to meet in person last year at the European Conference on Crystal Growth, ECCG-7 (<http://www.escg3-eccg7-paris2022.insight-outside.fr/>) in Paris, July 2022, which was very welcome after a long break.

G. Balakrishnan, IUCr Representative

Appendix 29 to Agenda

Bodies not belonging to the Union

29.1 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.

The only activity of the ICTNS during 2022 seems to have been a “Meet and Greet” Zoom meeting on 10 March (9 March in North America) that took place at a time when I had a previously scheduled activity.

Requests to referee papers and reports submitted to IUPAC arrive regularly because all submissions are sent to all members of the ICTNS. Most submissions are in specialized areas unrelated to crystallography. No reviews were written for IUPAC during 2022.

C. P. Brock, IUCr Representative

29.2 International Science Council (ISC)

The International Science Council has continued to develop into a grand unified force in science policy since its formation in 2018 from the merger of the International Council for Science (ICSU) and the International Social Science Council (ISSC). The joint effort of natural and social sciences gives voice to science in facing the challenges of a rather troubled world. Providing evidence-based advice and analysis during the crises we have faced and still face with a changing climate, the COVID pandemic and the war in the Ukraine is a key role for an organisation that spans a broad range of scientific expertise. The ISC assumes the important role of speaking for science as a whole and the ISC is certainly emerging as an organization that is well set to work on science for policy and policy for science.

During 2022, most meetings organized under the auspices of the ISC were still online, but the ISC has resumed physical meetings as well. During the year, the ISC hosted almost 200 meetings and webinars covering a broad swathe of subjects, some highly relevant to the IUCr covering such issues as managing and curating data, open access publishing, diversity in science and engagement with young scientists. There were no meetings during 2022 concerning ISC governance. As before, the ISC keeps up the impressive stream of publications on science policy. During 2022 the following titles emerged: In January, *The transformative potential of managed retreat in the face of rising sea levels*, in March, *Principles and Structures of Science Advice: An outline, The normalization of preprints and Briefing Note on Systemic Risk*, in May, *International Science Council Introductory Brochure 2022, Unprecedented & Unfinished: COVID-19 and Implications for National and Global Policy, Policy Brief: Using UNDRR/ISC Hazard Information Profiles to manage risk and implement the Sendai Framework for Disaster Risk Reduction, Policy Brief: Closing the gap between science and practice at local levels to accelerate disaster risk reduction and Policy Brief: Harnessing data to accelerate the transition from disaster response to recovery*, in June, *Position paper of the Scientific and Technological Community Major Group for the 2022 High-level Political Forum*, in July, *ISC Annual Report 2021* and in August, *Conference on the Ukraine Crisis: Responses from the European higher education and research sectors*.

The full activities of the ISC during 2022 will be detailed in the yearly report that is scheduled for publication in July this year.

S. Lidin, IUCr Representative

29.3 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. Full details of CODATA's activities are available from its website, <http://www.codata.org>.

In February 2022 we sought advice from the CODATA International Data Policy Committee and its subgroup on Data Rights and Responsibilities (<https://codata.org/initiatives/data-policy/international-data-policy-committee/>) on questions about rights and responsibilities of data 'ownership' arising from our Committee on Data Workshops at the IUCr Prague Congress. The details of these deliberations are described at <https://forums.iucr.org/viewtopic.php?f=39&t=445>. The conclusion was that before any data are measured all participants should agree a data management and sharing plan. We are very grateful to this CODATA Committee for their assistance in these matters.

In June 2022 International Data Week was hosted by the Korean Institute of Science and Technology Information (KISTI), in a hybrid conference format, on the overall theme of "Data to improve our world". I attended virtually, which saved attendance costs. The overall IDW 2022 Programme (including Plenary, SciDataCon and Research Data Alliance 19th Conference sessions) is described at https://idw2022.org/bbs/content.php?co_id=Agenda_en&lang=English. Within the CODATA Global Open Science Cloud (GOSC) IDW2022 conference session I presented a talk on our Diffraction Case Study contribution to the GOSC. Our Case Study focuses on an increased role for raw diffraction data, and is described at <https://codata.org/initiatives/decadal-programme2/global-open-science-cloud/case-studies/diffraction-data/>. As well as this global event there were also 'All GOSC Hands Meetings' hosted by CODATA specifically for the five case studies involved in this CODATA GOSC initiative. In October 2022 the GOSC International Programme Office Launch event was held, as a virtual event. This office is based in Beijing with expert information and data archiving staff provided by China (<http://english.cnic.cas.cn/>). The GOSC is a major initiative stemming from the <https://en.unesco.org/science-sustainable-future/open-science/recommendation>, which affirms the importance of Open Infrastructure as one of the key pillars of Open Science. Along with the Action Plan – International Science Council, the UNESCO Recommendation calls for the development of multinational, regional and national Open Science platforms, as integrated and federated e-infrastructures, and urges stakeholders to ensure both that these initiatives interoperate and that no one is left behind. Similarly, an idea to co-design and co-build the Global Open Science Cloud (GOSC) has now developed into a worldwide initiative to encourage cooperation, alignment, and interoperability among Open Science e-infrastructures. (See my report on the UNESCO Initiative on Open Science below.)

In August 2022 CODATA contacted its Representatives for a Research Data Terminology compilation. We provided detailed feedback.

I have kept CODATA informed about the new *IUCrData* Raw Data Letters article category, launched in September 2022, again indicating the increased role for raw diffraction data as the digital data archive technologies have considerably expanded in their capacity. The launch Editorial can be found at <https://iucrdata.iucr.org/x/issues/2022/09/00/me6192/index.html>.

J. R. Helliwell, IUCr Representative

Report on the UNESCO Initiative on Open Science

A UNESCO Recommendation on Open Science was adopted by the General Conference of UNESCO at its 41st session, on 23 November 2021. The Recommendation affirmed the importance of open science as a vital tool to improve the quality and accessibility of both scientific outputs and scientific process, to bridge the science, technology, and innovation gaps between and within countries and to fulfil the human right of access to science. Details of this are at <https://www.unesco.org/en/open-science?hub=686>.

UNESCO convened five ad-hoc Working Groups focusing on key impact areas, bringing together experts and open science entities, organizations, and institutions, according to their field of activity and expertise on:

- (i) Open Science Capacity Building
- (ii) Open Science Policies and Policy Instruments
- (iii) Open Science Funding and Incentives
- (iv) Open Science Infrastructures
- (v) Open Science Monitoring Framework

These have each had three virtual events. Recordings are available at <https://www.unesco.org/en/open-science/implementation>.

I attended these Working Groups and prepared reports for the Editor-in-chief and Managing Editor of IUCr Journals and the IUCr's CEO. A key output of the Working Groups assembled by UNESCO is a helpful toolkit, <https://www.unesco.org/en/open-science/toolkit>. Within this toolkit is a checklist for publishers: <https://unesdoc.unesco.org/ark:/48223/pf0000383327>.

A linked event to this UNESCO initiative and its various events was a three-day hybrid event on open science organised by the UN Library, <https://www.un.org/en/library/OS23>, with a focus on accelerating the UN's sustainable development goals and democratizing the record of science.

On behalf of IUCr I made specific inputs into these events on (i) the importance of global collaborative sharing of instrumentation [citing Warren, J. E., Diakun, G., Bushnell-Wye, G., Fisher, S., Thalal, A., Helliwell, M. & Helliwell, J. R. (2008). *Science experiments via telepresence at a synchrotron radiation source facility*. *J. Synchrotron Rad.* **15**, 191–194] and (ii) a fine example of open science in practice being the ESRF (European Synchrotron Radiation Facility) heritage database for palaeontology, evolutionary biology and archaeology (<http://paleo.esrf.eu/>). Basically, so much of these data can be measured quickly that Europe's palaeontologists decided to share all their data with the whole world's palaeontologists to analyse the data as promptly as possible.

A specific conclusion from the UN/UNESCO deliberations features a growing importance of, and seeking funds for, the prioritising of diamond open access for publications. ‘Diamond’ open access refers to a scholarly publication model in which journals and platforms do not charge fees to either authors or readers, e.g. see 202203-diamond-oa-action-plan.pdf (scienceeurope.org).

J. R. Helliwell, ad hoc IUCr Representative

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

In July 2020 the Chair of the Commission on Crystallographic Nomenclature was appointed to be the IUCr’s Ambassador to the DRUM initiative of CODATA. The official IUCr delegate to CODATA itself is John Helliwell. There does not appear to have been any DRUM activity in 2022.

C. P. Brock, IUCr Representative

29.4 ISC Committee on Space Research (COSPAR)

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

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

COSPAR President for the period 2022–2026 is Pascale Ehrenfreund (Netherlands/USA) and the Vice-Presidents are Catherine Césarsky (France) and Pietro Ubertini (Italy). Members of the Bureau are: Vassilis Angelopoulos (USA), Masaki Fujimoto (Japan), Manuel Grande (UK), Petra Rettberg (Germany), Iwona Stanislawska (Poland) and Chi Wang (China).

The most recent 44th Scientific Assembly of COSPAR was held in Athens, 16–24 July 2022, <https://www.cosparathens2022.org/>.

The 45th COSPAR Assembly will be in Busan, Korea, 13–21 July 2024, <https://www.cospar2024.org/>.

The 46th COSPAR Assembly will take place in Florence, Italy, 1–9 August 2026.

Following the success of the Capacity Building Workshop (CBW) on Crystallography for Space Science in April 2016 in Puebla, Mexico (<http://www.inaop.mx>), a similar workshop/school was proposed for Addis Ababa, Ethiopia, in 2022. However, owing to the deteriorating security situation, a change of venue has been considered. Yuki Kimura (IUCr) and Carlos Gabriel (COSPAR) will co-chair the workshop.

The Chair of the Scientific Commission on Material and Fluid Sciences in Space Conditions (Scientific Commission G) is M. Avila (Germany), and the Vice-Chairs are K. Brinkert (UK), J. Porter (Spain) and A. Romero-Calvo (USA).

The official journal of COSPAR is *Advances in Space Research (ASR)*, <https://www.journals.elsevier.com/advances-in-space-research>, and had an impact factor of 2.611 (in 2021). *ASR* includes COSPAR’s information bulletin *Space Research Today*. Another COSPAR journal, *Life Sciences in Space Research*, <https://www.journals.elsevier.com/life-sciences-in-space-research>, had an impact factor of 2.73 (in 2021), and is a quarterly peer-reviewed scientific journal covering astrobiology, origins of life, habitability, life in extreme environments, effects of spaceflight on the human body, radiation risks and other aspects of life sciences relevant in space research.

In 2022 COSPAR organized two CBWs:

- CRTS-COSPAR Workshop on Oceanography, 12–16 September 2022, Rabat, Morocco.
- Pan-Ocean-Remote-Sensing-Conference Tutorial, 3–6 December 2022, Johor Bahru, Malaysia.

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

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

Y. Kimura, IUCr Representative

29.5 International Organization for Standards (ISO)

The Chair of the Commission on Crystallographic Nomenclature is a member of the ISO. The group sends out e-mails once per week that list 25–50 reports on a very wide variety of topics (e.g., information technology, plastics and rubber, ships and marine technology, tobacco products, medicinal herbs, clothing, medical equipment).

A topic of interest to crystallographers seldom appears in these reports, but the report *Quantities and units –Part 1: General* that was adopted during 2022 has a statement that describes the use of non-standard units (e.g., the angstrom). The fourth paragraph of the first section of the Introduction of that report reads as follows:

It is inevitable that some readers working in particular specialized fields may find that the quantities they are interested in using may not be listed in this International Standard or in another International Standard. However, provided that they can relate their quantities to more familiar examples that are listed, this will not prevent them from defining units for their quantities.

It seems that the angstrom is safe; there just needs to be an exact conversion factor to a standard unit, which there is.

C. P. Brock, IUCr Representative

Appendix 30 to Agenda

Sponsorship of meetings: Sub-committee on the Union Calendar

During the IUCr Executive Committee meeting in Versailles in August 2022, the Sub-committee of the Union Calendar was renamed as the Meeting Support Committee (MSC). This renaming still needs to be approved by the General Assembly. Nonetheless, the working name of the committee is now the MSC. The new Chair of the MSC is Manfred Weiss, having taken over from Graciela Díaz de Delgado after the Versailles Executive Committee meeting.

The MSC received funding requests for a total of 19 events to take place during the calendar year 2022. Among these there were four meetings of the regional associates (ACA, ECA, AsCA and LACA), with zero, two, one and three associated satellite meetings, respectively, for which support was sought. The two ECA satellite meetings and the LACA satellite meeting were approved. AsCA failed to provide additional details for their three satellites, so no funding was allocated to them. Nine further events applied for IUCr funding, of which seven were approved. The remaining two cancelled their applications. One cancellation was received from a Gordon Research Conference meeting due to the inability to meet the IUCr sponsor requirements. The other cancellation came from the meeting of the International School on Synchrotron Radiation due to a too-late allocation of funds. The other seven events were approved and received funds. The total funds requested were USD 118,000, and the total funds allocated were USD 73,000 (62%).

During 2022 a workflow for streamlining the application process was developed between the MSC Chair and the IUCr CEO, Alex Stanley. The plan is to roll out the new scheme after the Melbourne Congress.

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

6th Conference of the Bangladesh Crystallographic Association, virtual, 15–16 January 2021.

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.)

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

2nd International School on Advanced Porous Materials (MOFSchool2021) – Virtual Meeting, 21–25 June 2021.

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

To.Sca.Land: Total Scattering for Nanotechnology in Al Andalus, University of Granada, Granada, Spain, 20–24 September 2021.

10th International Conference of the Hellenic Crystallographic Association, Athens, Greece, 15–17 October 2021 (originally scheduled for 2020).

Tunisian Powder Diffraction School, 21–24 January 2022.

LACA IV School on Powder Diffraction; Phase-ID & Microstructure, 24–28 January 2022.

56th Erice School: Crystallography Under Extreme Conditions, 3–11 June 2022.

57th Erice School: Diffuse Scattering, 3–11 June 2022.

Gordon Research Conference – Crystal Engineering, 19–24 June 2022 (withdrawn).

International Conference on the Chemistry of the Organic Solid State, ICCOSS XXV, 3–9 July 2022.

7th European Crystallography School, ECS-7, 10–15 July 2022.

16th International Conference on the Physics of Non-Crystalline Solids, PNCS-2022, 10–16 July 2022.

3rd European School on Crystal Growth, ESCG-3, 20–23 July 2022.
7th European Conference on Crystal Growth, ECCG-7, 25–27 July 2022.
72nd Annual Meeting of the ACA, ACA-2022, 29 July – 3 August 2022.
33rd European Crystallographic Meeting, ECM-2022, 23–27 August 2022.
ECM-2022 School on Spin and Charge Densities Modelling, 20–22 August 2022.
ECM-2022 School on Functional Materials under Pressure and Chirality in Crystals, 28–30 August 2022.
International School on Synchrotron Radiation, SILS-2022, 5–16 September 2022 (withdrawn).
XVIII International Small-Angle Scattering Conference, SAS-2022, 11–16 September 2022.
Asian Crystallographic Association Conference 2022, AsCA-2022, 30 October – 2 November 2022.
50th Annual Meeting of the Argentinian Biophysical Society, SAB-2022, 16–18 November 2022.
V Meeting of the Latin American Crystallographic Association, V-LACA, 28–30 November 2022.
LACA School: Polymorphism: Applications in Industry, 1–3 December 2022.
2022 IUCr Commission on High Pressure Workshop, CHP-2022, 6–10 December 2022.

Appendix 31 to Agenda

Date and place of Twenty-Seventh General Assembly

In accordance with By-Law 1.3, the Twenty-Fifth General Assembly in Prague in 2021 gave consideration to invitations that had been received to host the Twenty-Seventh General Assembly and International Congress of Crystallography in 2026. The General Assembly accepted the invitation from the three equal partners, Canadian National Committee for Crystallography (CNCC), the U.S. National Committee for Crystallography (USNC/Cr), and the American Crystallographic Association (ACA) to hold the Congress in Calgary, Alberta, Canada.

Appendix 32 to Agenda

Consideration of date and place of Twenty-Eighth General Assembly

By-Law 1.3 allows for consideration to be given by the General Assembly to an invitation for the next-but-one General Assembly. At the time of preparing these papers, one invitation to host the 2029 General Assembly and Congress has been received, from the German Society for Crystallography (DGK) to hold the Congress in Berlin, Germany.

The locations of earlier Congresses are:

1948 Cambridge, USA
1951 Stockholm, Sweden
1954 Paris, France
1957 Montreal, Canada
1960 Cambridge, UK
1963 Rome, Italy
1966 Moscow, USSR
1969 Stony Brook, USA
1972 Kyoto, Japan
1975 Amsterdam, The Netherlands
1978 Warsaw, Poland
1981 Ottawa, Canada
1984 Hamburg, Federal Republic of Germany
1987 Perth, Australia
1990 Bordeaux, France
1993 Beijing, People's Republic of China
1996 Seattle, USA
1999 Glasgow, UK
2002 Geneva, Switzerland*
2005 Florence, Italy
2008 Osaka, Japan

2011 Madrid, Spain
 2014 Montreal, Canada
 2017 Hyderabad, India
 2021** Prague, Czech Republic
 2023 Melbourne, Australia
 2026 Calgary, Canada

* To be considered as Jerusalem, Israel.

** Postponed from 2020 due to the pandemic.

Appendix 33 to Agenda

Determination of general policy and timetable for period to Twenty-Seventh General Assembly

Statute 5.10(l) requires the General Assembly to determine the general policy and timetable for the period to the next General Assembly. Several meetings to be held in this period have already requested IUCr sponsorship and financial support. These requests have been considered by the Sub-committee on the Union Calendar and the Executive Committee. Further requests may be received before the next General Assembly. The General Assembly may wish to consider the present policy of the IUCr in its various activities, including the size, scope and length of the triennial Congresses, the number of meetings sponsored by the IUCr and the level of financial support for such meetings.

Appendix 34 to Agenda

Preliminary consideration of activities for period 2026–2029

Statute 5.10(m) requires the General Assembly to give preliminary consideration to the activities of the IUCr for the three-year period following the next General Assembly.

Appendix 35 to Agenda

Budget estimates for period to Twenty-Seventh General Assembly: determination of unit contribution

(a) 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 2023 – 31 December 2026.

	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)

(b) 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.

Appendix 36 to Agenda

Confirmation of appointments of Editors of publications of the Union

Statute 7.1 of the Union prescribes that initial appointments and re-appointments of the Editors of the publications of the Union are made by the Executive Committee and are subject to confirmation by the General Assembly.

The Executive Committee intends to appoint (or re-appoint) A.J. Allen as Editor-in-Chief of IUCr journals; A. Altomare and S.J.L. Billinge as Editors of Section A of Acta Crystallographica; M. de Boissieu, L. Dawe and A. Nangia as Editors of Section B of Acta Crystallographica; A. R. Kennedy, A. Sarjeant and J. White as Editors of Section C of Acta Crystallographica; C.S. Bond, E.F. Garman and R.J. Read as Editors of Section D of Acta Crystallographica; G. Diaz de Delgado, C. Massera, S. Parkin and L. Van Meervelt as Editors of Section E of Acta Crystallographica; M.J. van Raaij as Editor of Section F of Acta Crystallographica; J. Hajdu, G.J. McIntyre and F. Meilleur as Editors of Journal of Applied Crystallography; Y. Amemiya, D. Bhattacharyya and K. Kvashnina as Editors of Journal of Synchrotron Radiation; D. Argyriou, E.N. Baker, C.R.A. Catlow, H. Chapman, S. Subramaniam and X. Zou as Editors of IUCrJ, W.T.A. Harrison, L. M. J. Kroon-Batenburg, E.R.T. Tiekink, L. Van Meervelt and M. Weil as Editors of IUCrData and E.V. Boldyreva, Th. Proffen and R. Steiner as Commissioning Editors.

The Executive Committee intends to appoint (or re-appoint) C.P. Brock as Editor-in-Chief of *International Tables*; M.I. Aroyo as Editor of Volume A; G. Chapis as Editor of Volume B; T.R. Welberry as Editor of Volume C; TBD as Editor of Volume D; G. Madariaga as Editor of Volume E; E. Arnold and L. Tong as Editors of Volume F; B. McMahon and J. Hester as Editors of Volume G; C.J. Gilmore and J.A. Kaduk as Editors of Volume H; C.T. Chantler, F. Boscherini and B. Bunker as Editors of Volume I; and TBD as Editor of Volume A1.

Appendix 37 to Agenda

Elections

The procedures for nominations and elections are described in Section 8 of the Union's By-Laws. Nominations shall be made by the Executive Committee; other nominations may be made by any six or more delegates to the General Assembly. The nominations by the Executive Committee for Officers of the Union are given in Appendix 37.3 to the Agenda. The nominations for Chairs and members of Commissions and for Representatives on bodies not belonging to the Union will be presented at the General Assembly. The Executive Committee will be meeting the Chairs of the Commissions and IUCr Representatives to discuss their work and, where appropriate, make recommendations for membership for the next triennium. In making their votes, delegates should remember that they are representing their Adhering Bodies, who may have provided guidance on how they should vote on certain items.

37.1 Chairs and members of Commissions

The numbers of elected members are determined by the General Assembly for each individual Commission. It should be noted that, according to By-Law 7.3, service on a Commission is limited to three consecutive full terms of office, except for Editors, Co-editors and *ex officio* members. A person who has already served for three full consecutive terms is still eligible as Chair for a fourth term.

The **present** memberships of Commissions (and the original years of election or appointment for non-publishing Commissions) are as follows:

Commission on Journals

Chair, Editor-in-Chief:	A. J. Allen (USA)
Editors of JAC:	J. Hajdu (Sweden) G. J. McIntyre (Australia) F. Meilleur (USA)
Editors of JSR:	Y. Amemiya (Japan) D. Bhattacharyya (India) K. Kvashnina (France)
Editors of IUCrJ:	D. Argyriou (Sweden) E. N. Baker (New Zealand) C. R. A. Catlow (UK) H. Chapman (Germany) G. R. Desiraju (India) S. Subramaniam (Canada) X. Zou (Sweden)
Editor of Acta Cryst. Section A:	A. Altomare (Italy) S. J. L. Billinge (USA)
Editors of Acta Cryst. Section B:	A. J. Blake (UK) M. de Boissieu (France) A. Nangia (India)

Editors of Acta Cryst. Section C:	L. R. Falvello (Spain) A. R. Kennedy (UK) P. R. Raithby (UK) A. Sarjeant (USA) J. White (Australia)
Editors of Acta Cryst. Section D:	C. S. Bond (Australia) E. F. Garman (UK) R. J. Read (UK)
Editors of Acta Cryst. Section E:	G. Diaz de Delgado (Venezuela) C. Massera (Italy) S. Parkin (USA) L. Van Meervelt (Belgium)
Editors of Acta Cryst. Section F:	J. Newman (Australia) M. J. van Raaij (Spain)
Editors of IUCrData:	W. T. A. Harrison (UK) L. M. J. Kroon-Batenburg (Netherlands) E. R. T. Tiekink (Malaysia) L. Van Meervelt (Belgium) M. Weil (Austria)
Commissioning Editors:	E. V. Boldyreva (Russia) T. Proffen (USA) R. Steiner (UK)
Co-editors of journals:	J. Agirre (UK, Acta F) F. A. Almeida Paz (Portugal, Acta C) M. A. G. Aranda (Spain, IUCrData, JSR) M. I. Aroyo (Spain, Acta A) A. Barty (Germany, JAC) A. S. Batsanov (UK, Acta E) T. Bekker (Russia, Acta B) A. Bergamaschi (Switzerland, JSR) A. M. Berghuis (Canada, Acta D) S. Bernes (Mexico, IUCrData) E. V. Boldyreva (Russia, IUCrData) M. Bolte (Germany, IUCrData) A. Borbely (France, JAC) P. Bordet (France, Acta B) S. Boutet (USA, JAC) M. Bowler (France, Acta F) H. Brand (Australia, JAC) A. S. Brewster (USA, IUCrData) A. Briceno (Venezuela, Acta E) I. Brito (Chile, IUCrData) E. Bullitt (USA, IUCrJ) R. J. Butcher (USA, IUCrData) R. Cerny (Switzerland, Acta B) Y. Chen (Sweden, Acta F) E. Y. Cheung (USA, Acta C) A. M. Chippindale (UK, Acta E) G. Cingolani (USA, Acta D) S. J. Coles (UK, IUCrData) R. I. Cooper (UK, Acta C) M. Czjzek (France, Acta D) L. Dawe (Canada, Acta C) M. L. A. N. De Las Penas (Philippines, Acta A) Z. S. Derewenda (USA, Acta D) K. Diederichs (Germany, Acta D) R. Diniz (Brazil, Acta C) K. Djinovic-Carugo (France, Acta D) P. M. Dominiak (Poland, Acta A) M. Du (People's Republic of China, Acta B)

P. Dunten (USA, Acta F)
M. Dusek (Czech Republic, Acta B)
M. Eddaoudi (Saudi Arabia, IUCrJ)
J. Ellena (Brazil, Acta E)
L. Fabian (UK, Acta E)
V. Favre-Nicolin (France, JSR)
A. Fitch (France, IUCrJ)
V. T. Forsyth (Sweden, IUCrJ, JAC)
C. S. Frampton (UK, Acta C)
J. M. Garcia-Ruiz (Spain, JAC)
M. Gardiner (Australia, Acta C)
R. C. Garratt (Brazil, Acta D)
M. Gemmi (Italy, IUCrJ)
E. P. Gilbert (Australia, JAC)
A. Gonzalez (Sweden, Acta D)
T. E. Gorelik (Germany, Acta A)
D. Gratias (France, IUCrJ)
D. Gray (USA, Acta E)
J. Hadermann (Belgium, Acta B)
Q. Hao (Hong Kong, Acta D)
W. T. A. Harrison (UK, Acta E)
J. R. Helliwell (UK, IUCrData)
M. Hough (UK, Acta F)
C. Hua (Australia, Acta C)
J. Ilavsky (USA, JAC)
W. Imhof (Germany, IUCrData)
T. Ishikawa (Japan, IUCrJ)
V. Jancik (Mexico, Acta E)
U-S. Jeng (Taiwan, JSR)
G. Joyce (USA, Acta F)
A. Katrusiak (Poland, Acta B)
J. Keckes (Austria, JAC)
D. A. Keen (UK, Acta A)
S. D. Kelly (USA, JSR)
V. Khrustalev (Russia, Acta E)
K. K. Kim (South Korea, Acta F)
K. E. Knope (USA, Acta B)
B. Kobe (Australia, Acta D)
W. Kuhlbrandt (Germany, IUCrJ)
G. Kurisu (Japan, Acta D)
P. Langan (USA, Acta D)
A. Lemmerer (South Africa, Acta C)
W. Lewis (Australia, Acta C)
P. Lightfoot (UK, IUCrJ)
J. Lipkowski (Poland, Acta B)
A. H. Liu (People's Republic of China, JAC)
Z.-J. Liu (People's Republic of China, IUCrJ)
A. J. Lough (Canada, Acta E, IUCrData)
T.-B. Lu (People's Republic of China, Acta C)
P. Macchi (Italy, Acta B)
L. R. MacGillivray (USA, IUCrJ)
J. T. Mague (USA, Acta E)
F. Maia (Sweden, IUCrJ)
I. Margiolaki (Greece, Acta A)
P. McArdle (Ireland, Acta E)
R. McKenna (USA, Acta D)
L. Meshi (Israel, IUCrJ)
P. Metrangolo (Italy, Acta B)
K. Moffat (USA, IUCrJ)
S. Moggach (Australia, Acta C, JAC)
A. Momose (Japan, JSR)
A. Nakagawa (Japan, Acta F)
R. B. Neder (Germany, Acta B)
P. D. Nellist (UK, IUCrJ)
J. Newman (Australia, Acta D)
M. Nespolo (France, Acta, JAC, JSR, IUCrJ) (Book Review Editor)
M. Nieger (Finland, Acta E, IUCrData)
T. Ohhara (Japan, Acta C)

A. G. Oliver (USA, Acta C)
 I. Oswald (UK, Acta C)
 L. Palatinus (Czech Republic, Acta A)
 S. Parkin (USA, IUCrData)
 L. A. Passmore (UK, IUCrJ)
 A. R. Pearson (Germany, JAC)
 V. K. Peterson (Australia, IUCrJ)
 G. Prive (Canada, Acta F)
 S. Raunser (Germany, IUCrJ)
 C. M. Reddy (India, Acta B)
 J. Reibenspies (USA, Acta E)
 E. Reinheimer (USA, Acta C)
 J.-P. Renaud (France, Acta F)
 C. Rizzoli (Italy, Acta E, IUCrData)
 I. Robinson (UK, IUCrJ)
 J. A. Rodriguez (USA, IUCrJ)
 M. Romao (Portugal, Acta F)
 M. Rosales-Hoz (Mexico, Acta C)
 M. Rudolph (Switzerland, Acta D)
 R. Sankaranarayanan (India, Acta F)
 T. J. Sato (Japan, JAC)
 M. Schiltz (Luxembourg, Acta D)
 C. Schulzke (Germany, Acta E)
 S. Sheriff (USA, Acta F)
 L. Shimon (Israel, Acta F)
 A. Singer (USA, Acta A)
 J. L. Smith (USA, IUCrJ)
 A. L. Spek (The Netherlands, Acta C)
 R. Stanfield (USA, Acta F)
 A. W. Stevenson (Australia, JSR)
 R. W. Strange (UK, JSR)
 N. Strater (Germany, Acta F)
 C.-Y. Su (People's Republic of China, IUCrJ)
 F. Sun (People's Republic of China, IUCrJ)
 J. Sun (People's Republic of China, IUCrJ)
 S. Svensson (Sweden, JSR)
 M. Takata (Japan, IUCrJ)
 B. Therrien (Switzerland, Acta E)
 A. Thorn (Germany, IUCrJ)
 F. Tsai (USA, Acta F)
 D. R. Turner (Australia, Acta C)
 I. A. Vartanians (Germany, Acta A)
 K. R. Vinothkumar (India, Acta D)
 S. Wakatsuki (USA, Acta D)
 M. Wang (Switzerland, JSR)
 X. Wang (USA, Acta C)
 M. Weil (Austria, Acta E)
 G. Williams (USA, IUCrJ)
 I. D. Williams (Hong Kong, Acta C)
 P. R. Willmott (Switzerland, Acta A)
 D.-J. Xu (People's Republic of China, IUCrData)
 M. Yabashi (Japan, JSR)
 O. V. Yakubovich (Russia, Acta B)
 M. Yamamoto (Japan, JSR)
 G. P. A. Yap (USA, Acta C)
 M. Yousufuddin (USA, Acta C)
 M. Zeller (USA, Acta E, IUCrData)
 X. Zhang (People's Republic of China, IUCrJ)

Commission on International Tables

Chair:	C. P. Brock (USA)
Editor of Volume A:	M. I. Aroyo (Spain)
Editor of Volume A1:	-
Editors of Volume B:	G. Chapuis (Switzerland)
Editor of Volume C:	T. R. Welberry (Australia)
Editor of Volume D:	-
Editor of Volume E:	G. Madariaga (Spain)

Editors of Volume F:	E. Arnold (USA) L. Tong (USA)
Editors of Volume G:	B. McMahon (UK) J. Hester (Australia)
Editors of Volume H:	J. A. Kaduk (USA)
Editors of Volume I:	F. Boscherini (Italy) B. Bunker (USA) C. T. Chantler (Australia)

Commission on Aperiodic Crystals

Chair:	O. Perez (France, 2011)
Elected members:	E. Abe (Japan; 2017) M. Dusek (Czech Republic; 2014) A. Goldman (USA; 2014) C.P. Gomez (Sweden; 2020) T. Leisegang (Germany; 2020) K. Pussi (Finland; 2017) S. Schmid (Australia; 2017) R. Strzalka (Poland; 2020)

Commission on Biological Macromolecules

Chair:	W. Minor (USA; 2014)
Elected members:	A. Buschiazzo (Uruguay; 2017) C.S. Bond (Australia; 2020) M. Nowotny (Poland; 2017) G. Kurisu (Japan; 2020) J. Sanz-Aparacio (Spain; 2014) W.-D. Schubert (South Africa; 2017) J. Smith (USA; 2020) N. Sträter (Germany; 2014) D. Tomchick (USA; 2017) B. Vallone (Italy; 2017) A. Vrielink (Australia; 2017) H. Wu (China; 2020)

Ex officio member: S. Burley (USA) (as Director of the PDB)

Commission on Crystal Growth and Characterization of Materials

Chair:	G. Balakrishnan (UK; 2020)
Elected members:	H. Fujioka (Japan; 2017) J. Kumar (India; 2014) M. Leszczyński (Poland; 2020) H. Luo (People's Republic of China; 2014) G.E. Narda (Argentina; 2020) J. Newman (Australia; 2017) A. Vecchione (Italy; 2020) S. Veessler (France; 2017)

Ex officio members: E. Vlieg (The Netherlands) (as Representative of International Organization of Crystal Growth)
J.M. Garcia-Ruiz (Spain) (as an Editor of *Journal of Applied Crystallography*)
T. Bekker (Russia)(as an Editor of Acta B)

Commission on Crystallographic Computing

Chair:	M. Lutz (The Netherlands; 2011)
Elected members:	P. Boyle (Canada; 2020) R. Giordano (France; 2017) B. Gopal (India; 2017) C. Millan (Spain; 2017) L. Palatinus (Czech Republic; 2014) S. Panjekar (Australia; 2014) P. Boyle (Canada; 2020) A. Thorn (Germany; 2017)

Commission on Crystallography of Materials

Chair: Changqing Jin (People's Republic of China; 2017)
 Elected members: A. Abakumov (Russia; 2020)
 V. Blatov (Russia; 2017)
 Y. Gogotsi (USA; 2017)
 C. Grey (UK; 2020)
 H. Hosono (Japan; 2020)
 S. Pan (China; 2020)
 M. Petrukhina (USA; 2015)

Commission on Crystallographic Nomenclature

Chair: C.P. Brock (USA)
 A.M. Glazer (UK) (consultant)
 M. Nespolo (France) (consultant)
 A.J. Allen (USA) (as Editor-in-Chief of IUCr journals)
 A. Altomare (Italy) (as Section Editor of *Acta Cryst.* Section A)
 S.J.L. Billinge (USA) (as Section Editor of *Acta Cryst.* Section A)
 A.J. Blake (UK) (as a Section Editor of *Acta Cryst.* Section B)
 M. de Boissieu (France) (as a Section Editor of *Acta Cryst.* Section B)
 A. Nangia (India) (as a Section Editor of *Acta Cryst.* Section B)
 L.R. Falvello (Spain) (as a Section Editor of *Acta Cryst.* Section C)
 P.R. Raithby (UK) (as a Section Editor of *Acta Cryst.* Section C)
 J. White (Australia) (as a Section Editor of *Acta Cryst.* Section C)
 C.S. Bond (Australia) (as a Section Editor of *Acta Cryst.* Section D)
 E.F. Garman (UK) (as a Section Editor of *Acta Cryst.* Section D)
 R.J. Read (UK) (as a Section Editor of *Acta Cryst.* Section D)
 G. Diaz de Delgado (Venezuela) (as a Section Editor of *Acta Cryst.* Section E)
 C. Massera (Italy) (as a Section Editor of *Acta Cryst.* Section E)
 S. Parkin (USA) (as a Section Editor of *Acta Cryst.* Section E)
 L. Van Meervelt (Belgium) (as a Section Editor of *Acta Cryst.* Section E and as a
 Section Editor of *IUCrData*)
 J. Newman (Australia) (as a Section Editor of *Acta Cryst.* Section F)
 M.J. van Raaij (Spain) (as a Section Editor of *Acta Cryst.* Section F)
 K. Chapman (USA) (as a Main Editor of *JAC*)
 J. Hajdu (Sweden) (as a Main Editor of *JAC*)
 G.J. McIntyre (Australia) (as a Main Editor of *JAC*)
 Y. Amemiya (Japan) (as a Main Editor of *JSR*)
 D. Bhattacharyya (India) (as a Main Editor of *JSR*)
 K. Kvashnina (France) (as a Main Editor of *JSR*)
 I. Lindau (USA) (as a Main Editor of *JSR*)
 D. Argyriou (Sweden) (as a Main Editor of *IUCrj*)
 E.N. Baker (New Zealand) (as a Main Editor of *IUCrj*)
 C.R.A. Catlow (UK) (as a Main Editor of *IUCrj*)
 G.R. Desiraju (India) (as a Main Editor of *IUCrj*)
 J.C.H. Spence (USA) (as a main Editor of *IUCrj*)
 S. Subramaniam (Canada) (as a main Editor of *IUCrj*)
 W.T.A. Harrison (UK) (as a Section Editor of *IUCrData*)
 E.R.T. Tiekink (Malaysia) (as a Section Editor of *IUCrData*)
 M. Weil (Austria) (as a Section Editor of *IUCrData*)
 E.V. Boldyreva (Russia) (as a Commissioning Editor for IUCr Journals)
 T. Proffen (USA) (as a Commissioning Editor for IUCr Journals)
 R. Steiner (UK) (as a Commissioning Editor for IUCr Journals)
 M.I. Aroyo (Spain) (as Editor of Volume A of *International Tables*)
 G. Chapuis (Switzerland) (as an Editor of Volume B of *International Tables* and
 as Editor-in-Chief of the Online Dictionary of Crystallography)
 T.R. Welberry (Australia) (as Editor of Volume C of *International Tables*)
 D.B. Litvin (USA) (as Editor of Volume E of *International Tables*)
 E. Arnold (USA) (as an Editor of Volume F of *International Tables*)
 L. Tong (USA) (as an Editor of Volume F of *International Tables*)
 B. McMahon (UK) (as an Editor of Volume G of *International Tables*)
 J. Hester (Australia) (as an Editor of Volume G of *International Tables* and as
 Chair of COMCIFS)
 U. Müller (Germany) (as Editor of Volume A1 of *International Tables*)
 C.J. Gilmore (UK) (as an Editor of Volume H of *International Tables*)
 J.A. Kaduk (USA) (as an Editor of Volume H of *International Tables*)
 F. Boscherini (Italy) (as an Editor of Volume I of *International Tables*)

B. Bunker (USA) (as an Editor of Volume I of *International Tables*)
C.T. Chantler (Australia) (as an Editor of Volume I of *International Tables*)
J. Helliwell (UK) (as Chair of IUCr/OUP Book Series Committee)
O. Asojo (USA) (as Chair of Commission on Crystallographic Teaching)

Commission on Crystallographic Teaching

Chair: O. Asojo (USA; 2017)
Elected members: A.J. Blake (UK; 2020)
C. Esterhuysen (South Africa; 2020)
A. Guerri (Italy; 2017)
T. Inoue (Japan; 2017)
P. Kashkarov (Russia; 2017)
D. Lamas (Argentina; 2017)
S. Lopez-Andres (Spain; 2017)
J. Moorthy (India; 2017)

Commission on Crystallography in Art and Cultural Heritage

Chair: G. Artioli (Italy; 2014)
Elected members: S. Bette (Germany; 2020)
J.M. Delgado (Venezuela; 2020)
K. Janssens (Denmark; 2020)
T. Kamiyama (Japan; 2020)
P.C. Ravines (USA; 2017)
S. Svarcova (Czech Republic)
E. Tereschenko (Russia; 2017)

Commission on Diffraction Microstructure Imaging

Chair: D. Pagan (USA; 2021)
A. Bucsek (USA; 2021)
M. Kobayashi (Japan; 2021)
E. Lauridsen (Denmark; 2021)
U. Lienert (Germany; 2021)
S. Merkel (France; 2021)
R. Pokhrel (USA; 2021)
H.F. Poulsen (Denmark; 2021)
L. Wang (China; 2021)

Commission on Electron Crystallography

Chair: M. Gemmi (Italy; 2020)
Elected members: K. Balzuweit (Brazil; 2014)
L. Bourgeois (Australia; 2017)
T. Gorelick (Germany; 2020)
D. Jacob (France; 2017)
P. Moeck (USA; 2017)
A. Stewart (Ireland; 2020)
J. Sun (China; 2020)
H. Young (Canada; 2017)
M. Zubko (Poland; 2020)

Commission on High Pressure

Chair: K.F. Dziubek (Italy; 2017)
Elected members: N. Dubrovinskaia (Germany; 2017)
N. Garg (India; 2017)
K. Komatsu (Japan; 2020)
A. Lazicki (USA; 2020)
S. Moggach (UK; 2017)
G. Shen (USA; 2014)
N.M. Souza-Neto (Brazil; 2017)
W. Yang (PR China; 2020)
B. Zakharov (Russia; 2017)

Commission on Inorganic and Mineral Structures

Chair: C. Ling (Australia; 2020)
Elected members: J.L Jorda (Spain; 2020)
M. Colmont (France; 2017)
A. Gagor (Poland; 2020)
V. Kahlenberg (Austria; 2017)
E.E. McCabe (UK; 2020)
M. Nespolo (France; 2017)
K. Sugiyama (Japan; 2020)
S. Tarantino (Italy; 2020)
N. Zubkova (Russia; 2017)

Commission on Magnetic Structures

Chair: B. Campbell (USA; 2011)
Elected members: G. Aurelio (Argentina; 2020)
M. Avdeev (Australia; 2017)
F. Damay (France; 2020)
M.T. Fernandez-Diaz (France; 2017)
O. Garlea (USA; 2017)
M. Henriques (Czech Republic; 2017)
D. Khalyavin (UK; 2020)
J.M. Perez-Mato (Spain; 2014)
N. Terada (Japan; 2020)
A. Wills (UK; 2017)
O. Zaharko (Switzerland; 2017)

Commission on Mathematical and Theoretical Crystallography

Interim Co-Chairs: L. Suescun (Uruguay; 2014)
Elected members: V.A. Blatov (Russia; 2017)
J. Hadermann (Belgium; 2014)
G. McColm (USA; 2014)
H.B. Napolitano (Brazil; 2017)
M. Nespolo (France; 2020)
M.L.A. de la Penas (Philippines; 2014)
Wei Ren (People's Republic of China; 2017)
B. Stöger (Austria; 2020)

Commission on Neutron Scattering

Chair: T. Ishigaki (Japan; 2014)
Elected members: C. Alba-Simoniesco (France; 2017)
S. Chaplot (India; 2014)
J. Hernandez-Velasco (Spain; 2014)
C. Hoffmann (USA; 2020)
M. Meven (Germany; 2017)
V. Peterson (Australia; 2017)
R. Przenioslo (Poland; 2014)
J. Santisteban (Argentina; 2020)

Commission on NMR Crystallography and Related Methods

Interim Chair: D. Bryce (Canada; 2017)
Elected members: S. Brown (UK; 2020)
A. Commoti (Italy; 2020)
Y. Khimyak (UK; 2020)
M. Leskes (Israel; 2020)
P.K. Madhu (India; 2020)
Y. Nishiyama (Japan; 2020)
T. Polenova (USA; 2014)
J. Senker (Germany; 2017)

Commission on Powder Diffraction

Chair: D.G. Billing (South Africa; 2011)
Elected members: I. Evans (UK; 2017)
F. Furlan- Ferreira (Brazil; 2020)
T. Ida (Japan; 2014)

D. Kovacheva (Bulgaria; 2017)
M. Leoni (Saudi Arabia; 2020)
C. Lind-Kovacs (USA; 2020)
A. Neels (Switzerland; 2020)
N. Sharma (Australia; 2020)
A. Wilkinson (USA; 2017)

Ex officio member: J.A. Kaduk (USA) (as Representative of ICDD)

Commission on Quantum Crystallography

Chair: P. Dominiak (Poland; 2014)
Elected members: J. Contreras-Garcia (France; 2020)
A. Gukasov (France; 2014)
J. Kozisek (Slovakia; 2014)
C. Matta (Canada; 2017)
P. Munshi (India; 2020)
E. Nishibori (Japan; 2014)
A Pendas (Spain; 2020)
J. Sabino (Brazil; 2017)
W. Scherer (Germany; 2014)

Ex officio member: T. Ishigaki (Japan) (as representative from Commission on Neutron Scattering)

Commission on Small-Angle Scattering

Chair: J. Ilavsky (USA; 2017)
Elected members: K. Djinovic Carugo (Austria; 2017)
E. Gilbert (Australia; 2017)
E. Kentzinger (Germany; 2020)
D. McGillivray (New Zealand; 2014)
F. Meneau (Brazil; 2020)
E. Shtykova (Russia; 2017)
M. Sugiyama (Japan; 2017)

Commission on Structural Chemistry

Chair: S.A. Bourne (South Africa; 2017)
Elected members: R. Banerjee (India; 2017)
M. Dakovic (Croatia; 2020)
A.J. Edwards (Australia; 2017)
J. Ellena (Brazil; 2014)
K. Fromm (Switzerland; 2017)
J. Harada (Japan; 2017)
L.R. MacGillivray (USA; 2017)
A. Maloney (UK; 2020)
P. Naumov (UAE; 2020)
S.M. Peng (Taipei; 2014)

Commission on Synchrotron and XFEL Radiation

Chair: M.A. Garcia-Aranda (Spain; 2011)
Elected members: S-I. Adachi (Japan; 2020)
A. Cohen (USA; 2020)
E. Granada (Brazil; 2014)
T. Hatsui (Japan; 2017)
L. Keefe (USA; 2020)
M. Kozak (Poland; 2017)
E. du Plessis (South Africa)
S. Ramaswamy (India; 2017)
T. Tschentscher (Germany; 2014)

Commission on XAFS

Chair:	S. Diaz-Moreno (UK; 2014)
Elected members:	H. Abe (Japan; 2020)
	G. Aquilanti (Italy; 2014)
	D. Bhattacharyya (India; 2017)
	V. Briois (France; 2017)
	S.M. Heald (USA; 2014)
	R. Loredo Portales (Mexico; 2020)
	G. Subia-Peruga (Spain; 2020)
	C.Q. Tran (Australia; 2020)
	E. Welter (Germany; 2020)
	A. Wolska (Poland; 2020)

37.2 Representatives of the Union on bodies not belonging to the Union

Statute 8.5 prescribes that representatives of the Union on bodies not belonging to the Union are elected at each General Assembly, and that for each body one representative shall be designated as the chief representative. By-Law 8.9 states that the procedure for nomination and election of the representatives is so far as is possible the same as that for the Commission memberships.

The bodies involved are as follows, together with the **present** representatives:

American Crystallographic Association (ACA) (REGIONAL ASSOCIATE)

Representative: T. Proffen (USA)

Asian Crystallographic Association (AsCA) (REGIONAL ASSOCIATE)

Representative: J. Martin (Australia)

European Crystallographic Association (ECA) (REGIONAL ASSOCIATE)

Representative: A. Altomare (Italy)

Latin-American Crystallographic Association (LACA) (REGIONAL ASSOCIATE)

Representative: G. Diaz de Delgado (Venezuela)

Worldwide Protein Data Bank (wwPDB)

Representative: J. Martin (Australia)

International Centre for Diffraction Data (ICDD) (SCIENTIFIC ASSOCIATE)

Representative: D.G. Billing (South Africa) (*ex officio* as Chair of Commission on Powder Diffraction)

International Organization of Crystal Growth (IOCG) (SCIENTIFIC ASSOCIATE)

Representative: G. Balakrishnan (UK) (*ex officio* as Chair of Commission on Crystal Growth and Characterization of Materials)

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

Representative: C.P. Brock (USA)

International Science Council (ISC)

Representative: S. Lidin (Sweden)

ISC Committee on Data for Science and Technology (CODATA)

Representative: J.R. Helliwell (UK)

ISC Committee on Space Research (COSPAR)

Representative: Y. Kimura (Japan)

International Standards Organization (ISO)

Representative: C.P. Brock (USA)

37.3 Officers of the Union

The **present** membership of the Executive Committee (constituting the officers of the Union) is:

President:	H.A. Dabkowska (Canada)	(1) (2)
Vice-President:	S. Garcia-Granda (Spain)	(1) (2)
General Secretary and Treasurer:	B. Brummerstedt-Iversen (Denmark)	(1)
Immediate Past President:	S. Lidin (Sweden)	(1) (2)
Ordinary members:	A. Altomare (Italy)	(3)
	G. Diaz de Delgado (Venezuela)	(1)(2)
	T. Proffen (USA)	(3)
	J.L. Martin (Australia)	(1)(2)
	M. Takata (Japan)	(1)(2)
	M.S. Weiss (Germany)	(3)

In addition, the Convenor of the Finance Committee (M.J. Cooper, UK) is *ex officio* a member of the Executive Committee (By-Law 6.1).

The members of the Executive Committee who will continue are, therefore:

Immediate Past President:	H.A. Dabkowska (Canada)
Ordinary members:	A. Altomare (Italy)
	T. Proffen (USA)
	M.S. Weiss (Germany)

Nominations presented by the Executive Committee for Officers of the Union

The Executive Committee met in Versailles, Paris, 22-25 August 2022. At the meetings all nominations for officers and members of the Executive Committee proposed by the National Committees of member countries were considered. The Committee agreed to put forward all the candidates proposed for each of the offices of President, Vice-President and General Secretary and Treasurer and it was further agreed that the nine candidates put forward by National Committees should be presented for Executive Committee membership for the three six-year vacancies. These

The nominations made by the Executive Committee are as follows:

President:	S. Garcia-Granda (Spain)	(3)	
Vice-President:	G. Diaz de Delgado (Venezuela)	(3)	
General Secretary and Treasurer:	T. Forsyth (Sweden)	(3)	
Ordinary members (six-year term):	H. Liu (China)	(4)	
	S.C. Mande (India)	(4)	
	A. Moreno (Mexico)	(4)	
	A. Nakagawa (Japan)	(4)	
	P. Naumov (UAE)	(4)	
	M. C. Nonato (Brazil)	(4)	
	S. Ravy (France)	(4)	Withdrawn
	D. Tomchick (USA)	(4)	
	K. Wozniak (Poland)	(4)	

- (1) until the close of the Twenty-Fifth General Assembly
 (2) not eligible for immediate re-election to the same office
 (3) until the close of the Twenty-Sixth General Assembly
 (4) until the close of the Twenty-Seventh General Assembly

Additional nominations for Officers of the Union

If any group of National Committees wishes to make **additional** nominations, could they please send these to the Chief Executive Officer (ceo@iucr.org) at least **one month before** the General Assembly, supported by curricula vitae (including nominees' reasons for standing) and the names of at least six delegates supporting the nominations (see By-Law 8.2). If the names of the delegates are not decided at that time, this group of National Committees should provide the Chief Executive Officer with the names of the dele-

gates as soon as they have been appointed (not later than three weeks before the date of the General Assembly). The Chief Executive Officer will circulate details of any additional nominations (including curricula vitae and nominees' reasons for standing) to the National Committees two weeks before the General Assembly.

An additional nomination for Ordinary Member was received for **S. Bourne (South Africa)** and supported by the National Committees of Canada, Cameroon, Morocco and South Africa fulfilling the requirement of at least six delegates. In addition, the Finnish Crystallographic Committee (although not an adhering body) lent their support.

According to By-Laws 8.2 and 8.4 additional nominations may still be made by delegates in Melbourne but it is hoped that the above procedure will make this unlikely.

Brief biographical details of all candidates nominated to serve on the Executive Committee are given below.

Santiago GARCIA-GRANDA *Physical and Analytical Chemistry Department, Faculty of Chemistry, University of Oviedo, Av. Julian Clavería, 8, 33006-Oviedo, Asturias, Spain*

Nationality: Spanish

Qualifications: Professor of Physical-Chemistry. Degree, 1980, and PhD, 1984, in Chemistry, Faculty of Chemistry, University of Oviedo. Postdoc Radboud University (The Netherlands), 1985/87 (Professor Paul T. Beurskens). Co-author of Program DirDif cited more than 3000 times. Responsible for the infrastructure of the Spanish Line of the Synchrotron of the ESRF-SpLine-. Creator of the X-Ray Diffraction unit at the University of Oviedo and director for 30 years. To mention some concrete personal contributions promoted from my positions in IUCr and ECA are the pioneering Gender Balance Statement and the Family friendly Conference with children care, in the ECM31 or the creation of the concept of General Interest groups (GIG), initiated with the Young Crystallographers GIG in the ECA. Total publications: 798; over 500Q1; H-index: 57 (Google Scholar) / 53(Scopus) / 51 (Wos); Total citations: 12029 (Wos). Crystallography and Structural Science is my vocation and the scientific place where I feel more comfortable.

Recent appointments held: Current Vice President of the IUCr, 2021-; Ordinary Member of the Executive Committee of the IUCr 2014/21; President of the ECA, 2009/12; Chair of the second European Crystallography School, 2015; Chair of the 31 European Crystallographic Meeting, ECM31, Oviedo (Spain) August 2018, with 1000 participants. Current Member of the Spanish National Committee of the IUCr, 2000-; President of the Specialized Group of Crystallography and Crystal Growth, 2000/10; Coordinator of the International Year of Crystallography - IYCr 2014, for Europe and Spain, 2013/15; Rector of the University of Oviedo, 2016/21; Current Officer of the Spanish Sustainable Development Council, 2019-; Current President of the Spanish Commission for the 2030 Agenda, 2019-; President of the CRUE-Sustainability Commission 2018/21; Vice-Chancellor for Research of the University of Oviedo, 2008/12; Executive Secretary of the R&D commission of the CRUE, 2012; Secretary of the Jury of the Princess of Asturias Award for Technical and Scientific Research, 2016/21.

Fields of research: Leads the research group of Synthesis, Structure and Technological Application of Materials at University of Oviedo and the CSIC Nanomaterials and Nanotechnology Institute. Crystallography, materials science, structural determination, diffraction, and calculations. Ten main fields (contributions): Chemistry (729), Crystallography (335), Physics (123), Polymer Science (110), Material Science (82), Spectroscopy (72), Biochemistry Molecular Biology (63), Engineering (43), Science Technology Other Topics (40), Pharmacology Pharmacy (24).

Personal statement: The 75th anniversary of the first IUCr congress and GA held at Harvard in 1948 gives us an opportunity to appreciate our bright past, but above all to think about the future of our Union. The Melbourne 26th Congress will hold the 75th anniversary MS and importantly, the Workshop on the Vision and Values to find the keys that will allow us to face with the illusion of the new generations, women and men, the new challenges to continue developing and leading structural science in a world very different from that of 1948.

The IUCr must keep going on and reinforce the initiatives started on the occasion of IYCr2014, focusing on: (i) Education, to provide new generations of crystallographers and structural scientists, (ii) Research, by fostering scientific collaboration and leadership in Structural Science through the Commissions and our Journals and Books, (iii) New generations, creating a young division to attract the early carrier scientist to have a strong voice in and from the IUCr, (iv) Society, by reinforcing the impact of crystallography in society to obtain the support of stakeholders and put crystallography and structural science, on the agenda of the decision makers, (v) Organization, favoring the links between the regional associations, boosting their influence within the IUCr, and reinforcing our team in the Chester Office (vi) Promoting, keeping the momentum and favor gender equality at all levels and activities. (vii) Attracting, extending the family and child friendly crystallographic conferences, as we initiated in ECM31.

After the 2014 IYCr and beyond the IUCr is more active in demonstrate, foster, and coordinate the impact of crystallography and structural science on humanity. Therefore, providing networking between scientists worldwide and having an active role in the ISC. Now, the hybrid IUCr25 in Prague, brings new opportunities to adapt the IUCr to the new environments. With my experience serving since 2006 on the ECA EC as Officer, President and Past-President, coordination IYCr activities, being

active part of the born of LACA and AfCA and representing the Executive Committee as liaison person with several IUCr Commissions and more recently updating the commission's guidelines. Now the possibility of continuing working on the IUCr Executive Committee as President is a huge challenge to renew serving crystallography and Structural Science worldwide.

Graciela DÍAZ DE DELGADO Universidad de Los Andes, Facultad de Ciencias, Departamento de Química, Lab. de Cristalografía-LNDRX. Mérida 5101. Venezuela

Nationality: Venezuelan

Qualifications:

Ph.D. in Chemistry, Brandeis University (USA). 1988. Research Director: Prof. Bruce Foxman, Master of Arts, Brandeis University (USA). Chemistry Dept. 198, Licenciatura en Química, Universidad de Los Andes. Facultad de Ciencias. Departamento de Química (Venezuela). 1979-1983. Attended advanced courses on Crystallography, Solid State Chemistry, among others.

Recent appointments held:

Prof. Titular (Full Professor) since 2002. Associate Prof. 1997-2002. Prof. Agregado 1995-1997. Assistant Prof. 1989-1995. All at Universidad de Los Andes (ULA), Mérida, Venezuela.

Director, Laboratorio Nacional de Difracción de Rayos-X, LNDRX. Since January, 2007.

Member of the Board of Directors of Orquesta Sinfónica del Estado Mérida. 2013-2015.

Visiting Professor, Universidad Industrial de Santander, Bucaramanga, Colombia. 2014.

Chair, Materials Science Division, Chemistry Graduate Studies Program, ULA. 1994-1998, 2011-2015.

Chair, Graduate Studies Division, Facultad de Ciencias, ULA. May 2004-2007.

Chair, Technical Committee of the Chemistry Graduate Studies Program, ULA. 2001-2004.

Visiting Professor, Materials Research Laboratory, University of California, Santa Barbara, USA. 1998-1999.

Fields of research:

Use of single crystal and powder diffraction techniques in the characterization of materials. Synthesis and characterization of organic-inorganic hybrid porous materials with potential applications in the pharmaceutical and oil industry, catalysis, gas storage, controlled release, among others. Solution, solvothermal, and mechanochemical synthesis. Supramolecular chemistry. Crystal Engineering. Hydrogen bonding patterns in crystalline carboxylic acids and metal carboxylates. Solid state chemistry of unsaturated carboxylic acids and metal carboxylates. Coordination geometry in metal carboxylates. Structural characterization of Active Pharmaceutical Compounds (APIs) and intermediates in the synthesis of APIs. Polymorphism in APIs. Metal derivatives and multicomponent materials involving APIs. Structural characterization of Natural Products isolated from medicinal plants of the Venezuelan Andes. Other interests: Science outreach, Symmetry and Art.

Personal statement: Since our Congress and General Assembly in Hyderabad, in 2017, our Union has experienced difficult unexpected situations and faced enormous challenges. A global health crisis made us postpone our most important event in 2020. In spite of all difficulties, the hybrid 25th Congress and General Assembly of 2021 was highly successful. As a member of the Executive Committee elected in 2017 in Hyderabad, I have had the unique opportunity to see how our Union works. I am honored to have been part of an excellent team that has worked hard to maintain the leadership of the IUCr as a scientific and publishing union and to contribute to increase the visibility of our field in the global scientific scenario. I would like the opportunity to continue working for our Union as Vice-president. Since 2017, we have seen the incorporation of new country members from all geographical areas in the IUCr, the consolidation of LACA, and the crystallization of AfCA (African Crystallographic Association) but we need to keep our efforts to include more countries from Africa, Asia, and Latin America and the Caribbean. My time on the Subcommittee on the Union Calendar has allowed me to get a good picture of the activities that need to be supported around the world to prepare the new generations of crystallographers. We also need to adapt to the new trends in publishing and access to publications but ensure our journals and books remain at the top of the list of choices for authors for the dissemination of quality work. Our Union should continue working towards more inclusion and equality among all members. We should also remain an amicable and collaborative home for ALL crystallographers even under the appalling and disheartening circumstances we are facing.

V. Trevor FORSYTH LINXS - Institute of Advanced Neutron and X-ray Science, Scheelevägen 19, Lund, Sweden and Faculty of Medicine, Lund University, Sweden

Nationality: Ireland & United Kingdom

Qualifications:

1976 Waterford-Kamhlaba United World College, Mbabane, Eswatini, A-Levels (Cambridge) Physics, Biology, Mathematics, 1976 - 1979 BSc (Physics & Biology) 1980, 1980 - 1983 PhD (Biophysics) 1984.

Recent appointments held: 2022 - Director, LINXS Institute of Neutron and X-ray Science, Lund, Sweden, 2022 - Professor of Biophysics, Faculty of Medicine, Lund University, Sweden, 2011 - 2021 Senior Fellow in Life Sciences, Institut Laue-Langevin, Grenoble, 2005 - 2021 Chair in Biophysics, School of Life Sciences & ISTM Research Institute, Keele University, Staffordshire, UK, 2005 - 2021 Head of ILL's Life Sciences Group at the Partnership for Structural Biology (PSB), Institut Laue-Langevin, Grenoble, France

Fields of research: Molecular Biophysics – amyloids and amyloidogenesis in relation to health pathologies, nucleic acid structure and polymorphism, redox proteins, lipid nanoparticle systems for mRNA delivery. Methodologies used include crystallography, fibre diffraction, solution scattering using X-rays, neutrons, electrons. Exploitation of biomolecular deuteration using neutron scattering and mass spectrometry. Extensive use of central facility infrastructures such as the Institut Laue-Langevin (ILL), the European Synchrotron Radiation Facility (ESRF), the ISIS Spallation neutron source, Diamond Light Source, MAX IV, ESS.

Personal statement The International Union of Crystallography (IUCr) plays a vital role in advancing scientific research and understanding in the field of crystallography and other techniques relating to diffraction and scattering. Essentially all of my research career has involved scientific results or method developments that fall within the broad remit of IUCr and it is a great pleasure to be considered as a candidate for General Secretary and Treasurer. As a global organisation, the IUCr fosters collaboration and knowledge sharing among scientists worldwide, serving as a key hub for scientific exchange. It promotes the development of crystallographic/diffraction/scattering techniques, methodologies, and standards, ensuring the accuracy and reliability of data and data interpretation. This enables and facilitates the work of many thousands of researchers involved in the exploration of atomic and molecular structure and dynamics for a wide range of materials, from minerals, metals, through complex compounds and polymers to biological molecules and complexes with therapeutic agents. IUCr also contributes importantly to education and outreach by providing a platform for scientists to connect, learn, and collaborate, spreading awareness and understanding of a broad range of scientific areas and inspiring the next generation of scientists.

Susan BOURNE Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa

Nationality: South African

Qualifications: Prof of Physical Chemistry and Director of Centre for Supramolecular Chemistry Research, University of Cape Town, 1986 BSc in Chemistry, with distinction, University of Cape Town, 1987 BSc Hons. in Chemistry, University of Cape Town. 1991 PhD in Chemistry, University of Cape Town, Inclusion compounds of Hydroxy Hosts

Recent appointments held: 2015-present Professor of Physical Chemistry, Department of Chemistry, University of Cape Town. 2012-2017 Head of Department, Department of Chemistry, University of Cape Town. 2013-2016 Deputy Dean, Faculty of Science, University of Cape Town. 2018-2019 Interim Dean, Faculty of Science, University of Cape Town. Fellow of the Royal Society of Chemistry (UK), 2014, Fellow of the African Academy of Sciences, 2018, Fellow of the South African Chemical Institute, 2019, IUPAC Distinguished Woman in Chemistry/Chemical Engineering, 2019

Fields of research: NRF rating: B2 (since 2008) "Researchers who enjoy considerable international recognition by their peers for the high quality and impact of their recent research outputs." Research interests: Supramolecular chemistry, particularly crystal engineering. Current projects include synthesis of functional metal-organic frameworks; applications of co-crystals to improve properties of pharmaceutical and nutraceutical agents. All of my research involves working with postgraduate students. Part of this work has been carried out in the form of international collaborations.

Personal statement:

I have been actively involved in the IUCr over my entire career. This has included several terms as chair of the South African national committee for the IUCr, one term on the Commission for Crystallographic Teaching and three terms on the Commission for Structural Chemistry, including as chair since 2017. The IUCr plays a crucial role in bringing together scientists working in crystallography and all aspects of diffraction and scattering technology. It also provides a meeting space for scientists across the globe, ever more important in our current difficult times. The 2023 IUCr Congress will consider the African Crystallographic Association (AfCA) as a regional affiliate. The United Nations estimates that, by 2050, 25% of the world's population will live in Africa which provides African scientists with both great challenges and opportunities. I have witnessed the growth of crystallography across Africa over the past thirty years and have played an active role in this growth. I have organised and participated in crystallographic conferences and schools and have trained postgraduate students from across the continent, many of whom are now academics in their home countries. Look out too for a virtual special collection of articles from African scientists across all IUCr journals, to be published this year. I am excited at the prospects for further growth

across the continent. I am deeply honoured to be considered as a candidate for the Executive Committee. If elected, I would continue to promote progress in crystallography across Africa and globally, with particular focus on developing opportunities and inclusivity for younger scientists.

Arthur Haozhe LIU, Center for High Pressure Science & Technology Advanced Research, HPSTAR, 10 XiBeiWang East Road, Room A-308, Haidian, Beijing, 100094, China

Nationality: Chinese

Qualifications: Ph. D., Material Sciences and Engineering, Institute of Metal Research, Chinese Academy of Sciences, China (1994-1997); M. S., Solid State Physics, Jilin University, China (1991-1994); B. S., Solid State Physics, Jilin University, China (1987-1991).

Recent appointments held: Staff Scientist, HPSTAR, Beijing, China (2014-present); Longjiang Distinguished Professor, Harbin Institute of Technology (HIT), China (2007-2022). Leader for HIT Overseas Collaborative Research Team at Argonne National Laboratory, USA (2010-2014); Visiting Scientist, X-ray Operation and Research/X-ray Science Division (XOR/XSD), Advanced Photon Source (APS), Argonne National Laboratory, USA (2009-2010); Research Scientist, HPCAT, Carnegie Institution of Washington, APS, Argonne National Laboratory, USA (2003-2007); Research Scientist, Mineral Physics Institute, State University of New York at Stony Brook, USA (2002-2003); Guest Scientist, Max Planck Institute for Solid State Research, Stuttgart, Germany (2000-2001); Postdoc, Institute of Physics, Chinese Academy of Sciences (CAS), Beijing, China (1997-1999). Chair of Commission on High Pressure (2017-2021); Co-editor of Journal of Applied Crystallography (2020-present); Associate Editor of American Mineralogist (2012-2022); Executive Committee Member of AIRAPT (2017-present); Executive Council Member of Chinese Crystallography Society (2016-2021); Secretary of Commission on High Pressure (2014-017); Committee Member of Commission on High Pressure (2008-2014); Co-Chair of AIRAPT-26 Conference, Beijing, Aug. 18-23, 2017; Co-Chair of LAM-15 Conference, Beijing, Sep. 15-20, 2013; SPring8 Proposal Review Panel (2019-2023).

Fields of research: Current scientific interest is the mineral physics and materials physics under high pressure conditions. Research topics include pressure induced transitions in crystalline and non-crystalline or melting samples; structure and property relationship for materials under high pressure extreme conditions, using multiples advanced synchrotron radiation techniques, such as X-ray diffraction and scattering, high energy X-ray PDF method, absorption base and diffraction base tomography, XPCS, etc.

Personal statement: As a US citizen who has worked in China for the last 16 years, my team and I have benefitted from the international collaborative program. However, the strained relationship between the USA and China in last 5 years has made collaboration in these two scientific communities quite challenging. I believe scientists can do a better job than politicians to improve this relationship. If I was elected as a IUCr Executive Committee member, I would focus on the mission to promote and coordinate scientific exchanges between various countries. This is one of the most important goals of the IUCr, and we need to further advance this mission.

I have served as co-editor of the Journal of Applied Crystallography since 2020, and would like to continue to contribute to the journal, since the publication is crucial to the financial health of IUCr. Another major component of IUCr activity is the Congress. I advocate that China should host the IUCr Congress in the near future. Nowadays, China has the largest crystallographic community, but it has only hosted the IUCr Congress once in 1993. Clearly, China is underrepresented in hosting Congress. If I was an EC member, I would strengthen ongoing collaborations and encourage new collaborations between colleagues in China and peers overseas, through the various local funding programs in China, and beyond.

Other personal mission: Since 2018, my wife and I started a family charity funding as our own Jubilee mission (Lev. 25: 8). This charity has been supporting the tuitions and needs of over 100 college students at HIT and Jilin University, China. We have plans to expand this charity effort to scientific communities in other countries.

Shekhar C. MANDE Academy of Scientific and Innovative Research (AcSIR), CSIR- Human Resource Development Centre, (CSIR-HRDC) Campus, Postal Staff College Area, Sector 19, Kamla Nehru Nagar, Ghaziabad, Uttar Pradesh- 201 002

Nationality: Indian

Qualifications: Ph.D.

Recent appointments held:

Secretary, Council for Scientific and Industrial Research, Government of India
Director, National Center for Cell Science, Pune
Scientist, Center for DNA Fingerprinting and Diagnostics, Hyderabad

Scientist, Institute for Microbial Technology, Mohali

Fields of research: Macromolecular Crystallography, Computational Biology and Bioinformatics

Personal statement I would like to be considered for the Executive Committee of IUCr as I have been closely associated with the Indian Crystallographic Association since its inception, and moreover, I was the Chair of the IUCr committee of the Indian National Science Academy, New Delhi for one term. In my capacity as the Chair, I attended the IUCr General Assembly at Hyderabad in 2017. Due to my administrative responsibilities in the Govt of India between 2018 and 2022, I was away from academics, but now being fully back in academics, I would like to contribute to the growth of structural sciences in India, and around the world in general. In the exciting times of new techniques including Cryo Electron Microscopy single particle analysis, electron tomography and free electron lasers, complementing X-ray single crystal methods, the awareness of the power of all these among scientists in general needs to be enhanced. I believe that my general academic background, and my vast administrative experience, will help me carry out this formally, if I were elected as a member of the EC of IUCr. Moreover, my exposure to South Asia and the region around us during my tenure as the Director General of CSIR (India), will be useful in taking these ideas in the regions geographically closer to mine.

Abel MORENO, Institute of Chemistry, National Autonomous University of Mexico, Av. Universidad 3000, Mexico City, 04510, Mexico

Nationality: Mexican

Qualifications: B.Sc. in Chemistry, Autonomous University of Puebla (Mexico) and University of Granada in Spain in 1990. Ph.D. in Chemistry, University of Granada (Spain), 1995. Currently, a full Professor of Biological and Physical Chemistry at the Institute of Chemistry of the National Autonomous University of Mexico (UNAM), Mexico City. Distinguished as a member of the National System of Researchers of Mexico (SNI) at level 3 (the highest category of Mexican scientists), a member of the Mexican Academy of Sciences, Mexican Society of Crystallography, Mexican Society of Synchrotron Light, the New York Academy of Sciences, and member of the Mexican and American Chemical Societies as well as the Spanish Royal Society of Chemistry. A visiting professor at the University of Cambridge (United Kingdom, 2009) and at the University of Strasbourg (France, 2003–2004). Dr. Moreno has been a visiting scientist at the University of Luebeck and at the Institute of Crystal Growth (IKZ) Berlin (Germany, February 2004), at the University of Tohoku (Japan, Autumn 2003), at Imperial College London (the United Kingdom in 1999 and 2000), and at the University of California Riverside (USA, 1997). Into the Academia he has graduated more than 30 students at all levels from BSc up to the PhDs and postdoctoral fellows. Former President of the International Organization for the Biological Crystallization from September 2010 to September 2012 (IOBCr). A member of the international advisory board of the Commission of Crystal Growth and Characterization of Materials of the International Union of Crystallography, member of the Executive Committee of the International Organization for Crystal Growth (2019–2022). President of the Mexican Society of Crystallography from 2018–2019, currently the vice-President of Mexican Society of Synchrotron Light from 2019–2023. Member of the Advisory board of the Latin America Asia Africa and Middle East Program (LAAAMP) of the IUCr–UNESCO–IUPAP. Member of the Editorial Board of the journal *Progress in Crystal Growth and Characterization of Materials* (ELSEVIER). Editor for the Latin America section of the Newsletter of the International Union of Crystallography, and Editor-in-Chief of the section *Biomolecular Crystals* of the journal *Crystals* (MDPI, Switzerland). Recently was assigned associate editor of the journal *Revista Mexicana de Física* (Mexican Journal of Physics, Mexico).

Recent appointments held: Full Professor of Biological and Physical Chemistry; Chair of the Lectures on Physical Chemistry for Biomedical Sciences (1997–2002), and from 2010 the Chair of the Course: Equilibrium and Kinetics in the undergraduate level at the Faculty of Chemistry UNAM. Habilitated to supervise students into the PhD Graduate Programs in Biomedical, Biological, Chemical and Materials Sciences since 2000.

Fields of research: Published more than 115 papers in prestigious international journals cited 2500 times having a H-index of 25. Author of 15 book chapters and 7 books on his specialties in Biological Crystallogeneses, Crystallochemistry, and Bio-mineralization processes.

Personal statement: I would like to be a member of the Executive Committee (EC) of the IUCr for several reasons: the first is because of the prestige of this organization whose reach in the world is impressive. I am convinced that the geographical distribution of the members of the EC is very important, not only to disseminate Crystallography but also to be able to carry out many activities such as courses, workshops, and congresses world-wide. The EC is the brain of the organization, where the central decisions are taken on where the future of this International Union should go. Another reason is that the EC must coordinate and rely on the sub-committees to carry out its work. According to the statutes of the IUCr, the EC must carry out the decisions of the General Assembly and make them effective immediately. The EC must respect and follow up all the guidelines in order to organize the budget between the current Assembly and the one that will come into the immediate board members of the EC. Thirdly, I know that one of the responsibilities of this EC is to make nominations for the heads of the commissions their

activities and their responsibilities. It is my commitment that when these decisions are made, they will consider a gender balance and an appropriate international distribution. Finally, if I would be selected, I would like to be a bridge in communication with the board of directors of LACA to support the development of crystallography in this geographical area.

Atsushi NAKAGAWA, Institute for Protein Research, Osaka University, 3-2 Yamadaoka, Suita, Osaka 565-0871, Japan

Nationality: Japanese.

Qualifications: B.S. in Science from Nagoya University (1984) with Professor Jiro Tanaka and Professor Noriyoshi Sakabe, M.S. in Science from Osaka University (1986), and Ph.D. in Science from Osaka University with Professor Hideaki Chihara and Professor Noritake Yasuoka (1989). Research Associate with Professor Noriyoshi Sakabe in the Photon Factory of the National Laboratory for High Energy Physics, KEK (1987-1995). Associate Professor at Hokkaido Univ. (1995-1999) with Professor Isao Tanaka. Associate Professor (1999-2003), Professor (2003-), a Director of the Institute for Protein Research, Osaka University (2018-2022). Author and co-author of more than 240 research publications in the field of crystallography, structural biology, synchrotron radiation science, life sciences, and chemistry (H-index 54, Citation Index: 12104 in Google Scholar). Reception of the Young Scientist Award (1993) and the Prize for Science (2009) from the Crystallographic Society of Japan (CrsJ). Chair of SPring-8 Users Community (2016-2018). The president of the CrsJ (2022-present) and the president of the Protein Science Society of Japan (2022-present).

Recent appointments held:

IUCr Commission member of the Crystallographic Computing Commission (2005-2008), Consultant of the Crystallographic Computing Commission (2008-2011), Commission member of the Crystallographic Computing Commission (2011-2014), Member of the Meeting Support Committee (formerly the Sub-committee on the Union Calendar) (2016-present), Local Organizing Committee of IUCr2008 (2008)

AsCA Council member (2008-2014)

CrSJ Secretary of Editorial Committee (1998-2000), Council member (2001-2007, 2008-2014, 2015-present) President (2022-present)

Others Secretary of Accounting of the Japanese Society for Synchrotron Radiation Research (JSSRR) (2005-2006) Secretary of Promotion of Use of SPring-8 Users Society (2010-2012), Council member of SPring-8 Users Community (SPRUC) (2012-present), Secretary of Facility Use of SPRUC (2012-2014), Vice-Chair of SPRUC (2014-2016), Chair of SPRUC (2016-2018), Auditor Secretary of SPRUC (2018-present), Councilor of Japan Synchrotron Radiation Institute (JASRI) (2016-present), President of the Protein Science Society of Japan (2022-present), Council member of the Protein Society, USA (2022-present)

Fields of research: Dr. Nakagawa is interested in structural biology on voltage-sensing protein family proteins, multidrug efflux pumps, viruses, and other biologically important targets, together with the development of macromolecular crystallography techniques. In the early stage of his scientific carrier, he was interested in the application of wavelength tunability of SR for macromolecular crystallography and succeeded to solve the structure of cytochrome c-553 from *Desulfovibrio vulgaris* Miyazaki F strain, which was the third novel structure solved by MAD, in 1990. He then succeeded to determine the structure of macrophage migration inhibitory factor, which was the first selenomethionine labeled structure determined by the MAD method from Japan in 1996. Since then, he has solved and deposited more than 130 protein structures to the PDB.

Dr. Nakagawa also contributed to the development of a synchrotron radiation beamline using a Weissenberg camera for macromolecular crystallography (commonly called Sakabe camera) (BL6A) in the Photon Factory in the middle of the 1980s with professor Noriyoshi Sakabe. He also contributed to the development of a drum scanner-type Imaging Plate reader with Dr. Yoshiyuki Amemiya in the Photon Factory. After he moved to the Institute for Protein Research, Osaka University, he is in charge of the contract beamline in SPring-8 (Beamline for Macromolecular Assemblies, BL44XU). The beamline is designed to collect high-precision diffraction data from large unit cell crystals.

Personal statement: It is my great honor to be nominated as a candidate for the IUCr Executive Committee.

Crystallography is a powerful technique for solving the atomic structure of molecules. However, especially in the field of structural biology, it is becoming increasingly important to combine it with other complementary techniques such as cryo-electron microscopy, NMR, and AI-based structure prediction to better understand molecular mechanisms. The IUCr aims to promote the advancement of crystallography and its related topics including non-crystalline states. Traditional "Crystallography" is now expanding as a "Molecular Science based on atomic structures," which forms the foundation of all fields of natural sciences and the development of functional materials. Based on my experiences as the current president of the Crystallographic Society of Japan, the president of the Protein Science Society of Japan, a council member of the Protein Society in the USA, and a former Chair of the SPring-8 Users Community, I am eager to contribute to expanding the IUCr's activities in promoting scientific endeavors based on atomic structures.

Panče NAUMOV New York University Abu Dhabi, Experimental Research Building (C1), office 151, P.O. Box 129188 Abu Dhabi, United Arab Emirates

Nationality: Macedonian

Qualifications:

Radcliffe Fellow, Harvard University

Friedrich Wilhelm Bessel Fellow, Alexander von Humboldt Foundation

Japanese Ministry of Education, Culture, Sports, Science & Technology Scholar

Founder, American Chemical Society (ACS) Chapter of the UAE

Founder and President, Emirates Crystallographic Society (ECS)

President, Division of Crystallography, Society of Chemists and Technologists of Macedonia

Fellow, American Chemical Society (ACS)

Fellow, the Royal Society of Chemistry (RSC)

Councilor, the European Crystallographic Association (ECA)

Consultant and a member, Commission on Structural Chemistry, IUCr

Regional Editor, IUCr Newsletter

Member, Natural Sciences Advisory Board, Emirates Science Council

Member: ACS, RSC, ECA, ACA, MBRAS, ECS

Recent appointments held:

Associate Professor (tenured), New York University Abu Dhabi

Associate Professor, Osaka University

Associate Professor, Kyoto University

Research Fellow, National Institute for Materials Science

Fields of research: The research of Panče Naumov Group focuses on smart crystalline materials, adaptive and dynamic crystals, photocystallography, emissive materials, and petroleomics.

Personal statement Coming with an upbringing in South-Eastern Europe, being educated in small-molecule crystallography in far-East Asia (Japan), and currently working in an American university in the Middle East, my professional background reflects a unique cultural diversity that has benefitted from very different academic settings and aligns with some of the main goals of the IUCr's mission. With the financial support of the Japanese Government, I had the honor of working on my Ph.D. with Yuji Ohashi, one of the world's most eminent small-molecule crystallographers and a former President of the IUCr. In over two and half decades of active crystallographic research, I have contributed not only to the promotion of crystallography in South-Eastern Europe by establishing the first crystallographic division in Macedonia but also by establishing the first laboratory for single-crystal diffraction analysis in the United Arab Emirates (UAE) and the Emirates Crystallographic Association (ECS), a milestone in the development of the crystallography in the Middle East. From the many esteemed colleagues I had the privilege of working with in my past career, I am especially indebted to Yuji Ohashi (Japan), Joel Bernstein (Israel), Gautam Desiraju (India), and Elena Boldyreva (Russia). If I am elected a member of the IUCr's Executive Committee, I hope to be able to capitalize on my creative potential that brings crystallography closer to the wider materials science research community. I believe that the gap between crystallographers and others who align better with materials research can be bridged by effectively integrating contemporary, sophisticated automated crystallographic methods deeper into the educational curricula at all levels and providing employment opportunities for young crystallographers.

Maria Cristina NONATO, Department of Biomolecular Sciences, School of Pharmaceutical Sciences, University of São Paulo, Laboratório de Cristalografia de Proteínas, FCFRP-USP, Av. Café S/N, Bloco M, Sala 57, 3 andar. Bairro: Monte Alegre

Nationality: Brazilian

Qualifications: She has over 25 years of experience in the field of Structural Biology, integrating biophysics chemistry and biology with the goal of advancing human health, in particular in the fields of neglected and rare diseases. Dr. Nonato's research is focused on Structural Biology applied to drug discovery with special emphasis in Protein Crystallography, Enzyme kinetics, Biophysical and Biochemical characterization of protein targets, and ligand screening by both *in silico* and *in vitro* techniques as a tool for the design of lead compounds for the treatment of neglected and rare diseases. She is a world expert in dihydroorotate dehydrogenases, an important drug target for many diseases, having published over 20 papers in this specific field. She has also introduced the study of oxygen-sensitive proteins by X-ray crystallography in Brazil and solved the first crystal structure of a class I fumarase enzyme that revealed a new protein fold (PNAS, 2017). She pioneered the use of X-ray

crystallography fragment screening in Brazil and is now leading a project to establish this technique for the Brazilian scientific community. Dr. Nonato has a dedicated career as research mentor, having supervised 9 MSc, 7 PhDs as supervisor and 3 PhDs as co-supervisor, 7 pos-docs and 20 undergraduates, with attraction to young women to science. Her laboratory has established a fruitful network of national and international scientific collaborations, including the University of Zaragoza, Broad Institute at MIT and Harvard, Universities of Dundee, Durham and Aberystwyth (UK), University of Utah (USA), Drug Discovery Unit (UK) and H3D (South Africa). She is a disseminator of science, giving speeches to highlight the important role of women in science, including motivational speeches for young girls.

Recent appointments held:

Full Professor at University of São Paulo, President of the Research Committee at School of Pharmaceutical Sciences, President of the Brazilian Crystallographic Association

Fields of research: protein crystallography, medicinal chemistry, enzymology

Personal statement As a passionate advocate for the advancement of crystallography in Latin America, I am thrilled to present myself as a candidate for the Executive Committee of the International Union of Crystallography (IUCr). Latin America boasts a vibrant scientific community, filled with untapped potential and groundbreaking research. However, there remains a critical need to bridge the gap between the scientific advancements made by the global crystallographic Community and developing countries. If elected to the Executive Committee, I am committed to not only strengthening connections between Latin America, Southern Hemisphere, and the IUCr but also leveraging my experience to contribute to the formulation of policies that shape the future of crystallography.

By fostering dialogue and cooperation, we can create a global network that facilitates the exchange of ideas and research, ensuring a more inclusive and diverse approach to the field. Special emphasis will be placed on advocating for women in the field of science.

I am committed to representing Latin America and promoting the progress of crystallography within the region. In particular, Latin America has never hosted an IUCr congress and general assembly. Based on preliminary considerations, my feeling is that Brazil could be a suitable candidate for hosting the event in 2035. If I get elected I will do everything to work towards that goal

Thus, If elected to the Executive Committee, I will actively contribute with my experience, while working to strengthen connections, foster collaborations, and create an interconnected scientific community. I humbly request your support in electing me to the Executive Committee of the IUCr, as together we can advance the field of crystallography and create a more inclusive and prosperous future.

Thank you for considering my candidacy.

Diana TOMCHICK UT Southwestern Medical Center, Department of Biophysics/Biochemistry, 5323 Harry Hines Blvd., Dallas, TX 75390-8816, U.S.A.

Nationality: USA

Qualifications:

Member of the IUCr Commission on Biological Macromolecules (2017 – present)

Member, International Program Committee, IUCr 26th Congress and General Assembly, Melbourne Australia (2023)

Past President, ACA (2023)

President, ACA (2022)

Member, U.S. National Committee on Crystallography (2021 – 2022)

Vice President, ACA (2021)

Member, Bid Committee for IUCr 27th Congress and General Assembly, Calgary Canada (2021)

Secretary, ACA (2015 – 2020)

Ph.D. Chemistry, University of Wisconsin, Madison WI (1990)

B.S. Chemistry, Washington State University, Pullman WA (1983)

Recent appointments held:

Professor, UT Southwestern Medical Center, Dallas TX (2011 – present)

Director, Structural Biology Laboratory core facility, UT Southwestern Medical Center, Dallas TX (2000 – present)

Fields of research:

I am the Director of the Structural Biology Laboratory (SBL) at UT Southwestern Medical Center, which is a campus-wide core facility that provides expertise and assistance in all matters pertaining to X-ray crystallographic as well as Cryo-EM structure determination. Since the establishment of the SBL in 2000, we have collaborated with more than 70 groups on campus on over 140 projects. We have guided dozens of graduate students, postdoctoral fellows and technicians through all stages of the structure determination process, resulting in 163 peer-reviewed publications and over 257 X-ray crystal structures as well as 15 Cryo-EM structures deposited to the Protein Data Bank to date. I am a co-investigator on several NIH-funded grants in which I provide structural biology expertise, and I have been involved with several fragment-based lead discovery studies that have included X-ray crystallography as a critical component. The SBL also provides services to various regional academic institutions and has contracts with several industrial partners.

Personal statement I began my career as an inorganic small molecule crystallographer in graduate school, during which time I attended the 14th IUCr Congress in Perth Australia in 1987. After receiving my Ph.D., I became a Structural Biologist with an emphasis in protein crystallography. In the intervening years I have attended an additional nine IUCr Congresses and have been a witness and participated first-hand in three decades of remarkable technological and scientific progress in the imaging of biological macromolecules. The IUCr and its regional affiliates serve a critically important function in promoting best practices as well as educational opportunities, especially during times of rapid changes in science and technology. In 2017 I successfully campaigned to establish the Cryo-EM Scientific Interest Group (SIG) in the American Crystallographic Association (ACA) and have supported the recently inaugurated MicroED SIG. I have been a voice in support of including Cryo-EM technology and scientific applications in the IUCr Commission on Biological Macromolecules, as well as in the scientific program for the IUCr2023 Congress. It is critical for the IUCr to maintain its position as the standard bearer for data integrity, quality publications, educational opportunities, and cutting-edge science for macromolecular crystallography, Cryo-EM and AI methods used for structure elucidation. The IUCr has an important role in promoting structural science worldwide, to a diverse group of scientists, non-scientists, public policy makers and government officials. As a member of the EC I would continue to lobby for an inclusive approach to addressing the evolution of the field of structural biology and to all the structural disciplines in the IUCr.

Krzysztof WOŹNIAK Department of Chemistry, University of Warsaw, Pasteura 1, 02093 Warszawa, Poland

Nationality: Polish

Qualifications: 1998 Habilitation "On Weak Interactions in Organic Solids" awarded the Prime Minister Prize for the Best Habilitation, Chemistry Department, UW (UW stands for the University of Warsaw), Poland; 1992 PhD "On Influence of H-Bonding on Properties of Molecules, Promoter: Prof. Tadeusz Krygowski, Chemistry Department, UW, Poland; 2000 – 2018, Promoter of 20 PhDs completed and another 6 currently in progress, >30 MSc theses. Supervisor of ca. 30 postdoctoral fellows including Marie Curie Fellows Dr Maria Gorna and Dr Katarzyna Bandyra (currently supervisor of 10 postdoctoral fellows), host of Prof. D. Haynes (Stellenbosch, SA) and Dr hab. Julian Henn (Germany)) during their sabbatical stays in my group (2018 and 2020-2021) >410 refereed publications in learned scientific journals, ca. 8868 citations, H-index =46 (Google Scholar 06/2022), >100 invited lectures in total,

Recent appointments held: (2008-) Head of Crystallochemistry Laboratory and Laboratory for Structural Research at the Department of Chemistry, Univ. of Warsaw, Poland; (2016-) Head of Laboratory for Structural and Biochemical Research, Biological and Chemical Research Centre, Warsaw, Poland; (2018-2021) Research expert in WPD Pharmaceuticals, Warsaw, Poland; (2020-) Head of the Cryo-Electron Microscopy and Electron Diffraction Core Facility at the Center for New Technologies, Warsaw, Poland; (2013 – 2016) and (2020-2024) Member of the Scientific Council of the Department of Chemistry, UW, and its several committees; (2007-2010) Member of the Scientific Council of the Institute of Organic Chemistry PAS, Warsaw, Poland; (2011-2016) Member and (2020-2024) vice-Chairman of Committee for Crystallography of the Polish Academy of Sciences. (2017-2020) Chairman of the Scientific Council of Pharmaceutical Institute, Warsaw, Poland. (2017-2018) Co-chairman and (2018-2022) Chairman of the European Crystallographic Association Special Interest Group on Charge Spin and Momentum Densities (SIG2) presently named Quantum Crystallography. (2022-2026) Member of the Scientific Council of the Centre for New Technologies, Warsaw, Poland.

Fields of research: Scientific interests; Crystallography beyond Independent Atom Model, Hirshfeld Atom Refinement, experimental studies of charge densities in crystals of interesting organic, inorganic compounds and minerals, polymorphism and interactions in pharmaceutical substances and different forms of ice, supramolecular compounds, model systems with interesting weak and strong interactions (proton sponges, Schiff bases, etc), biological compounds, artificial molecular machines. I am also interested in methodological aspects of X-ray scattering, neutron diffraction and electron diffraction and in high pressure studies of particularly minerals and different forms of ice in particular – especially Quantum Crystallographic methods under high pressure.

Ca, 10 years ago, I also organised a wet macromolecular lab. and we have now several macromolecular projects regarding small pharmaceutical molecules and their interactions with macromolecular receptors (potential drug moieties).

Personal statement: As a global crystallographic community, we should look to the future. IUCr should anticipate developing trends in crystallography and stimulate the most interesting directions. We all have seen the amazing developments in scientific infrastructure which have not yet been accompanied by similar progress in theory and applications. For example, we have now plenty of new tools: modern diffractometers, electron microscopes, the newest generations of synchrotrons, and XFELs which all supply accurate and precise information but still ca. 99.7% of all ca. 1.5mln X-ray structures are refined with the 100-year-old IAM. Isn't this the greatest paradox of modern crystallography? IUCr should initiate and stimulate the modernisation of crystallographic approaches. I also believe that the crystallographic standards promoted by the IUCr should be reviewed and updated. IUCr should also react to global challenges such as, for example, war in Ukraine. Organisations which represent aggressor countries which commit war crimes cannot be formal members of IUCr. We as a crystallographic community should solve the problem of storage of original/primary measured data. Most structural information measured and refined in the past could now be improved by re-refinement and reused using more modern models of electron density and more attention could be paid to the analysis of systematic effects both in measured data and in residuals obtained after model fitting.

The next important issue is the social role of IUCr. IUCr should initiate and stimulate activities in these parts of the world that require both infrastructure and organizational assistance. I also see a chance for some improvements in the review procedures for publications in the IUCr journals.

Appendix 38 to Agenda

Any other business