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**Twenty-Fourth General Assembly and International Congress of  
Crystallography, Hyderabad, India, 21–28 August 2017**

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

### A1. Report of the Executive Committee

#### A1.1. Executive Committee and Finance Committee meetings

The Executive Committee met in Montreal, Canada, in August 2014 before and during the General Assembly, in Rovinj, Croatia, in August 2015 at the time of the European Crystallographic Meeting, and in Denver, USA, in July 2016 at the time of the American Crystallographic Association Meeting. The Finance Committee met in March 2015, August 2015, March 2016, July 2016 and March 2017, 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 triennium at these meetings, and in postal and e-mail ballots between meetings, were:

editorial policy, pricing policy and subscription rates, review of work of Journals Management Board, development of *IUCrJ*, launch of *IUCrData*, approval of appointments of Editors, approval of appointments of Co-editors, re-launch of *Acta E*, archival policy, 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;

General Fund estimates and level of unit contribution, status of membership subscriptions;

investment policy;

funding and uses of Publications and Journals Development Fund, Research and Education Fund and President's Fund;

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

establishment of Outreach and Education Fund and guidelines for its use;

cooperation with databases;

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

*IUCr Newsletter*, *World Database of Crystallographers*;

marketing and promotional activities;

introduction of an IUCr Associates Programme;

events and outcomes from the International Year of Crystallography;

OpenLabs and other activities;

appointment of the Selection Committee for eleventh Ewald Prize;

sponsorship of other prizes;

discussion of arrangements for Hyderabad Congress;

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

level of financial support for Hyderabad Congress;

consideration of progress with arrangements for Prague Congress;

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

Other items dealt with in this way were:

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

IUCr 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;

establishment of the wwPDB as a Scientific Associate;

appointment of an IUCr Representative to the International Standards Organization (ISO);

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

relations with other Scientific Unions;

review of work of Diffraction Data Deposition Working Group, formation of Committee on Data;

Items concerning the Chester office were:

staffing requirements in the IUCr office in Chester;

retirement of, and appointment of successor for, Executive Secretary;

risk analysis;

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

## A1.2. Publications

The subscription prices of *Acta Crystallographica*, the *Journal of Applied Crystallography* and the *Journal of Synchrotron Radiation* were increased each year during the triennium. *IUCrJ* and *IUCrData* were launched during the triennium.

The total annual number of pages published in 2014, 2015 and 2016 were:

	2014	2015	2016
<i>Acta Crystallographica</i> Section A	686	630	705
<i>Acta Crystallographica</i> Section B	1,036	813	933
<i>Acta Crystallographica</i> Section C	1,180	1,117	1,011
<i>Acta Crystallographica</i> Section D	3,329	2,542	1,309
<i>Acta Crystallographica</i> Section E	2,351	2,931	1,874
<i>Acta Crystallographica</i> Section F	1,713	1,540	911
<i>Journal of Applied Crystallography</i>	2,115	2,044	2,282
<i>Journal of Synchrotron Radiation</i>	1,385	1,560	1,563
<i>IUCrJ</i>	613	690	467
<i>IUCrData</i> (launched 2016)			1,396
Total	14,408	13,867	12,471

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

From January 2014 all journals have been available online only. Section F is available free of charge to subscribers to Section D. *IUCrJ*, *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.); Education (including the *Online Dictionary of Crystallography*); People (including the photographic archive); Resources (including discussion lists); and the International Year of Crystallography.

Full details on the publication of volumes of *International Tables for Crystallography* are given in the Triennial Report of this Commission (Appendix A6.2).

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

The *IUCr Newsletter* is distributed electronically free of charge to 587 libraries and more than 18,000 crystallographers and other interested individuals in 102 countries. W.L. Duax is the Editor with the editorial office at the Hauptman–Woodward Medical Research Institute at Buffalo, New York, USA. A report on the *IUCr Newsletter* is given in Appendix A8.

The IUCr/Oxford University Press Book Series continues to be successful. Details are given in Appendix A19.

### A1.3. Sponsorship of meetings

The Sub-committee on the Union Calendar considers and advises the Executive Committee on requests for IUCr sponsorship and financial support of meetings. The Chair of the Sub-committee is W. Depmeier. A list of IUCr-sponsored meetings is given in Appendix A11.

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

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

Meetings (other than satellite meetings) scheduled to be held within one month before or after an IUCr Congress will not be considered for sponsorship. For any meetings scheduled to be held between one and two months before or after a Congress, the application for sponsorship requires the approval of the Chair of the Congress Programme Committee. For meetings (other than satellite meetings) scheduled to be held, in the respective region, within one month before or after a meeting of a Regional Associate (American Crystallographic Association, Asian Crystallographic Association, European Crystallographic Association, Latin-American Crystallographic Association), the applicants for sponsorship must seek the approval of the Chair of the Regional Associate Organizing Committee.

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

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

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

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

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

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

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

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

#### *Visiting 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. Visiting Professorships will not normally be awarded for workshops or schools held in BRICS countries (Brazil, Russia, India, China, South Africa). These schools or workshops may have national or international character. Up to a maximum of three Visiting Professorships (VPs)

can be granted for a single event. Travel and insurance costs will be met by the IUCr, while the local organizers cover the accommodation/subsistence expenses. Support from at least one IUCr Commission is required.

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

#### A1.4. Commissions of the IUCr

Each Commission Chair is required to provide a written triennial report to the General Assembly. These reports are included as Appendix A6. 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.

#### A1.5. Regional Associates, Scientific Associates, and other bodies

The reports of the Representatives on these bodies are given as Appendices A12 and A13.

#### A1.6. IUCr staff

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

#### A1.7. Acknowledgements

On behalf of the IUCr, the Executive Committee wishes to express its deep gratitude to the Indian National Science Academy and the Indian Crystallographic Association for the invitation to hold the Twenty-Fourth General Assembly and International Congress of Crystallography in Hyderabad.

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

### A2. Financial Report

Extracts from the full financial statements for the three years 2014, 2015 and 2016 are summarized in Tables 1–4. All amounts are expressed in Swiss Francs. The notations used in this report for the various currencies of the IUCr's activities are CHF = Swiss Franc, GBP = Pound Sterling, USD = US Dollar.

#### A2.1. General financial development

Table 1 shows a comparison of the fund accounts at the beginning and the end of the triennium. The total assets have decreased by CHF 1,550,038 from CHF 4,596,542 to CHF 3,046,504, or 33%, over the triennium. These figures include the fluctuations in exchange rates. If the exchange-rate fluctuations are disregarded, the total assets decreased by CHF 1,509,375 from CHF 4,685,759 to CHF 3,176,384, or 32%, over the triennium.

Table 2 shows the distribution of the assets. The great majority of the amounts under debtors and creditors have been settled since year-end.

The total holding of investments at 31 December 2016 is CHF 2,571,596 at market value, as shown in Table 2. 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. 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 account*

In order to present an overall picture of the state of the Union's affairs an income and expenditure account for the triennium is included as Table 3. This shows that the Union was operating with deficits in each year of the triennium. The losses are largely a result of additional expenditure connected with the International Year of Crystallography, *IUCrJ*, creation of the position of Business Development Manager and the loss of open-access income when *Acta E* lost its ISI impact factor. Steps have been taken to address this drop in income by a re-design of *Acta E*, launch of *IUCrData*, introduction of the IUCr Associates Programme, review of the production and financing of the *IUCr Newsletter*, reduction of and/or and strict adherence to other budgets, and eventually optimizing investments. The Union is predicted to return to operating with a profit in the coming triennium.

#### **A2.2. General Fund**

This Fund carries the income and expenditure related to the IUCr's administration and its regular scientific activities, other than publications. Table 4 shows a comparison of the budget and accounts for the triennium. The income has two main sources, the subscriptions from Adhering Bodies and the interest income from investments and bank accounts. The subscriptions from Adhering Bodies are based on the unit contribution, which was CHF 1,000 for 2014, 2015 and 2016. The income is 23% lower than the budgeted amount and the expenditure is 16% lower. It should be noted that the investments are held primarily for long-term gain. All investment income is assigned to the General Fund.

The administration expenses for the journals are calculated as 45% of the general administration costs of the IUCr, including the work of the Executive Secretary and his office and of the General Secretary and Treasurer. The Executive Committee met annually, while the Finance Committee held two meetings in each of 2014, 2015 and 2016. The cost of these meetings varies depending on the location and the circumstances. In Table 4 these costs are included in the expenses of administrative meetings, together with the costs of the IUCr representatives on other bodies. The expenses of scientific meetings in Table 4 include the travel grants and other expenses for the Montreal Congress in 2014, the cost of the 2016 meeting of the Programme Committee for the Hyderabad Congress, the expenses of the non-publishing Commissions, financial support to meetings and schools, and the IUCr/FIZ Agreement (which generated income in each year of the triennium), and sales from miscellaneous books. Proportions of the Research and Development, Promotion and Business Development costs are charged to the General Fund. The financial support for young scientists attending meetings and schools is charged to the Research and Education Fund.

In Table 4, the favourable deviation from budget of CHF 127,673 is mainly accounted for by lower administration expenses, which were 12.5% lower than predicted.

#### **A2.3. President's Fund**

This Fund is intended mainly for use in emergencies and under special or difficult circumstances, to help crystallographers from countries with currency problems to take part in the activities of the IUCr (especially in connection with the triennial Congresses).

#### **A2.4. Journals Fund**

The total number of pages printed for *Acta*, *JAC*, *JSR*, *IUCrJ* and *IUCrData* were 14,408, 13,867 and 12,471 in 2014, 2015 and 2016, respectively. The Finance Committee and the Executive Committee have monitored the financial development for all journals very closely. The **Crystallography Journals Online** service has been available throughout the triennium and is a

great success. All journals have been available online only from January 2014. For further details see the Triennial Report of the Commission on Journals (Appendix A6.1).

#### A2.5. International Tables Fund

The eight-volume *International Tables* series was completed in 2005 with the publication of Volume G *Definition and Exchange of Crystallographic Data*. The new Volume H *Powder Diffraction* will be published in 2017. The new Volume I *XAFS* is in preparation. **International Tables Online** was launched in 2007. For further details see the Triennial Report by the Chair of the Commission on International Tables (Appendix A6.2).

#### A2.6. Publications and Journals Development Fund

This Fund was established in 1984 and has been built up through transfers from other funds. During the triennium the major expenses have been related to the purchase of computer hardware and software, programming and development, promotion, Special Issue costs and projects related to the development of CIF-related products to facilitate deposition of data in crystallographic databases and submission to IUCr journals. It remains the policy of the Executive Committee to support and encourage the IUCr's highly qualified staff by supplying them with the best equipment. Also charged to this Fund are costs of inputting news items on the IUCr web site and archiving. As the programming and development activities underpin much of the Union's activity, in 1997 the Executive Committee decided that the associated costs should be assigned to the Journals Funds, the *International Tables* Fund and the General Fund. This principle has been extended to the promotion and business-development expenses.

#### A2.7. Research and Education Fund

The fund was also established in 1984 and, like the Publication and Journals Development Fund, has been built up through transfers from other funds. CHF 532,673 was given as young scientists' support during the triennium. Other expenditure involved the Visiting Professorship Programme (CHF 48,139), the inter-regional bursary scheme (CHF 10,249), the Crystallography in Africa initiative (CHF 78,639) and support for the International Year of Crystallography (CHF 348,880).

#### A2.8. Ewald Fund

This fund is used to finance the triennial Ewald Prize.

#### A2.9. Newsletter Fund

The fund was established in 1994 following the successful launch of the *IUCr Newsletter* in 1993. The *IUCr Newsletter* is currently distributed electronically free of charge to 587 libraries and more than 18,000 crystallographers and other interested individuals in 102 countries. The costs to the IUCr were CHF 136,839 for the triennium.

#### A2.10. General Assembly and Congress Fund

The fund was established in 2007 so that the costs associated with the General Assembly and Congress could be spread over the triennium.

#### A2.11. Outreach and Education Fund

This fund was established in 2016 so that initiatives begun during the International Year of Crystallography could be maintained.

TABLE 1. BALANCE SHEET, FUND ACCOUNTS. Swiss Francs

	<i>31 December 2013</i>	<i>Fluctuations in rates of exchange</i>	<i>31 December 2016</i>
General Fund	(2,787,889)	76,035	(3,727,383)
President's Fund	133,611	2,233	158,216
Journals Funds	5,251,599	111,390	5,238,446
International Tables Fund	(548,618)	(9,964)	(745,368)
Publications and Journals Development Fund	877,647	14,373	765,606
Research and Education Fund	822,231	17,022	577,773
Ewald Fund	522,023	(9,452)	539,280
Newsletter Fund	37,479	2,154	(97,252)
General Assembly and Congress Fund	288,459	5,464	262,043
Outreach and Education Fund	-		75,143
TOTAL ACCUMULATED BALANCE	4,596,542	209,255	3,046,504
Excluding exchange rates	4,685,759		3,176,384

TABLE 2. BALANCE SHEET, ASSETS. Swiss Francs

	<i>31 December 2013</i>	<i>31 December 2016</i>
FIXED ASSETS		
Tangible fixed assets	40,994	13,299
Investments at market value	2,626,051	2,571,596
	2,667,045	2,584,895
CURRENT ASSETS		
Stock	119,459	79,102
Cash at banks and in hand		
Current accounts	115,221	48,541
Deposit and savings accounts	1,542,174	767,701
Cash with Union officials	18,237	14,564
	1,675,632	830,806
Debtors, accrued income and payments in advance	428,093	245,521
Subscriptions due	18,686	57,862
Total current assets	2,241,870	1,213,291
Deduct Creditors and accrued charges	(312,373)	(751,682)
NET CURRENT ASSETS	1,929,497	461,609
TOTAL ASSETS	4,596,542	3,046,504

TABLE 3. INCOME AND EXPENDITURE. Swiss francs

	2014	2015	2016
<b>I. INCOME</b>			
Membership subscriptions	163,689	170,463	160,407
Sales			
Journals, back numbers and single issues	3,141,732	3,093,214	2,733,262
Books	106,883	102,717	114,144
	3,248,615	3,195,931	-
Investment income			
Income from investments	31,810	13,667	21,041
Bank interest	1,145	483	504
Profit/(loss) on sale of investments	64,190	(1,745)	(21,643)
	97,145	12,405	(98)
Other income			
Royalties and copyright fees	7,213	11,349	27,632
Advertising income	128,368	95,853	85,371
STAR/CIF income	-	-	36,535
Congress income	48,910	184,491	149,538
<b>TOTAL INCOME</b>	<b>3,693,940</b>	<b>3,486,001</b>	<b>3,157,253</b>
<b>II. EXPENDITURE</b>			
Journals			
Publication costs	418,442	381,466	371,493
Editorial expenses	201,127	191,906	203,699
Technical editing	1,382,539	1,354,281	1,134,961
Subscription administration	118,161	2,120,269	120,326
Books			
Publication costs	6,124	52,472	21,602
Editorial expenses	27,282	26,048	33,166
Technical editing	67,605	67,407	63,556
Newsletter			
Publication costs	17,176	2,343	25,258
Editorial expenses	99,762	94,867	94,867
International Year of Crystallography/Outreach	269,320	115,091	75,823
President's Fund, other grants and young scientist support	226,612	200,523	207,605
General Assembly and Congress costs	74,970	19,196	32,652
Committee meetings and expenses	147,834	60,877	76,486
Ewald Prize	38,894		
Publications and journals development			
General	422,124	483,196	367,199
Business development	112,001	153,734	110,959
Editor meetings	14,593	14,901	11,955
STAR/CIF	7,695	2,404	-
IUCrJ development	165,619	178,468	128,835
Promotion	184,223	906,255	1,000,625
Subscriptions paid	4,219	4,787	5,117
Visiting Professorship Programme	10,893	9,891	16,134
Administration expenses			
General Secretary and Treasurer, including honorarium	4,907	5,946	7,081
Audit and accountancy charges	45,487	46,440	37,538
Legal and professional fees	4,765	1,487	20,102
Travelling expenses	16,500	6,495	9,222
Bank charges	8,725	80,384	73,291
Executive Secretary's office			
Salaries and expenses	314,835	299,601	254,261
Travel expenses of IUCr representatives on other bodies	12,802	10,417	6,978
Commission (income)/expenses	-	(195)	-
Sponsorship of meetings	2,018	4,052	3,029
President's secretary	4,605	-	-
IUCr/FIZ Agreement	(18,171)	(13,797)	(14,930)
Bad debts	1,484	317,573	-
Depreciation	41,744	36,442	29,848
<b>TOTAL EXPENDITURE</b>	<b>4,456,916</b>	<b>4,109,241</b>	<b>3,574,511</b>
EXCESS (DEFICIT) OF INCOME OVER EXPENDITURE	(762,976)	(623,240)	(417,258)
REALISED FLUCTUATIONS IN RATES OF EXCHANGE ON TRADING ACTIVITIES	39,946	2,846	2,845
(DEFICIT)/SURPLUS OF INCOME OVER EXPENDITURE (AFTER REALISED EXCHANGE LOSSES)	(723,030)	(620,394)	(414,413)
MOVEMENT IN MARKET VALUE OF INVESTMENTS	95,044	(86,731)	6,435
UNREALISED FLUCTUATIONS IN RATES OF EXCHANGE			
TRADING ACTIVITIES	117,582	12,482	(66,670)
INVESTMENT ACTIVITIES	213,403	(17,692)	(66,055)
	330,985	(5,210)	(132,725)
TOTAL RECOGNISED (LOSSES)/GAINS RELATING TO THE YEAR	(297,001)	(712,335)	(540,703)
ACCUMULATED BALANCE AT 1 JANUARY	4,596,542	4,299,541	3,587,206
ACCUMULATED BALANCE AT 31 DECEMBER	4,299,541	3,587,206	3,046,503

TABLE 4. GENERAL FUND, COMPARISON OF BUDGET AND ACCOUNTS  
FOR THE YEARS 2014-2016 INCLUSIVE. Swiss Francs

	<i>Budget</i>		<i>Accounts</i>		<i>Difference</i>
<b>INCOME</b>					
Subscriptions from Adhering Bodies	474,000		491,713		17,713
Yield from investments and bank accounts (including profit/loss on disposal of investments)	300,000	774,000	109,453	601,166	(190,547) (172,834)
<b>EXPENDITURE</b>					
Administration (net)	1,555,000		1,362,157		(192,843)
Subscriptions to ICSU/ICSU bodies	36,000		14,123		(21,877)
Administrative meetings	305,000		313,858		8,858
Scientific meetings	54,000	1,950,000	(40,645) <sup>a</sup>	1,649,493	(94,645) (300,507)
FAVOURABLE VARIANT FROM BUDGET					127,673
ESTIMATED PROFIT OR DEFICIT		(1,176,000)			(1,176,000)
DEFICIT OF INCOME OVER EXPENDITURE				(1,048,327)	(1,048,327)

### A3. Ewald Prize

The establishment of the Ewald Prize, for outstanding contributions to the science of crystallography, was announced in February 1986. The name of the Prize was chosen with the kind consent of the late Paul Peter Ewald, to recognize Professor Ewald's significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography, especially 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 an award of USD 30,000 (if there is more than one awardee, USD 40,000 is shared). It is presented once every three years during the triennial International Congresses of Crystallography. The first Prize was presented during the Perth Congress, being awarded jointly to J.M. Cowley and A.F. Moodie. The second Prize was presented during the Bordeaux Congress to B.K. Vainshtein. The third Prize was presented during the Beijing Congress to N. Kato. The fourth Prize was presented during the Seattle Congress to M.G. Rossmann. The fifth Prize was presented during the Glasgow Congress to G.N. Ramachandran, the sixth Prize was presented during the Geneva Congress to M.M. Woolfson. The seventh Prize was presented during the Florence Congress to P. Coppens. The eighth Prize was presented during the Osaka Congress to D. Sayre. The ninth Prize was presented during the Madrid Congress to E. Dodson, C. Giacovazzo and G.M. Sheldrick. The tenth Prize was presented during the Montreal Congress to A. Janner and T.W.J.M. Janssen.

The eleventh Ewald Prize has been awarded to

#### **Professor Sir Tom Blundell**

for his work as one of the worldwide leaders in crystallographic innovation, especially at the interface with life sciences; starting with his work on determining the structure of insulin with Dorothy Hodgkin, he determined an exceptionally broad array of medically critical human protein structures, championing methods enabling drug design and discovery through structural optimization, crystallographic fragment screening, and computational modelling, and for being a leader in advanced crystallographic education internationally.

The presentation of the Ewald Prize was made during the Congress Opening Ceremony.

#### A4. International Year of Crystallography

In January 2014, the United Nations Educational, Scientific and Cultural Organization (UNESCO) and the International Union of Crystallography (IUCr) launched a number of activities to support the United Nations Resolution A/RES/66/284 of 3 July 2012 proclaiming the International Year of Crystallography.

The significance of the International Year was summarized in a booklet entitled *Crystallography Matters!*, distributed worldwide in 16 different languages. Over the course of the year, hundreds of activities, initiatives and publications brought the importance of crystallography to new audiences, actively trained new crystallographers, and raised the profile of a science that is central to so much of our understanding and interaction with the world around us.

The conference Crystallography for the Next Generation, held in Rabat, Morocco, in April 2015, under the High Patronage of His Majesty King Mohamed VI, reviewed with pride the accomplishments achieved during the International Year, with a forward-looking focus on how to sustain momentum and build on success. At a time when scientific endeavour is critical for societal benefit and the importance of crystallography is greater than ever, crystallography remains a science that still has lower visibility than it should.

An outcome of the conference was the IYCr2014 Legacy Resolution, which was signed by representatives from the IUCr, UNESCO, TWAS, ICSU-ROA, IUBMB, IUPAP, IMA and IUPAC who committed:

(1) to enhance the stature of crystallography

- ∞ by maintaining close liaison and representation between our individual organizations
- ∞ by collaborating on relevant programmes of science policy at regional, international and global scales
- ∞ by forging closer links between the IUCr and other International Scientific Unions
- ∞ by encouraging the recognition of crystallography as an essential component of physics, materials science, chemistry and structural biology, and of its inclusion in curricula for secondary and tertiary-level education
- ∞ by continuing to protect the integrity of science through publication of peer-reviewed journals and reference works of the highest quality;

(2) to build capacity in developing regions of the world

- ∞ by continuing implementation of the OpenLabs and related training initiatives
- ∞ by coordinating strategic projects based on available funds and resources, such as the IUCr Crystallography in Africa and the IUCr–ICSU Building Science Capacity in Africa via Crystallography programmes, and supporting similar initiatives in Latin America and South-East Asia
- ∞ by encouraging talented students to take advantage of opportunities such as the TWAS Fellowships for Research and Advanced Training
- ∞ by continuing to transfer expertise through Visiting Professorship programmes and regional schools or workshops
- ∞ by working to reduce barriers to the free movement of scientists;
- ∞

(3) to extend further the public understanding of science in general and crystallography in particular

- ∞ by maintaining and expanding educational and public awareness materials and making them freely available in many languages
- ∞ by direct engagement of practising crystallographers with active school outreach programmes such as UNESCO Associated Schools Network
- ∞ by on-going development of local crystal-growing activities for schoolchildren and the permanent establishment of a global coordination;

and called upon associates, scientific practitioners and educators worldwide to join these organizations in these efforts to sustain and build on the momentum of the International Year of Crystallography in the spirit that now *Crystallography Matters ... More!*

This resolution was subsequently signed by a further 275 individuals.

The IUCr has established an Outreach and Education Fund through which support for the IUCr OpenLabs and other individual projects (crystal-growing competitions, for example) may be supported.

## A5. IUCr Associates Programme

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

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

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

The IUCr is therefore officially launching its new 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. There will also be tools for professional networking such as access to the IUCr LinkedIn group, a jobs board and opportunities to participate in the IUCr Outreach and Education programme.

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).

## A6. Reports of the Commissions of the Union

### A6.1. Commission on Journals

*Acta Crystallographica Section A*

	2011	2012	2013	2014	2015	2016
No. of submissions	134	143	97	119	95	120
Rejection rate (%)	40	33	39	32	27	38
No. of published papers	68	83	71	72	70	74
research papers – foundations – advances	56	64	58	52 4	47 8	42 5
short communications	5	5	1	4	3	3
lead articles	0	0	0	0	0	3
feature articles	0	1	0	0	1 (advances)	1
editorial	0	0	2	1	2	1
commentaries				2	2	2

abstracts	2087	527	599	1832	789	647
other	7	13	10	9	7	17
No. of open-access papers	6	3	4	4	9	7
No. of pages	565	787	623	686	630	705
Average length (pages)	9	10.2	9.6	10.8	10.1	10.3
Average publication time (months)	4.7	5.1	5.3	5.7	4.8	5.6
Impact factor	2.07	2.24	2.07	2.33	2.33	
5 year impact factor	30.65	18.32	17.24	2.26	2.17	
Cited half life (years)	3.9	>10.0	>10.0	>10.0	>10.0	

Just before the start of the triennium, the subtitle of *Acta A* was changed from *Foundations of Crystallography* to *Foundations and Advances*, and a new *Advances* section of the journal was launched. As described in the November 2013 Editorial, *A New Vision for Acta Crystallographica Section A* [Acta Cryst. (2013), A69, 533–534], the aim of the *Advances* section is to offer rapid publication of high-impact papers. The first *Advances* article, *Magnetic Pair Distribution Function Analysis of Local Magnetic Correlations*, by B. Frandsen *et al.*, with an accompanying commentary article, *Reflections on the Magnetic Pair Distribution Function* by W. Ratcliff, went online at the very end of 2013 as part of the January 2014 issue. It was followed in July by *On the Temperature Dependence of H-U<sub>iso</sub> in the Riding Hydrogen Model* by J. Lübben *et al.*, and in November by two more: *Atomic Scale Study of Polar Lomer–Cottrell and Hirth Lock Dislocation Cores in CdTe* by T. Paulauskas *et al.*, which was highlighted in the scientific commentary *New Capabilities for ‘Colouring in’ the Chemistry of Crystal Defects Atom-by-Atom* by S. J. Haigh, and *Unconstrained and X-ray Constrained Extremely Localized Molecular Orbitals: Analysis of the Reconstructed Electron Density* by L. H. R. Dos Santos *et al.*

2014 also saw the publication of a Special Issue on mathematical crystallography, with Guest Editors Massimo Nespolo and Greg McColm. This featured eight articles gathered in part from the 2013 SIAM Conference on Mathematical Aspects of Materials Science: these were published as regular articles over the first three issues of the year and then gathered together into a virtual Special Issue in December. The publication of the virtual Special Issue generated significant interest on social media.

The first issue of 2015 started with an Editorial, *Celebrating the Past, Looking to the Future*. In this we reiterated our plans for *Acta A*, explaining the aims of the new *Advances* section and emphasizing the fact that we were adopting higher standards for acceptance of articles across the board. In particular, beyond just describing a development, it is our aim that each article should identify the rationale for making the development and how it would be used by the crystallographic community.

Eight *Advances* papers were published during 2015: *SHELXT – Integrated Space-Group and Crystal-Structure Determination* (G. M. Sheldrick); *Nuclear-Weighted X-ray Maximum Entropy Method – NXMEM* (Christensen *et al.*); *Diffuse Multiple Scattering* (Nisbet *et al.*); *Partial Order Among the 14 Bravais Types of Lattices: Basics and Applications* (H. Grimmer); *Identification of Inversion Domains in KTiOPO<sub>4</sub> via Resonant X-ray Diffraction* (Fabrizi *et al.*); *Interpretation of Angular Symmetries in Electron Nanodiffraction Patterns from Thin Amorphous Specimens* (Liu *et al.*); *Solution of the Phase Problem at Non-Atomic Resolution by the Phantom Derivative Method* (C. Giacovazzo); and *Complex Modelling: a Strategy and Software Program for Combining Multiple Information Sources to Solve Ill-Posed Structure and Nanostructure Inverse Problems* (Juhás *et al.*).

We also published a Feature Article on *MicroED Data Collection and Processing* (J. Hattne *et al.*), which was highlighted in the scientific commentary *Accessible Atomic Structures from Sub-Micron Protein Crystals* by J.A. Rodriguez. Howard Flack explained the utility of Grimmer's approach to order among the Bravais lattices in his Commentary *The Revival of the Bravais Lattice*.

2016 was also a good year with the *Advances* section featuring five standard research articles (*Bragg–von Laue Diffraction Generalized to Twisted X-rays* by D. Jüstel *et al.*; *On the Possibility of using X-ray Compton Scattering to Study Magnetoelectrical Properties of Crystals* by S. P. Collins *et al.*; *Dynamic Quantum Crystallography: Lattice-Dynamical Models Refined Against Diffraction Data. I. Theory* by A.A. Hoser and A.Ø. Madsen; *Coherent Diffraction Imaging:*

*Consistency of the Assembled Three-Dimensional Distribution* by M. Tegze and G. Bortel; and *Miniaturized Beamsplitters Realized by X-ray Waveguides* by S. Hoffmann-Urlaub and T. Salditt), three Lead Articles (*Computation in Electron Microscopy*, by E.J. Kirkland; *Topological Features in Crystal Structures: a Quotient Graph Assisted Analysis of Underlying Nets and Their Embeddings*, by J.-G. Eon; and *Observing Structural Reorientations at Solvent–Nanoparticle Interfaces by X-ray Diffraction – Putting Water in the Spotlight*, by M. Zobel) and a Feature Article (*Cryogenic Coherent X-ray Diffraction*

*Imaging of Biological Samples at SACLA: a Correlative Approach with Cryo-Electron and Light Microscopy*, by Y. Takayama and K. Yonekura). Two of these were highlighted in accompanying scientific commentaries (*Cryo-Coherent Diffractive Imaging of Biological Samples with X-ray Free-Electron Lasers*, by H. Jiang; and *Simple Graphs that Guide Combinatorial Materials Design*, by P.M. Duxbury).

In the November 2016 issue we also published a Special Issue of six articles and an editorial celebrating *100 Years of the Debye Scattering Equation*, based on talks given at the DSE2015 workshop held in Trentino, Italy, in 2015, with Guest Editors P. Scardi, R. Neder and A. Cervellino. This continued the theme of celebrating centennials (after Special Issues devoted to Laue and Bragg in 2012 and 2013, respectively) but with an emphasis on how the Debye scattering equation has recently enjoyed widespread use in research into the structure of nanomaterials.

The wide range of papers that we have published as *Advances* since the launch of this new section gives a good feel for the breadth of topics covered by the journal. It also seems that this initiative has led to our being able to attract and retain new authors.

We have continued to promote our top papers through social media. We are finding that scientific commentaries that help to explain and highlight the potential uses of techniques described in some of our more mathematical papers are particularly useful. Our news items and press releases were appreciated by authors and their institutions alike, and some were picked up by several other publications. The number of people following us on Twitter has also increased. Submissions to *Acta A* have remained fairly steady over the triennium. The editorial board have worked tirelessly with authors to ensure that all papers now explain the wider significance of the work, and to encourage authors who had previously been publishing frequent but rather incremental pieces of research to consider combining these into one longer article describing the whole body of work and its possible significance in more detail.

Vaclav Petricek retired from the Editorial Board during 2015, and John Miao stepped down as a Main Editor of *Acta A* at the end of 2016. I would like to thank him and the rest of the Editorial Board for all their hard work and support over the year.

S.J.L. Billinge, Editor

#### *Acta Crystallographica Section B*

	2011	2012	2013	2014	2015	2016
No. of submissions	121	112	167	126	157	171
Rejection rate (%)	40	34	36	28	32	31
No. of published papers	57	79	73	117	93	106
research papers	52	67	63	98	72	81
short communications	1	4	3	6	3	3
lead articles	0	0	3	1	0	0
feature articles	1	1	0	2	5	5
editorial	0	0	1	2	2	1
commentaries				3	5	6

other	3	7	3	5	6	10
No. of open-access papers	5	0	6	8	9	10
No. of pages	581	685	633	1036	813	933
Average length (pages)	10.7	9.6	9.3	9.7	9.6	10.3
Average publication time (months)	4.6	4.7	4.9	5.7	4.4	5.3
Impact factor	2.29	2.18	2.10	2.18	2.9	
5 year impact factor	2.00	1.89	1.83	2.21	2.50	
Cited half life (years)	>10.0	>10.0	>10.0	>10.0	>10.0	

During the 2014–2016 triennium *Acta B* continued to publish six issues per year, the numbers of articles (pages) published in 2014, 2015 and 2016 being 117 (1036), 93 (813) and 106 (933), respectively. These numbers are highly dependent on the number and size of Special Issues published in a particular year, but the average numbers for the previous triennium were 61 (633). Over the period 2011–2016 the rejection rate has been relatively stable within the range 28–40%. The average article length during the triennium (9.7, 9.6 and 10.3 pages, respectively) is in line with previous data. The average time between submission and publication (around 5 months) rises and falls in response to the number of Special Issues published. There have been slight increases in the number of open-access papers but the proportion is still only around 10%.

Having risen slowly to around 2.2 during the previous triennium, the journal's impact factor reached 2.9 in 2015, in part due to the effect of several highly cited Feature Articles. These articles moved out of the citation window in 2016, so a modest dip in the impact factor for that year might be anticipated before some very highly cited articles published in 2016 should significantly increase the impact factors for 2017 and 2018.

During the triennium *Acta B* underwent major changes in order to increase the quality and quantity of science it publishes, signalled by the change in subtitle to *Structural Science, Crystal Engineering and Materials*. The journal has developed a strong programme of Invited Articles and Special Issues in order to announce its renewed interests in these areas.

The following Special Issues have been published since August 2014: *Energy Materials* (Guest Editors: Simon Parsons, Richard Walton, Karena Chapman), *Crystal Structure Prediction* (Guest Editors: Graeme Day and Carl Henrik Görbitz). Forthcoming Special Issues for 2017 include: *Halogen Bonding* (Guest Editors: Pierangelo Metrangolo and Mate Erdelyi) and a Special Issue to mark the retirement of Professor Philip Coppens entitled *Charge Density and Photo-/Time-Resolved Crystallography: a Tribute to Professor Philip Coppens* (Guest Editors: Claude Lecomte, Jason Benedict and Yu-Sheng Chen). A Special Issue on *Mineralogy and Related Phases* (Guest Editors Sergey Krivovichev, Janusz Lipkowski and Stuart Mills) is scheduled to appear in early 2018. We wish to record our thanks to these Guest Editors for their exceptional efforts in bringing about the Special Issues. Special Issues add to the number of articles in the journal: they do not appear to reduce the number of other submissions.

Invited Articles are regularly sought from prominent scientists, including Keynote Lecturers at IUCr Congresses and Regional Associate Meetings. Analysis suggests that our programme of Invited Articles has had higher impact than our Special Issues: we intend to pursue both in the next triennium but will aim to publish only one or two Special Issues per year while vigorously pursuing a larger number of high-quality Invited Articles in the period 2017–2020. The journal is also experimenting with new categories of article such as the Opinion and Research Perspective articles.

Co-editors regularly report difficulties in identifying willing, qualified and competent reviewers. The Section Editors are available to advise as required. The contributions of reviewers are invaluable and we wish to express our deep thanks for their efforts in improving the quality of articles in *Acta B* and in identifying outstanding science. Among the many Chester staff who have contributed to *Acta B*, we particularly appreciate the many contributions of our Managing Editor Jill Bradshaw, from editing articles to coordinating the work of the Section Editors.

We note the retirement from the Editorial Board of *Acta B* of Andrew Bond during this triennium, whilst Dave Billing, Elena Boldyreva, Nadezhda Bolotina, T. N. Guru Row, Chris Howard, Alan Pinkerton and Richard Welberry are due to retire after

the 2017 Congress. We thank them warmly for all their contributions to the work of the journal and we are pleased to welcome several new Co-editors to the Board. Whilst preparing this report Professor Ashwini Nangia joined us as a Main Editor and we look forward to working together.

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

*Acta Crystallographica Section C*

	2011	2012	2013	2014	2015	2016
No. of submissions	479	504	609	479	407	335
Rejection rate (%)	50	49	41	50	52	47
No. of published papers	239	232	354	238	198	162
research papers	234	229	345	231	194	158
feature articles	0	0	0	0	2	0
editorial	2	2	4	2	1	1
commentaries				0	0	0
other	3	1	5	5	1	3
No. of open-access papers	0	0	0	1	3	0
No. of pages	993	984	1566	1180	1117	1011
Average length (pages)	4.2	4.2	4.5	5.0	5.7	6.4
Average publication time (months)	2	2	2.1	2.1	2.2	2.7
Impact factor	0.52	0.49	0.54	0.33	0.48	
5 year impact factor	0.44	0.4	0.44	0.32	0.41	
Cited half life (years)	>10.0	>10.0	>10.0	>10.0	>10.0	

In 2014, *Acta C* began a transformation to bring the journal to the forefront of publishing in the broad field of structural chemistry. This evolution is progressing slowly but steadily and it is pleasing to see that an increasing number of papers include a broader spectrum of science in the discussion in addition to the crystal structure determinations. To restate the journal's remit: *Section C is the journal of choice for the rapid publication of articles that highlight interesting research facilitated by the determination, calculation or analysis of structures ... Authors are encouraged to include mainstream science in their papers, thereby producing manuscripts that are substantial scientific well-rounded contributions that appeal to a broad community of readers and increase the profile of the authors.*

Efforts have been made to promote the journal directly to the chemistry community, such as having a presence at some chemistry-related conferences, including two American Chemical Society meetings. It is also felt that one of the main ways to improve the journal's visibility and sustainability is to have regular Special Issues and invited papers. To this end we were very excited that George Sheldrick and Ton Spek accepted our invitation to submit a paper each, which were published at the beginning of 2015, are key papers for the chemical crystallography community, and are very highly cited.

In late 2016, we published a Special Issue on Scorpionates: a Golden Anniversary, which is the second Special Issue on scorpionates within three years, emphasizing the interest in this class of structures. We are most grateful to Glenn Yap (University of Delaware, USA) and Kiyoshi Fujisawa (Ibaraki University, Japan) for putting together this excellent collection of 17 papers.

In March 2017, a Special Issue on NMR Crystallography was published. The Guest Editors, David Bryce (University of Ottawa, Canada) and Francis Taulelle (Université de Versailles Saint Quentin en Yvelines, France), worked hard on this substantial Special Issue containing one editorial, two Topical Reviews and 11 research papers. NMR crystallography has become a very important field where the marriage of traditional crystallography with the results from solid-state NMR can be very powerful for structure elucidation. The importance of the field was recognized at the Montreal Congress by the establishment of the Commission on NMR Crystallography and Related Methods.

Plans for the NMR Crystallography Special issue were initiated even before the Montreal Congress. That it took about three years to bring the issue to fruition demonstrates the long lead-time sometimes needed and other difficulties that can be encountered along the way with Special Issues. Among other things, one has to identify Guest Editors who are not only well connected and

respected within their field, but also have the time and energy needed to get the work of a Special Issue started and then keep up the momentum and interaction with authors to bring the project to completion within a reasonable time; potential Guest Editors often already have very full schedules. This means that it can be difficult to plan for regular Special Issues as they tend to appear just when they are ready.

Our efforts over the last three years, including the publication of Feature Articles, have already started to show a substantial increase in the journal's impact. This can be seen by looking at the Scopus CiteScore for the journal, which was 0.57 in 2015 and was showing an interim value of 3.17 for 2016 in March 2017. We hope that this will make the journal attractive to many new authors and readers. Of course, raising the impact is only a start and we will be striving to sustain this by continuing to publish Special Issues on eminent topics, solicit Feature Articles of significant and general interest to those in the field of structural chemistry, as well as attracting scientific comments of appeal to the readership. As a first step in this direction, Horst Puschmann (*Olex<sup>2</sup>*) and Mathias Meier (*CrysAlisPro*) were recently invited to submit Feature Articles highlighting some of the uses of their software to solve chemical crystallography problems. They accepted the invitations and we expect to publish their papers towards the end of 2017.

A Review Board with over 60 members was introduced during 2016. This should reduce the severe challenges some Co-editors had been facing with finding a quality reviewer who responds within a reasonable time, if at all. Members of the Review Board agree to review a certain number of papers each year.

The positive tone of the above developments is somewhat tempered by the continued decline in the total number of papers submitted to the journal. This number fell from 479 in 2014 to 335 in 2016. It is a stark contrast to the 751 submitted papers in 2008, especially as the rejection rate hovers near 50%. It is hoped that a positive effect will result when the journal's latest impact statistics are released in mid-2017 and that prospective authors will then feel more inclined to submit papers to *Acta C*. In addition, with the impact factor now likely to be on a par with that of *Acta B*, we can start to apply the keywords defining the focus areas of *Acta B* and *Acta C* more strictly when assessing the topics of submitted papers and distribute the papers accordingly between the journals with less likelihood of displeasing authors. Although the *Acta C* rejection rate is high, it should be noted that many of the rejected papers have been written in a style that is clearly more appropriate for *Acta E* and such papers are usually recommended for resubmission there.

After a nine-year term of office, Anthony Linden will retire as a Main Editor. The IUCr recently appointed two additional Main Editors: Larry Falvello (University of Zaragoza, Spain) and Jonathan White (University of Melbourne, Australia), who are teaming up with Paul Raithby to lead the journal into the coming triennium. We are extremely grateful to the team of Co-editors, both current and past, for their support, dedication and energy over the last triennium and even beyond. The journal would not exist without their valued contributions. The hard work, support, friendship and congeniality of the Chester Editorial Office staff cannot be praised highly enough, as it is they who ultimately get the accepted papers through production into the final product that we all read.

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

*Acta Crystallographica Section D*

	2011	2012	2013	2014	2015	2016
No. of submissions	239	340	433	429	272	158
Rejection rate (%)	26	29	27	32	27	24
No. of published papers	131	193	274	297	239	132
research papers	119	173	250	280	230	123
short communications*	5	8	9	3	0	0
feature articles	0	0	1	2	1	0
editorial	0	2	2	0	1	1
commentaries				1	1	2
other	7	10	12	11	6	6
No. of open-access papers	27	39	78	101	84	59
No. of pages	1077	1700	2584	3329	2542	1309
Average length (pages)	8.8	9.4	10.1	10.9	10.8	10.4
Average publication time (months)	4.0	5.1	5.5	5.5	5.2	5.6
Impact factor	12.62	14.10	7.23	2.68	2.51	
5 year impact factor	7.04	7.54	9.41	9.59	8.75	
Cited half life (years)	6.9	6.6	5.4	5.0	5.8	

\* The Short Communications category has been removed from 2015.

*Acta D* is experiencing challenging times. The impact factor has remained static over the period 2014–2015 (2.5–2.7) but is down from values of 7–14 in the three years before that. We note that this metric was artificially high owing to a few exceptionally highly cited methods papers, and that the historic value has been ~2–3. However, we are in different times now. Whereas in the past, authors submitted papers to *Acta D* because they fit the scope of the journal (biological crystallography) we are now competing with many more journals for the same papers – and many have a higher impact factor. The impact factor is now followed much more closely by potential authors, a substantial number of whom have to satisfy institutional requirements based on threshold values of impact factor. Targeting of journals by impact factor is borne out by the statistics table that shows that the number of submissions to *Acta D* appears to be correlated with impact factor, though with a two-year delay. We note that the impact factor is a flawed metric and does not measure the quality of individual papers in a journal. On the other hand we also recognize that a universal change to the impact factor metric or how it is perceived is out of our control. In addition, we are cognisant of the fact that there is significant pressure on young researchers and their careers to publish in journals with a high impact factor. That means that without increasing the impact factor of the journal it will be increasingly difficult to attract papers to *Acta D*.

Notwithstanding, we have been working to increase the impact factor of the journal by expanding the scope – with a concomitant change in name in 2016 (to *Acta D Structural Biology* from *Acta D Biological Crystallography*). In terms of the expanded scope, in 2015 we published a CCP4 proceedings issue on complementary methods that included papers on SAXS, sometimes in combination with fibre diffraction or DEER spectroscopy, and a paper describing the structural results of cryo-electron sub-tomogram averaging. We wrote an editorial that highlighted the new scope (published in the January 2016 issue), developed a workflow summary for Co-editors, and have been working closely with *Acta F* Section Editors to streamline the protocol and processes for transferring between the journals.

During the period 2014–2016, we have published four invited scientific commentaries and three invited Feature Articles. We are continuing to commission new articles from all areas of structural biology. In 2016, we published papers that included a broad range of structural methods including neutron crystallography, SAXS, EM and reflectometry.

We have also invited authors to write articles from Biology and Synchrotron Radiation 2016, ISDSB 2016, the 50th Erice International School of Crystallography, CCP-EM spring symposium, and the IUCr Congress. We will report on these in next year's report.

We now take the opportunity to remind the IUCr community that the IUCr journals are there to support them, but in the same way the journals need the community's support to continue.

A popular feature of *Acta D* has been the Special Issues. In October 2014 the topic was Diffraction Data Deposition from the IUCr working group of the same name, and began with an overview of the process from Tom Terwilliger. In 2015 the theme was Crystallography and Complementary Methods, from the proceedings of the CCP4 weekend. The conference Special Issue was published in January 2015, guest edited by Ivo Tews and Jon Cooper. Most recently, the 2016 CCP4 Study Weekend Special Issue, guest edited by Charles Ballard, Airlie McCoy and Thomas Schneider, was on the topic of Advances in Experimental Phasing and was published in the March 2016 issue.

The rejection rate of papers has stabilized to about a quarter of submitted manuscripts, which we consider to be a reasonable cut-off. We have removed the Short Communications category – and this will not be reported in future statistics tables.

Pleasingly, the proportion of open-access papers (an author-selected option requiring an additional payment) has increased considerably over the past few years. The percentages open access in 2010–2012 were relatively static in 2011/2012 at ~20% of accepted papers; this rose to 34% in 2014 and 35% in 2015 and a record high of 45% in 2016. Open access in *Acta D* is competitively priced compared with other journals that publish structural biology papers. This pricing structure provides an opportunity for encouraging new submissions and we propose that IUCr journals should actively promote that aspect.

The average publication time for *Acta D* remains steady at ~5 months, and this is in large part due to factors outside of our control (time required for authors to revise, time required for reviewers to provide their comments).

While the excellent panel of *Acta D* Co-editors represents the span of expertise and geography in our community, we are keen to see that the historic gender imbalance of editors in our sub-discipline is addressed. In our view, it is an urgent priority to re-evaluate the policies and procedures underlying Co-editor appointments, to address this imbalance. This will be critical to the future of the field and this journal. We need to ensure that the next generation is fully engaged in the discipline for healthy growth of the Union.

The electronic system of submissions continues to work very well for authors as well as the editors and reviewers. The quality of the journal is very high owing to the expert work of Louise Jones and Simon Glynn at the Chester Office. We thank them, Executive Managing Editor Peter Strickland, and Samar Hasnain, Editor-in-Chief, for their valuable help.

*J.L. Martin, R.J. Read and S. Wakatsuki, Editors*

*Acta Crystallographica Section E*

	2011	2012	2013	2014	2015	2016*
No. of submissions	5471	4605	2123	1478	1273	542
Rejection rate (%)	19	17	15	13	15	17
No. of published papers	4444	4047	1964	1336	1168	450
structure/data reports	4434	4039	1961	1165	768	0
research communications				164	395	441
editorial	0	0	0	3	0	1
other	10	8	3	4	5	8
No. of open-access papers	4444	4047	1964	1336	1168	450
No. of pages	5523	5171	2637	2351	2931	1874
Average length (pages)	1.2	1.3	1.3	1.8	2.5	4.2
Average publication time (months)	0.7	0.7	0.8	0.8	0.8	0.9
Impact factor	0.35					
5 year impact factor	0.28					
Cited half life (years)	3.3					

\*For 2016, the total of *IUCrData* and *Acta Cryst. E* papers are around 90% of 2015.

The years 2014–2016 have seen a number of developments for the journal, especially in 2016. Short Data Reports are now published in *IUCrData* while full papers are accepted for *Acta E, Research Communications*. The aim of this reorganization is to regain coverage of *Acta E* in the *Science Citation Index Expanded*, as soon as possible.

Because of the reorganization, the number of papers submitted to *Acta E* was down from 1,478 in 2014 to 542 in 2016. With 585 submissions to *IUCrData* in 2016, the total number of submissions is 1,127, compared to 1,273 in 2015, a decrease of *ca* 11%.

The distribution of papers by country remained approximately constant for 2014 to 2016, with the top 5 countries in 2016 being the USA, India, Germany, People's Republic of China and Republic of Korea. Authors from more than 70 countries continue to publish with *Acta E*.

The pre-review system, whereby the Section Editors preview the submissions to consider the quality of the paper and make sure that it is in the appropriate format, is working well. The Section Editors can decide if a submission should be published as a Research Communication in *Acta E* or if it should be transferred, subject to the agreement of the authors, to *IUCrData*. The introduction of a new version of *publCIF* has made it easy for authors to prepare both types of publication and we must put more emphasis on the use of this software and its functionality to generate the correct format for the submission.

The new web site for the journal is an added plus, and makes attractive reading.

#### *Significant developments in 2014*

2014 was another challenging year for *Acta E*, with a fall in submissions from 2,123 in 2013 to 1,478 in 2014. The relaunch of *Acta E* in June 2014 heralded its transformation from *Structure Reports Online* to *Crystallographic Communications* and saw

the publication of the first papers in the new Research Communication format designed to bring out the science behind the structure determination. We were delighted to see that an increasing number of authors are choosing to publish their work as a Research Communication, with the numbers of these articles increasing every month. The November issue included the one hundredth paper to be published in this format.

Overall, the proportion of organic (73%), metal-organic (22%) and inorganic (4%) papers was approximately the same as in 2013. However, the proportions were different for the Research Communications with 52% organic, 39% metal-organic and 9% inorganic papers.

In 2014 Luc Van Meervelt joined the Section Editor team, and an Advisory Board was established – we appreciate and thank the various members for their confidence and support.

#### *Significant developments in 2015*

2015 saw the completion of the transformation of *Acta E* from *Structure Reports Online* to *Crystallographic Communications*. The subtitle was changed in January and the final Data Reports were published in the December issue. The average number of Research Communications published each month rose by 20% compared to 2014 with a total of 395 published in 2015. The average length of a Research Communication also increased (from 3.7 pages in 2014 to 3.9 pages in 2015). We were pleased to see that papers reporting two or more structures are a now regular feature and that more authors are choosing to discuss complementary techniques, and take the opportunity to include extra tables and figures in the published paper to illustrate their results and enhance the discussion of the underlying science. We also noticed that the Research Communications format is attracting new authors to the journal and that the range of structures is far broader. The change in subject matter is reflected by the far higher proportion of metal-organic (39%) and inorganic (10%) papers compared to Data Reports where the proportion of organic (80%), metal-organic (19%) and inorganic (1%) papers is much the same as in recent years.

Although there was a further fall in submissions from 1,478 in 2014 to 1,273 in 2015, for the first time since 2011 the number of pages published increased compared to the previous year. The total of 2,931 was up 25% on 2014 (2,351 pages).

#### *Significant developments in 2016*

From January 2016 the journal only published Research Communications, and Data Reports are now published in *IUCrData*. Because of this reorganization, the number of papers submitted to *E* was down from 1,273 in 2015 to 542 in 2016. The quality of papers has increased with authors often reporting two or more structures and choosing to discuss complementary techniques, and include extra tables and figures to illustrate their results and enhance the discussion of the underlying science. The proportion of papers from India in Section E decreased (down 10%) while the proportion of papers from the USA increased. The top three countries for Section E were the USA (15%), India (9%) and Germany (9%).

#### *IUCrData – 2016*

585 data articles were submitted to *IUCrData* in its first year of publication. A total of 512 data articles were accepted and published in 2016 in 1,396 pages. The highest proportion of data articles came from India (26%) followed by Morocco (12%), the USA (12%), People's Republic of China (8%) and Germany (7%). The average length was 2.7 pages and the average publication time was 0.8 months. The rejection and withdrawal rate was 12%.

One of the stated aims of the relaunch of *Acta E* has been to regain indexing in the *Science Citation Index*. We are therefore delighted that the journal was included in the new *Emerging Sources Citation Index (ESCI)* when it was launched in November 2015. This means that articles published in *Acta E* can now be found in searches of the *Science Citation Index*. Importantly, it also means that the journal is under consideration for inclusion in the *Science Citation Index Expanded*. We hope that the final phase of the transformation of *Acta E* outlined above will herald the early re-indexing of the journal.

In 2016, the Advisory Committee was asked for a review of the performance of *Acta E*. Several recommendations made in that report are already being implemented and as always there is scope for improvement in view of obtaining inclusion in the *Science Citation Index Expanded*.

We are extremely grateful to our Co-editors for the excellent work they have done and cannot thank them enough; without their commitment this journal would not exist. We have been particularly fortunate in the past three years to recruit a number of new Co-editors to join the journal's hard working team that now numbers 58, including the four joint Section Editors. We also gratefully acknowledge the work of several Co-editors who have retired over the past three years. Thanks also to a number of Main Editors and Co-editors who, having achieved nine years of tireless service to the journal, will also be leaving the team after the Hyderabad Congress. As always, we are extremely grateful for the excellent support that we receive from the staff in Chester, in particular Gillian Holmes, Sean Conway and Mike Hoyland, for their constant help and support, and to Peter Strickland for his sound advice and expert guidance.

*W.T.A. Harrison, H. Stoeckli-Evans, E.R.T. Tiekkink, L. Van Meervelt and M. Weil, Editors*

*Acta Crystallographica Section F*

	2011	2012	2013	2014	2015	2016
No. of submissions	401	375	380	411	328	189
Rejection rate (%)	8	9	8	16	34	34
No. of published papers	385	362	335	344	251	136
research papers	365	351	321	339	247	130
editorial	3	3	5	2	2	0
commentaries				0	0	0
other	17	8	9	3	2	6
No. of open-access papers	42	15	22	36	41	27
No. of pages	1674	1576	1442	1713	1540	911
Average length (pages)	4.4	4.4	4.4	5.0	6.2	6.9
Average publication time (months)	3.9	3.2	2.8	2.9	3.2	2.7
Impact factor	0.51	0.55	0.57	0.52	0.65	
5 year impact factor	0.46	0.49	0.50	0.45	0.50	
Cited half life (years)	3.2	3.5	3.7	4.0	4.2	

*Acta F* was launched as the IUCr's first online-only biological journal in 2005 with the title *Crystallization and Structural Biology Communications*. Close to the end of its third triennium, at the beginning of 2013, the title of the journal was changed to simply *Structural Biology Communications* in order to reflect the changes that have happened in the structural biology scientific landscape. Now, in its fourth triennium, the journal has solidified its position as the home for the rapid publication of all structural biology communications. In the years 2014–2016 the journal published 731 papers (4,361 pages). This represents a decrease of about 30% in the number of papers and of about 10% in the number of pages compared to the third triennium. The main reason for this decrease is undoubtedly the demand for more information in manuscripts focused on crystallization and initial characterization of the crystals. The average time from submission to publication, including peer review, decreased to a record low of 2.7 months in 2016, although the average number of pages per paper increased to 6.9. This shows that the increasing length of the papers does not adversely affect publication time. However, it does put an increasing burden on referees, Co-editors and the editorial staff in Chester.

An important aspect in the last triennium was the consolidation of *Acta F*'s publication tool *publBio*. *publBio* has been developed to streamline short manuscripts describing the crystallization and/or the structure determination of a macromolecule.

It is available to authors as an online tool as well as in the form of publication templates. Although, the structural biology community has been slower than expected in adapting this new tool, about 20% of all papers appear to be assembled and submitted nowadays using *publBio*. It will be an important responsibility of the Section Editors in the next triennium to make *publBio* even more popular in the structural biology community and to expand its use among *Acta F* authors. With their more or less standardized content, we expect that these *publBio*-generated papers will prove to be even more useful to our readers and to the scientific community as a whole.

Another very positive development that we set out to achieve in the last triennium is the increase in papers describing a structure determination. While in 2014, only about 20% of all papers in *Acta F* described a structure, this number rose to 42% in 2015 and 69% in 2016. This is clearly the result of the new requirements for crystallization papers as laid down in the Notes for Authors.

A very successful endeavour of the journal in the last triennium was the publication of the IYCr series of papers dealing with various aspects of macromolecular crystallization. Twenty fine papers commissioned by our former Section Editor colleague Howard Einspahr appeared in the journal between 2014 and 2016. These papers are among the most downloaded ones of the journal and we anticipate that they will be highly cited. Plans to republish them as a book in time for the Hyderabad Congress are under way.

Although we have not been as successful as we would have liked to have been in commissioning Special Issues, we can report on one spectacular success, which was the May 2015 issue on molecular parasitology comprising fifteen original papers and two review articles.

Most importantly, though, the journal has become and remains a high-quality structural biology journal. Its current impact factor (for 2015) is 0.65. Initial estimates for the 2016 IF suggest that it will be higher than that for 2015. Our ambition is still to increase our visibility and raise the journal impact factor to 1.0 or above. We do feel that by mandating more information content in the papers published, we have taken a good step towards that goal. However, it will take another two or three years to see the full impact of this.

The referee panel, which was created in the second triennium, continues to function well. This group of about 30 experienced scientists, who have agreed to referee 12 papers a year, to reply to requests promptly, and to return reports within two weeks, can potentially provide half the number of referee reports needed in any publication year. Unfortunately, we have not been able to recruit as many new Co-editors from the panel or from outside as we would have liked in order to replace the retiring members and in order to fill the geographic gaps on the editorial board. With respect to the Section Editor team, we managed to recruit Zbigniew Dauter in 2016 after the term of our former colleague Howard Einspahr, who was one of *Acta F*'s founding Editors, ended in 2014. Now, with the conclusion of the Hyderabad Congress in August 2017, we will face the situation that all three current Section Editors will resign from their position. This will mark a significant gap in *F*'s history, but it will also give the new editorial team a chance to start afresh and with new vigour and ideas. Finally, a mention of the staff at Chester. Their input, advice and all the hard work that the Chester team, in particular Louise Jones, put into the journal is hugely important and highly valued and will be important in helping the new team. All three retiring Section Editors wish this team the luck and the stamina they will need to develop *Acta F* into an even more important and prominent structural biology publication.

Z. Dauter, W.N. Hunter and M.S. Weiss, Editors

*IUCrJ*

	2013	2014	2015	2016
No. of submissions	28	100	82	74
Rejection rate (%)	0	28	25	24
No. of published papers		70	81	57
research papers		34	38	37
feature articles		17	16	1
topical reviews		0	5	1
short communications		0	0	0
editorial		6	6	6
commentaries		7	12	8
other		6	4	4
No. of open-access papers		70	81	57
No. of pages		613	690	467
Average length (pages)		10.7	10.9	10.5
Average publication time (months)		3.7	4.6	4.5
Impact factor			5.3	
5 year impact factor			5.3	
Cited half life (years)			1.3	

To coincide with the International Year of Crystallography (IYCr2014), IUCr Journals launched the comprehensive open-access journal *IUCrJ* in January 2014. The journal has had a successful triennium, and has started to establish itself within the wider scientific communities that use results obtained from diffraction methods. All the indications are good in terms of the journal making a strong impact in attracting high-quality science papers of wide scientific significance from these communities. Impressions from authors, readers, referees and commentators are very positive with a number of papers receiving high downloads in line with high-impact publications.

Five Main Editors were appointed for the launch of *IUCrJ* (Ted Baker, Richard Catlow, Gautam Desiraju, Sine Larsen and John Spence). The journal also appointed 20 Co-editors and an Advisory Board (T.L. Blundell, P.M. Colman, J.B. Hastings, W.A. Hendrickson, B. Kobilka, Y. Ohashi, J.R. Schneider, W.G. Stirling and M.J. Zaworotko). In addition to providing high-impact high-profile publication, *IUCrJ* also aims to provide fast publication for authors. Submissions undergo preliminary screening by a panel consisting of the five Main Editors and the Editor-in-Chief (Samar Hasnain), and this has helped to provide a rapid and efficient review process. Preliminary screening is generally complete within 72 hours, and any articles that do not meet the journal's requirement for broad scientific significance are usually transferred, with the agreement of the authors, to one of our other journals. Such transfers are seamless and do not require any further work by the authors.

The 18 issues of *IUCrJ* published in the triennium have featured papers from a wide variety of areas including biology, chemistry, crystal engineering, materials, physics and FELs. The number of articles submitted to the journal in its first year

was 128; this was well ahead of our target of 100 articles. Overall 208 papers were published in the triennium. A number of papers have been highlighted in each issue *via* an in-depth commentary in a manner similar to other comprehensive journals such as *Nature* and *PNAS*.

In 2015, the journal was included in the *Science Citation Index* and in 2016 received its first impact factor of 5.3. This is very encouraging for such a newly launched journal, with *IUCrJ* currently ranked first out of 25 journals listed in the *Science Citation Index* Crystallography category.

The Biology and Medicine section of the journal has published 71 papers so far. These have given us glimpses into an exciting future, in which complementary approaches will substantially widen the reach of structural biology. Primary among these are the new advances in cryo-electron microscopy (cryoEM) and the growing applications of free electron lasers (FELs). Both approaches have a natural home in *IUCrJ*.

In the Chemistry and Crystal Engineering section a large number of submissions have been received; we have published 72 papers in this section since the inception of the journal. The crystal engineering papers are of a high quality and the community feels the journal is doing well relative to competitors. We expect more papers of general chemical interest to be submitted as researchers become familiar with the broader scope of the journal.

The 37 papers published so far in the Materials and Computation section of *IUCrJ* illustrate well the challenges posed by structural problems in the science of materials and the key role that computation can play in this and related fields in structural science. They demonstrate the continuing developments in techniques and instrumentation and the increasingly complex structural problems that these developments now make accessible.

The other sections of the journal, covering Neutron and Synchrotron Science and Technology, and Physics and Free Electron Laser Science and Technology, have published 25 and 36 papers, respectively, and have illustrated the rapid advances that are being made in these fields.

During the triennium, Sine Larsen retired as Main Editor and was replaced by Dmitri Argyriou, former Science Director of the European Spallation Source. In addition, one Co-editor (D. Bushnell) and three members of the Advisory Board (Y. Ohashi, J.R. Schneider and W.G. Stirling) stepped down. The Board and the Union express their gratitude to all these Editorial Board members for playing an active role in helping establish the journal. In 2016, new Co-editor and Advisory Board appointments were made to cover cryoEM (R. Henderson, W. Kühlbrandt and S. Subramaniam), chemistry and crystal engineering (P. Lightfoot and L.R. MacGillivray) and FELs (E.E. Lattman).

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

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

#### *Journal of Applied Crystallography*

	2011	2012	2013	2014	2015	2016
No. of submissions	266	321	432	410	360	380
Rejection rate (%)	34	30	36	38	29	30
No. of published papers	180	180	255	264	249	271
research papers	131	127	193	210	183	198
short communications	8	6	11	9	11	9
feature articles	0	0	0	1	1	0
computer programs	24	26	22	23	25	38

editorial	0	0	2	1	3	1
commentaries				3	2	0
other	17	21	27	17	24	25
No. of open-access papers	6	7	42	20	55	60
No. of pages	1306	1338	1913	2115	2044	2282
Average length (pages)	8.1	8.4	8.3	8.8	9.2	9.3
Average publication time (months)	5.1	5.4	5.7	5.7	5.5	5.4
Impact factor	5.15	3.34	3.95	3.98	2.57	
5 year impact factor	5.66	4.48	4.79	4.90	5.11	
Cited half life (years)	>10.0	>10.0	>10.0	>10.0	>10.0	

Over the past three years, *Journal of Applied Crystallography* has seen the number of submissions stabilize at just under 400 per year, of which about 250 are accepted for publication, accounting for just over 2,000 published pages. As in previous triennial periods, the impact factor has shown some fluctuation. However, the 5-year impact factor remains very solid and the citation half-life continues to exceed 10 years. The number of computer program submissions, which generally attract above average citations, remains at a healthy level. Furthermore, the fraction of published papers that are open access has doubled over the last 3 years, and now stands at more than 20 %.

Several virtual Special Issues have been published since 2014. The first, featuring some highlights of the 12th Biennial Conference on X-ray Diffraction and Imaging (XTOP 2014) held in Villard-de-Lans and Grenoble, France, in September 2014, was published in June 2015. Guest Editors were Vincent Favre-Nicolin and András Borbély. A Special Issue not associated with a conference: CCP-FEL: a Collection of Computer Programs for FEL Research, was published in August 2016 with Guest Editors: Filipe Maia, Thomas White, Duane Loh and Janos Hajdu. Finally, a Special Issue: Small-Angle Scattering, associated with the 16th International Conference on Small-Angle Scattering (SAS 2015) held in Berlin, Germany, in September 2015, was published in December 2016. Guest Editors were Michael Gradzielski and Andrew Allen. Work is currently under way on an issue associated with the XTOP 2016 conference held last September in Brno, Czech Republic (Guest Editors Václav Holý and Virginie Chamard). Further new Special Issues are planned, with a current call for papers for a Special Issue on Advanced Neutron Scattering Instrumentation with Dimitri Argyriou and Andrew Allen as Guest Editors.

Since 2014, we have bidden farewell to three long-serving Co-editors: John Helliwell and Walter Reimers, and to Katherine Kantardjieff, who also served as our Teaching and Education Editor. One of our existing Co-editors, Juan Garcia-Ruiz, kindly agreed to succeed Katherine as Teaching and Education Editor. Meanwhile, during this triennium, we have welcomed several new Co-editors to help us more fully address the scope and reach of the journal: Anton Barty, Sébastien Boutet, Karena Chapman, Elliot Gilbert, Flora Meilleur, Arwen Pearson and Dmitri Svergun. We would like to thank our Co-editors, whether retired or current, who have served the journal during this triennium for their hard work and dedication.

*A.J. Allen, J. Hajdu and A.R. Kaysser-Pyzalla, Editors*

#### *Journal of Synchrotron Radiation*

	2011	2012	2013	2014	2015	2016
No. of submissions	191	228	245	262	258	262
Rejection rate (%)	28	22	26	22	19	28
No. of published papers	146	154	155	187	210	198
research papers	123	124	130	147	164	157

short communications	8	6	8	9	9	10
feature articles	0	0	0	1	2	1
lead articles	0	0	0	1	2	1
beamlines	1	9	4	12	15	16
editorial	2	1	1	0	2	1
commentaries				0	0	1
other	12	14	12	17	18	11
No. of open-access papers	64	29	71	52	84	31
No. of pages	948	1066	1012	1385	1560	1563
Average length (pages)	7	7.3	7.0	8.1	8.1	8.3
Average publication time (months)	5.4	4.9	4.7	5.4	5.1	5.0
Impact factor	2.73	2.19	3.02	2.79	1.88	
5 year impact factor	2.57	2.23	2.73	2.67	2.32	
Cited half life (years)	6.6	7.5	8.1	8.9	8.3	

In this triennium, the *Journal of Synchrotron Radiation* welcomed Yoshiyuki Amemiya and Mikael Eriksson as Main Editors. As a Professor of Materials Science at the University of Tokyo and a renowned expert in the use of synchrotron diffraction techniques, Professor Amemiya, in collaboration with his fellow Co-editors in Japan, helps the rapidly growing community of synchrotron radiation and XFEL users in Asia find their way to the journal as authors. Given the rapidly rising availability of facilities in Asia, it is important to have strong representation from this continent on the Editorial Board. Mikael Eriksson is an accelerator physics expert from MAX IV in Sweden and was one of the Guest Editors of the Diffraction-Limited Storage Rings Special Issue published in September 2014. With many synchrotron radiation sources undergoing upgrade we hope that Mikael will attract advances in this field. During this triennium, the following Co-editors were appointed to the journal: Makina Yabashi (XFELs and instrumentation) and Masaki Yamamoto (structural biology), both from RIKEN SPring-8 Center, Japan. In 2017, Gene Ice will complete his Main Editor tenure and J. Friso van der Veen will resign as Main Editor. Currently there are vacancies for Main Editor positions notably in the area of soft X-ray applications and imaging.

The past years have seen a continuously rising number of submissions, as in the previous triennial period. The journal's impact factor dropped in 2014 and 2015 and appears to have recovered in 2016. Although it is difficult directly to relate the fluctuating impact factor to our editorial actions, the published Special Issues with invited high-quality papers on XFELs and Diffraction-Limited Storage Rings have certainly helped to curb the trend of declining impact, as have the two Special Issues on Radiation Damage in 2015 and 2017. Therefore, our policy of publishing Special Issues on hot topics is to be continued. In 2018 a Special Issue will appear on the latest developments in the science of extremely bright synchrotron and XFEL sources. In addition, we consider publishing news and views summaries and editorial overviews, similar to what is being done in *IUCrJ*. Finally, we believe that a prescreening of submitted papers by the Editors will benefit the overall science quality of the journal and its impact. Prescreening tools should be available on the Main Editors's web portal as of 2018.

Y. Amemiya, M. Eriksson, G.E. Ice, I. Schlichting and J.F. van der Veen, Editors

## A6.2. Commission on International Tables

*International Tables for Crystallography* is a book series published by the IUCr in conjunction with Wiley. Eight volumes designated A (and A1) through G are currently in print, a ninth (H, on powder diffraction) is expected to appear during 2017, and a tenth (I, on X-ray absorption spectroscopy and related techniques) is being written. Printed volumes can be purchased individually; online access is by subscription to the entire series. A new, considerably revised edition of the low-cost, printed *Brief Teaching Edition* of Volume A (*Space-Group Symmetry*) should appear in late 2017 or early 2018.

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

Additional information of a general type is included in Volumes B (*Reciprocal Space*) and C, which can be traced back to Volume II of the original series (1937) and Volumes II – IV of the series with red covers (1959–1974). The other volumes of the series can be described as comprehensive handbooks that cover more specific areas. These volumes are F (*Crystallography of Biological Macromolecules*), G (*Definition and Exchange of Crystallographic Data*), the nearly finished H (*Powder Diffraction*), and I (*X-ray Absorption Spectroscopy and Related Techniques*), which is being written.

In common with print sales for many other major reference works, sales of the print editions of the volumes have continued to decline. However, sales of subscriptions to *International Tables Online* have increased. The issue of whether to continue printing all the volumes will need to be addressed quite soon: it might be possible to continue to make some volumes available by ‘print on demand’. Several volumes in the series now contain or plan to include content that will only be available in the online version.

Developments in the triennium 2014–16 include:

- (1) Completion of the sixth edition of Volume A. It is a great pleasure to thank Mois Aroyo for bringing this major project to fruition. Details of how this new edition differs from the fifth can be found at <http://it.iucr.org/Ac/newedition>.
- (2) Very considerable development of the *Symmetry Database* (also edited by Mois Aroyo). This electronic resource simplifies discussion of non-standard space-group settings, which are often appropriate when phase sequences are being considered, and facilitate identification of group/subgroup/supergroup relationships. The Editor of Volume A1 (Ulrich Müller) is also involved in the development of this database.
- (3) Revision of the *Brief Teaching Edition* of Volume A. With the completion of the new Volume A, attention can be focused on the associated teaching edition, which should become available within the next 12 months. Part of the text will be a shorter and less complex version of Part 1 of Volume A, and will be supplemented by a number of current and accessible references. New text introducing less familiar topics, like the subperiodic and magnetic groups, will be added.
- (4) Work on revised editions of Volumes B and C. These two volumes are the successors of Volume II of the original series (1937) and Volumes II – IV of the ‘red’ series (1959–1974). Both (but especially C) are in need of reorganization and updating. Plans for both volumes have been drawn up, authors have agreed to write sections, and some new sections have been received and reviewed. The material on incommensurate structures and quasicrystals, which is currently split between B and C, will be consolidated into B and expanded.
- (5) Publication of the second edition of Volume D. This went online at the end of 2013 and appeared in print during 2014.
- (6) Near completion of a new Volume H (*Powder Diffraction*) under the direction of Chris Gilmore, Henk Schenk, and Jim Kaduk. Publication is expected in 2017–2018. The online version will include extensive digital material that readers can use to develop their skills.
- (7) Important progress on a new Volume I (*X-ray Absorption Spectroscopy and Related Techniques*) being developed by Chris Chantler, Federico Boscherini, and Bruce Bunker. Nearly half of the ca 150 experts who agreed to submit material have already done so.

- (8) Further discussions with the Commission on Magnetic Structures about a volume covering their field.
- (9) Addition of Seitz symbols to the online versions of Volumes A and E. Minor corrections to the online versions of Volumes B and D.
- (10) Appointment of two new Editors: Michal Dusek for Volume B and James Hester for Volume G. Their willingness to accept the positions is greatly appreciated.

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

It is with sorrow that the passing of Hans Wondratschek in October 2014, Theo Hahn in February 2016 and Vojtech Kopsky in May 2016 is noted. Theo Hahn chaired the Commission on International Tables in the periods 1972–1981 and 1993–2003. He edited five editions of Volume A, created its *Brief Teaching Edition*, and was very involved with the sixth. Hans Wondratschek may be best known as the co-creator of Volume A1 but he was also very involved for many decades with Volume A and he contributed to Volume B. Vojtech Kopsky was the co-creator of Volume E and took a lively part in discussions of symmetry and its notation. The contributions of these three to the *International Tables* were enormous; their active involvement will be greatly missed.

During 2016 André Authier asked to retire as Editor of Volume D, which he has piloted since about 1990, when it was first being discussed. A search for a successor is underway but Volume D is so much his book that it will be difficult to replace him.

The staff in Chester, and especially Nicola Ashcroft, are absolutely central to the development and advertisement of this series. They advise Commission members on historical precedents and conventions, and they provide guidance on English usage, always in a very tactful and encouraging way. And they set all the type, layout the pages, and insert links. It is difficult to thank them enough for their contributions.

*C.P. Brock, Chair*

### A6.3. Commission on Aperiodic Crystals

The award of the *2011 Nobel Prize in Chemistry* to our colleague Dan Shechtman for his discovery of quasicrystals continues to provide a great inspiration for the community. It gave rise to further special meetings, honorary awards and Plenary Lectures on aperiodic crystals, promoting the notion of aperiodic crystals to the wider scientific community as well as to the general public. This included various activities that formed part of the International Year of Crystallography (IYCr2014), which provided a framework for activity aimed at promoting crystallography to the public. With the award of the 10th Ewald Prize to our colleagues Aloysio Janner and Ted Janssen for their development of superspace crystallography, aperiodic crystals took centre stage at the Montreal Congress in 2014, followed by Dan Shechtman's Plenary Lecture the next day. More recently, the 9th Max Perutz Prize of the European Crystallographic Association was awarded to Vaclav Petricek, in recognition of his practical application of the theory of aperiodic structures in the widely used computing system *JANA*. The prize was awarded at the 30th Meeting of the European Crystallographic Association (ECM30) in Basel, Switzerland, 28 August – 1 September 2016. We hope that these recognitions will continue to have a lasting effect in promoting the study of aperiodic crystals within the wider community.

Official meetings of Commission on Aperiodic Crystals (CAC) in the last triennium took place during the Montreal Congress in 2014, and during the 8th International Conference on Aperiodic Crystals (Aperiodic 2015), Břevnov Monastery, Prague, Czech Republic, 30 August – 4 September 2015. Other Commission business was conducted via e-mail, as well as through informal meetings of Commission members and consultants at various national and international conferences and workshops. As always, the Commission continued actively to promote aperiodic crystallography, in organizing, supporting, and promoting meetings, workshops, and educational activities worldwide. In doing so, CAC continued its ongoing coordination of

interaction between the various sub-communities and disciplines involved in the different aspects of research in aperiodic crystals. The next meeting of the Commission will take place at the Hyderabad Congress.

The central activity for the Commission in 2014 was its active participation and promotion of aperiodic crystals at the Montreal Congress. This was preceded by the very successful satellite workshop Introduction to Aperiodic Crystals, organized by Ron Lifshitz (as the then Chair of the Commission). Leading experts in the field provided an excellent exposition of research on aperiodic crystals, attracting a large audience of crystallographers, many new to the topic. The satellite workshop was followed by the opening of the Congress and the Ewald Prize ceremony with Ted Janssen's Ewald Prize lecture. Aperiodic crystals remained a strong thread throughout the Congress, with no fewer than twelve Microsymposia and five Keynote Lectures related to aperiodic crystals, which the Commission helped to organize. The Keynote Lectures and Microsymposia were very well received, attracting large audiences and inspiring discussions among delegates.

Our flagship scientific event in 2015 was the 8th International Conference on Aperiodic Crystals (Aperiodic 2015), which was held at the beautiful venue of the Břevnov Monastery in Prague, Czech Republic, 30 August – 4 September 2015. The conference, which was chaired by Michal Dušek and Václav Petříček, is the eighth in the series of triennial conferences organized under the auspices of the Commission, this time with the Czech and Slovak Crystallographic Association as the local organizer. The conference was attended by 134 delegates from 25 countries, among them 22 young scientists who were supported by IUCr funding. In the five conference days, a broad range of topics including classical modulated structures, quasicrystals and magnetic structures, symmetry aspects, mathematical aspects, tiling theory, high-pressure crystallography, diffuse scattering, lattice dynamics, physical properties, and commercial aspects were covered. The programme included the honorary lecture *Usefulness and Unusefulness of the Superspace Approach to Aperiodic Crystals*, given by the 2014 Ewald Prize winner Ted Janssen. A special session was devoted to the memory of Chris Henley, one of the pioneers of quasicrystal theory, who had sadly passed away on 29 June 2015.

Our central activity in 2016 was the 13th International Conference on Quasicrystals ICQ13, which was chaired by Hem Raj Sharma and An Pang Tsai and took place in September 2016 at Dhulikhel Lodge Resort near Kathmandu, Nepal. The conference was attended by 98 researchers from 22 countries, including 26 postgraduate students. There were 13 invited talks (including a public lecture by Dan Shechtman), 3 tutorial lectures, 50 contributed talks and 36 poster presentations. The conference was truly interdisciplinary, comprising theoretical and experimental physicists, chemists, material scientists and mathematicians. The 2016 Jean-Marie Dubois Award for Excellence in Quasicrystals was presented to Marek Mihalkovič, for his theoretical work that has enabled and demonstrated the simulation of thermodynamic and dynamic properties of quasicrystals, based on realistic atomic-scale models and energetics. The proceedings of the conference have been published in the Institute of Physics open-access *Journal of Physics: Conference Series* as volume 809 (2017).

In addition to these main events, the Commission contributed to many other conferences and sessions on aperiodic crystals. The next main conferences will be: the Hyderabad Congress in August 2017; the 9th International Conference on Aperiodic Crystals (Aperiodic 2018), Ames, Iowa, USA, 13–18 July 2018, with local organizers Alan Goldman, Gloria Borgstahl and Pat Thiel, with Andreas Kreyssig acting as the conference administrator; and the 14th International Conference on Quasicrystals ICQ14, Bled, Slovenia, 26–31 May 2019, with lead organizer Janez Dolinšek.

#### *International schools and workshops*

Our central educational activity of the triennium was the 3rd International School on Aperiodic Crystals. This was organized by Joke Hadermann in Antwerp, Belgium, in July 2016, with the support of the CNRS (formation permanente), the European CMAC network and the European Crystallographic Association. Material and organizational support was provided by the University of Antwerp and specifically the Antwerp Summer University. The School, which followed on from the successful Schools in Carqueiranne, France, in 2010 and in Bayreuth, Germany, in 2013, attracted 33 participants from 14 different nations, 18 of which were aged below 30. Teaching at the School was provided by 9 lecturers. This School is our central educational activity, with the objective of providing an overview of aperiodic order, of the basics of the mathematical description of both modulated structures and quasicrystals, of physical properties and chemical understanding of aperiodic crystals, as well as a working knowledge of structural analysis of aperiodic crystals. Successful participation at the school was acknowledged with three ECTS (European Credit Transfer System) credits, which students could obtain by passing an online test within a month after the school. The next school is planned to be held in France in 2019.

There is a continuing series of *ad hoc* JANA2006 workshops in Prague, Czech Republic, as well as a number of workshops at conferences, such as at the 6th and the 7th Shanghai Workshops on X-ray Crystallography in 2015 and 2016, which attracted

about 50 and 70 participants, respectively. In addition, Commission members were involved in various workshops. Some examples with direct involvement in the organization of the event are: a Workshop on Dynamical versus Diffraction Spectra in the Theory of Quasicrystals at the Mathematisches Forschungs-Institut Oberwolfach in December 2014, which was co-organized by the Chair; the 8th Workshop on Structural Analysis of Aperiodic Crystals in Bayreuth, Germany, 12–15 March 2015, with local organizers Andreas Schönleber and Sander van Smaalen; and a Workshop on Spectral Theory of Aperiodic Systems at the Heinrich-Fabri-Institut in Blaubeuren, Germany, June 2015, which was co-organized by the Chair.

*U. Grimm, Chair*

#### A6.4. Commission on Biological Macromolecules

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

*Standards for information to be provided to reviewers of macromolecular structures*

The Commission has continued to work with the American Crystallographic Association, the Asian Crystallographic Association, the European Crystallographic Association, and the worldwide Protein Data Bank ([www.PDB.org](http://www.PDB.org)) to begin the development of standards for information that reviewers of scientific publication related to macromolecular structures should receive. The key ideas in these draft standards are that reviewers of manuscripts pertaining to macromolecular crystal structure should receive (1) the PDB validation report and (2) pictures of omit maps for any ligands and unusual structural elements. Additionally, the draft standards suggest the idea of making the data (structure factors, coordinates) available to reviewers. In 2015 Commission members were part of a wwPDB workshop to further develop standards for ligand validation. The results from this workshop were published [Adams *et al.* (2016). *Structure* **24**(4), 502–508] and the PDB is currently implementing these recommendations.

*IUCr Diffraction Data Deposition Working Group*

The Commission has worked with the IUCr Diffraction Data Deposition Working Group (DDDWG) to evaluate theoretical and practical reasons for the deposition of raw diffraction images that constitute the primary data in a macromolecular X-ray diffraction experiment. In 2015 a workshop was held during the European Crystallographic Association Annual Meeting in Rovinj, Croatia, and the DDDWG and Commission members further discussed the necessity of archiving results of diffraction experiments in the form of original diffraction data. Major progress during 2015 included the implementation of a new public server where anyone can upload and download many crystallographic raw datasets ([https://www.youtube.com/watch?v=eQbs9sB\\_pOM](https://www.youtube.com/watch?v=eQbs9sB_pOM)). An extensive discussion of the issues is available on the DDDWG forums page at: [www.iucr.org/forums/dddwg](http://www.iucr.org/forums/dddwg) and in recent publications [Grabowski *et al.* (2016). *Acta Cryst. D* **72**(11), 1181–1193; Kroon-Batenburg *et al.* (2017). *IUCrJ* **4**(1), 87–99; Meyer *et al.* (2016). *Nature Commun.* **7**, 10882].

*Proposed mechanisms for enhancing ease of identification and correction of PDB deposits with errors*

The Commission is beginning discussions of mechanisms for making it easier for researchers to correct errors in the PDB and for users of the PDB to identify problematic or non-problematic entries in the PDB.

The principal goals of this proposal are:

- (1) to allow users of the PDB readily to identify and filter out the structures that have exceptionally poor validation statistics including geometric or data-based validation criteria;
- (2) conversely, to allow users of the PDB readily to identify experimental data in the PDB that is represented by more than one interpretation, compare these interpretations and select a single best interpretation based on the user's validation preferences;
- (3) to provide users of the PDB with validation of individual ligands in a structure separately evaluating the geometric plausibility of each ligand and the evidence for the ligand coming from the data;

(4) to provide researchers with straightforward mechanisms for depositing new and hopefully improved interpretations of data in the PDB and associating the new deposits with this data.

*Endorsement of Letter to the Editor of Acta D on definitions of ‘resolution’*

The Commission considered a Letter to the Editor on definitions of ‘resolution’ by Dauter and Wlodawer and endorsed the letter with the following text:

The IUCr Commission on Biological Macromolecules endorses the concepts in the Letter to the Editor by Dauter and Wlodawer [Wlodawer & Dauter (2017). *Acta Cryst. D* **73**, 379–380] and in particular supports the idea of developing community-agreed working definitions of ‘atomic resolution’ and ‘near-atomic resolution’. The Commission notes that although there are limitations in the definition of ‘resolution’ itself these limitations should not prevent the X-ray, neutron, XFEL, cryo-EM and other communities from coming to a consensus on the use of the terms ‘atomic resolution’ and ‘near-atomic resolution’, as suggested in the Letter.

*Meetings, workshops and other outreach activities*

The CBM has recommended support from the IUCr for a number of meetings and workshops that can provide a teaching or major dissemination role for macromolecular crystallography.

*T. Terwilliger, Chair*

#### **A6.5. Commission on Charge, Spin and Momentum Densities**

This triennium has been particularly lively for the Commission, with many activities ongoing and significant renovation of the profile in the field.

Some specific actions to be taken were identified, after some discussion carried out at meetings where some members of the Commission could take part:

(1) The field of charge, spin and momentum density is identified by the crystallographic community as ‘European centred’, although historically fundamental contributions came and still come also from North America, Asia and Australia. For this reason, some workshops and schools were organized with the purpose of educating young scientists especially in those areas where lack of basic knowledge may prevent research groups from undertaking projects in this field. In this respect, the First Asia Charge Density Workshop organized in Bangalore (India, 2015) was very important, as were similar events in Brazil and Mexico (see below) – as well as dedicated sessions in some new regional meetings, such as the first Pan-African Conference on Crystallography, organized in Dschang (Cameroon, 2016).

(2) The rapid growth of the emerging field of quantum crystallography fosters important renewal in this community. The definition of this field is under debate. Quantum crystallography is not only the improvement of ‘approximate wavefunctions by constraining them to reproduce observations derived from diffraction and scattering experiments’ or the improvement of ‘complete charge density models by supplementing diffraction experiments with quantum chemically calculated, tailor-made electron densities’. Quantum crystallography encompasses several quantum phenomena occurring in crystals and merges theoretical calculations and many kinds of experiments, not only X-ray diffraction. Two forthcoming meetings will be dedicated to define the field in more detail: the CECAM Discussion Meeting on Quantum Crystallography: Current Developments and Future Perspectives, Nancy, France 19–20 June 2017; and The Erice School on Quantum Crystallography, Erice, Italy, 1–10 June 2018. The Commission considered therefore urgently adapting its name to the ongoing transformation, also taking into account that the current name is itself inappropriate. In fact, the electron density distribution may refer to the total electron charge or the electron spin excess/defect and, given quantum mechanics, they can be represented in position space or in momentum space. Thus, ‘momentum density’, although easily identified as electron density in momentum space, is not an accurate definition. A new name for the Commission is proposed: Commission on Electron Densities and Quantum Crystallography, which merges all the definitions and representations of the electron density and includes research that is not a direct investigation of electron density distribution but, more generally, of the phenomena in crystals that require a quantum mechanical approach, hence the calculation or refinement of a periodic wave function.

(3) Collaboration with other Commissions has been strengthened, especially with the Commission of Neutron Scattering, with which some meetings have been jointly supported.

#### Conferences

Montreal Congress. The Commission organized or co-organized five scientific Microsymposia (MS19, MS35, MS65, MS89, MS106) that received a large audience. Discussions concerned new methods to compute electron density distributions from X-ray diffraction, combined refinements to determine simultaneously the charge and the spin density, new sources and detectors and new opportunities at large-scale research facilities. The Commission was also represented by Wolfgang Scherer (Germany), who gave a Keynote Lecture, where he reported on recent advances in charge density studies for inorganic materials. Mark Spackman (Australia) also gave a Keynote on application of charge density partitioning for crystal engineering purposes, invited by the Commission on Structural Chemistry.

Sagamore XVIII Conference on Charge, Spin and Momentum Densities, Santa Margherita di Pula, Italy, 6–12 June 2015. This is the only conference that covers all the aspects of the community represented by the Commission and that investigates electron charge and spin distribution in position or in momentum density. The meeting was organized by Carlo Gatti (past Commission Chair) and his colleagues and co-workers from the University of Milan and the CNR-ISTM of Milan. The participation was very large and, as usual, the scientific talks were accompanied by long discussions, favoured by the pleasant atmosphere of the venue. The scientific programme encompassed various fields of electron density in life and materials science; in particular, new experimental probes and theoretical methods, chemical and crystal engineering, functional materials and nanoscale, structure evolution and densities, topological approaches, extreme conditions and biochemical applications.

29th European Crystallography Meeting (ECM29), Rovinj, Croatia, August 2015. The Special Interest Group on Charge, Spin and Momentum Density (SIG2) of the European Crystallographic Association directly organized one Microsymposium on Charge Density Studies and one Keynote Lecture, given by C. Gatti, honouring his receiving the Aminoff Prize in 2013. Moreover, some other Microsymposia were co-organized by SIG2.

9th International Conference of Inelastic X-ray Scattering, Taiwan, 22–26 November 2015. The meeting programme included: Compton scattering and extreme conditions; Energy materials; Emergent two-dimensional materials; Low-energy excitations of correlated electron systems; Magnetism; Molecules and liquids; Time domains and new frontiers of theory and experimental techniques.

7th European Charge density Meeting (ECDM7), Warsaw, Poland, June 2016. The meeting was organized by K. Wozniak and P. Dominiak, in conjunction with the annual Polish Crystallographic Meeting. There were a large number of participants and the meeting was attended by many experts worldwide as well as by many young researchers. The charge density community in Poland is in fact quite large and this was very important for the attendance and the organization. During the meeting, very intense discussions took place also concerning the future of this field in view of the new opportunities.

30th European Crystallographic Meeting (ECM30), Basel, Switzerland, August 2016. The Commission organized three Microsymposia (Charge and Spin Density of Materials at Extreme Conditions; Beyond Multipolar Refinement; Measuring Data Quality) and one Keynote Lecture given by Birger Dittrich. During this conference, the board of the Special Interest Group on charge spin and momentum density was renewed. During the discussion, it was also suggested to review the name of this special interest group in keeping with the similar modification of the name of the IUCr Commission.

#### Schools and workshops

The Commission supported some workshops and schools in related fields and directly organized some schools.

1st Asian Charge Density Workshop, Bangalore, India, February 2015. This was the inaugural event of a possible long series of workshops, organized by Professor Guru Row (Commission consultant, from the Indian Institute of Science) in collaboration with Commission member Dr Louis Farrugia, from the University of Glasgow. The school covered the basic aspects of charge density refinement and analysis, with hands-on tutorials using the most common programmes *MO-PRO* and *XD*. The workshop was attended by more than 40 students, mainly from Asia. It was followed by a special session on charge density within the National Symposium on X-ray Diffraction and Recent Advances in Crystallography, organized by Professor Poomani Kumaradhas (Periyar University, Salem India).

Workshop on Charge Density Determination, Belo Horizonte, Brazil, September 2015. This was organized by B. Rodrigues and P. Macchi at the University of Minas Gerais and consisted of a series of lectures and tutorials. The charge density community in Brazil may also be growing in view of the new synchrotron facility available at Campinas; therefore this workshop was important to start building up a community.

The First Robert F. Stewart School on Electron Density and Related Properties, Nancy, France, 22–26 August 2016. As a satellite of the European Crystallographic Meeting in Basel, Switzerland, Professor M. Souhassou and Dr P. Macchi organized, with the collaboration of the LCRM2 of the University Lorraine, the first Robert F. Stewart School on Electron Density and Related Properties. This was the inaugural school of a hopefully long series dedicated to the memory of Professor R.F. Stewart, who made enormous contributions in the field and unfortunately passed away in 2015. The aim of this school was to teach all participants the basic knowledge about paired and unpaired electron density distributions using neutron and X-ray diffraction methods and to practise using existing refinement software. The school ended with a round-table discussion about the application of topological analysis and electrostatic properties of a charge distribution in chemistry, biochemistry and physics. The audience consisted of early career scientists, post-doctoral research fellows, and graduate students of crystallography, solid state and materials science, biochemistry, theoretical, quantum and computational chemistry.

#### *Commission projects*

Two projects, established in the previous triennium, were carried out by Commission members or consultants.

Professor P. Nakashima (Monash University, Australia) led the project on electron distribution in the metallic bond by QCBED techniques and X-ray diffraction, in conjunction with the Commission on Electron Crystallography. The results of the project are not ready and an extension will be granted to Profesosr Nakashima for completing the experiments and data analysis and reporting.

A round-robin test on charge density studies on a coordination network, Mn(HCOO)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>, using synchrotron radiation and laboratory sources was undertaken in collaboration with the Commission on Synchrotron Radiation. During this triennium, data were collected at different sources and analysed by project leader Dr Jacob Overgaard (University of Aarhus, Denmark), in cooperation with Professor Enrique Espinosa. Dr Overgaard is currently producing the final report.

Given the fundamental changes that are occurring in the Commission, a project will be launched for the definition of the field of quantum crystallography, to be carried out within the next triennium.

*P. Macchi, Chair*

#### **A6.6. Commission on Crystal Growth and Characterization of Materials**

Members and consultants of the Commission had the chance to meet three times: in 2014 during the Montreal Congress, in 2015 in Bologna, Italy, during the 5th European Conference on Crystal Growth, and in 2016 in Nagoya, Japan, during the 18th International Conference on Crystal Growth and Epitaxy (ICCGE-18). All the reports of these meetings can be found at the Commission web site. Apart from these events, discussion among members was carried out by e-mail. The next Commission meeting will take place during the Hyderabad Congress.

The activities of the Commission in 2014 were dominated by the occurrence of the International Year of Crystallography. Concerning IYCr2014, the Commission supported different activities at national level. Moreover, with the help of the IUCr webmaster, Brian McMahon, and of Michele Zema, the Commission realized a web site with the purpose of collecting crystal images from crystal growers worldwide. The web site (<http://www.iycr2014.org/participate/crystal-growing>) is active and keeps on growing with new images.

Also, the Commission was very active in the organization of the Montreal Congress. All the Microsymposia organized by the Commission were quite successful. I take the opportunity to thank Edmondo Gilioli, Tatyana Bekker, Antoni Dabkowski, Joseph Ng, Janet Newman, Detlef Klimm and Y. Mori for their enthusiastic efforts in the organization of these sessions. Also, Juan Garcia Ruiz and Peter Rudolph gave excellent Plenary and Keynote Lectures.

One of the main tasks for our Commission in the last triennium was to promote crystal-growth-related conferences and schools. This was done also by strengthening even more the cooperation with the International Organization for Crystal Growth (IOCG). Many Commission members/consultants (K. Kakimoto, T. Kuech, J. Wang, S. Baldochi, T. Duffar, A. Moreno and E. Vlieg) are active inside the IOCG.

In 2015 the Fifth European Conference on Crystal Growth and the First European School on Crystal Growth in Bologna, Italy, took place. Many Commission members and consultants were involved in the organization of these events; for example, Elias Vlieg and myself, as Chairs of the School and Conference, respectively. It has been decided that both the European School and Conference will take place in three years time in Bulgaria. We are very happy that the tradition of European Crystal Growth Conferences has been established again and that together with it also the tradition of European Schools on Crystal Growth.

In 2016, the most important meeting for the crystal-growth community was the 18th International Conference on Crystal Growth and Epitaxy (ICCGE-18), Nagoya, Japan, 7–12

August. The opening ceremony of the Conference took place in the presence of His Imperial Highness, The Crown Prince of Japan. A lecture was given by the Nobel Laureate Isamu Akasaki. 11 general sessions and 10 topical sessions were organized. The Conference was very successful (about 1,400 participants) and very well organized. The 16th International Summer School on Crystal Growth (ISSCG-16), Lake Biwa, Shiga, Japan, with the participation of 120 students, was organized in the week before the Conference. Both the Conference and the School were supported by the IUCr. Many members and consultants of the Commission were involved in the organization of the Conference and the School, but I would like to underline, in particular, the contribution of Koichi Kakimoto, Chair of ICCGE-18 and a member of this Commission. Moreover, three symposia of the IOCG Conference have been officially co-organized by representatives of the IUCr, namely Janakiraman Kumar (Defect Formation), François Puel (Industrial Crystallization), and Juan Manuel Garcia Ruiz (Organic and Biological Crystallization).

Of course, much of the work of the Commission was devoted to the organization of the Hyderabad Congress. Our Commission suggested and actually supports several MS. Among them: (i) Topological Insulators, co-Chaired by J. Kumar; (ii) Hybrid Perovskites, co-Chaired by R. Mosca; (iii) Macromolecular Crystal Growth, co-Chaired by Abel Moreno; (iv) Polymorphism and Solid-Form Investigations, co-Chaired by S. Cuffini; (v) Crystal Growth and Nucleation, co-Chaired by Jaime Gomez Morales; and (vi) Multiferroic Materials, co-Chaired by G. Mezzadri.

In the triennium the Commission recommended IUCr support for the following conferences (most were organized by Commission members and consultants):

First Pan-African Conference on Crystallography (PCCr1), Dschang, Cameroon, Central Africa, 6–11 October 2016.

16th International Conference on the Crystallization of Biological Macromolecules (ICCBM-16), Prague, Czech Republic, 2–7 July 2016.

Of more concern to the Commission was the organization of schools on crystal growth. The planning for organization of schools is always the first topic of discussion during the CCGCM meetings. The schools in Bologna, Italy, in 2015, and in Shiga, Japan, in 2016, have already be mentioned. Also I wish to mention the International School organized each year in Granada, Spain, with the presence of several members/consultants from this Commission, and, in particular:

4th International School on Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials (ISC2014), Granada, Spain, 26–30 May 2014.

5th International School on Biological Crystallization (ISBC2015), Granada, Spain, 24–29 May 2015.

5th International School on Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials (ISC2016), Granada, Spain, 22–27 May 2016.

Moreover, the Commission requested IUCr support for the following schools, inherent to the subject of crystal growth and with a strong participation of members/consultants of CCGCM:

1st International School of Crystallization and Polymorphism, San José, Costa Rica, 27–31 January 2014.

48th Course of the International School of Crystallography, Erice, Italy, 5–14 June 2015.

First Workshop on Crystallography for Space Sciences, Puebla, Mexico, 17–30 April 2016.

Finally, on a personal note, I wish to underline that it has been a great pleasure and honour for me to Chair the Commission during the period 2014–2017. I believe that promotion of the understanding of crystal growth is essential for progress in materials science, and I wish the Commission the best in the future challenges.

*A. Zappetini, Chair*

#### **A6.7. Commission on Crystallographic Computing**

*Activities during the triennium*

(1) The Commission had organized a Computing School to be held at la Cité Collégiale, Ottawa, Canada, 29 July – 4 August 2014, immediately prior to the Montreal Congress. This was cancelled owing to the very low number of applications (i.e. 2) for the event. The reasons discussed centred on the late organization of the meeting. Fortunately, the Commission was able to withdraw its booking for the venue without incurring a cost.

(2) The Commission has organized a Computing School to be held in Bangalore, India, 15–21 August 2017, immediately prior to the Hyderabad Congress. The School will be structured to have formal lectures and tutorials, so that ideas can be exchanged between new students and established programmers. More detailed information is available on the web pages of the School at <http://www.iucr.org/resources/commissions/crystallographic-computing/schools/bangalore2017>.

A Scientific Programme Committee composed of Patrick Mercier (Ottawa, NRC Canada), Arie van der Lee (Montpellier, France) and Garib Murshudov (MRC, Cambridge, UK) was set up to develop the course and choose speakers. I joined in with the e-mail discussions.

A Local Organizing Committee was set up, comprising B. Gopal (IISc, Bangalore), Santosh Panjikar (Australian Synchrotron, Melbourne). Garib Murshudov and I joined later for discussions.

(3) Organization of sessions related to crystallographic computing at the Hyderabad Congress. Professor Patrick McArdle of the National University of Ireland, Galway, was the Commission's representative for the IPC. It is very disappointing that the Commission will have only one MS (which is shared) at the Congress, since the Commission's MS are usually amongst the best attended.

*H.R. Powell, Chair*

## A6.8. Commission on Crystallographic Nomenclature

In 2014 André Authier resigned after more than 12 years as Chair of this Commission (the CCN). We thank him for his many years of hard work, good judgment and wise counsel. Under André's leadership the Commission prepared three formal reports that were published in Section A of *Acta Crystallographica*, the most recent in 2014 (see below). André was also the Founding Editor (and first General Editor) of the *Online Dictionary of Crystallography*, which was established according to distributed authorship principles similar to those of Wikipedia.

The members of the CCN are the Editors of the Union's journals and the Editors of the volumes of *International Tables*, the Chair of the IUCr/OUP Book Series Committee, the Chair of the Commission on Crystallographic Teaching, the Chair of the Committee for the Maintenance of the CIF Standard, the President of the IUCr and the General Secretary of the IUCr. The total number of members and appointed consultants exceeds 50. This number is somewhat unwieldy but there seems to be no good way to reduce it. In the case of a matter needing the vote of the whole Commission, a Working Group composed of members representing all important viewpoints would be asked to prepare a report to be circulated to the CCN in advance of the vote.

### I. Nomenclature problems

The Commission's web page invites crystallographers to bring nomenclature problems to the attention of any Commission member. The problems considered during 2014–2017 are listed below.

#### (1) Standardization of Seitz symbols

In May 2014 the CCN's report on the standardized Seitz notation for symmetry operations was published in *Acta Cryst.* [Glazer, Aroyo & Authier (2014). *Acta Cryst.* **A70**, 300–302].

#### (2) Nomenclature for reticular chemistry

At the 2014 Commission meeting in Montreal, M. Nespolo described work by M. O'Keeffe and associates on a graph-theoretic description of bonding in crystal structures. This group had developed a full terminology to be approved by IUPAC. It was suggested that the IUCr should also consider approving this terminology, but attempts to set up a joint working group were unsuccessful.

#### (3) Nomenclature for the field of crystal engineering

In 2014 ICSU funded a project titled CONcepts and termINology in Crystal Engineering (CONvINCE). The Lead Applicant for the project was IUPAC; the IUCr was listed as a Supporting Applicant. G.R. Desiraju (then IUCr President) was named as the IUCr contact. After the Montreal Congress the CCN became involved.

In August 2015 the CCN Chair attended a meeting connected with the project in Como, Italy, but no written definitions have yet been circulated. A special-activities Microsymposium (Terminology Issues in Crystals Engineering) will be held at the Hyderabad Congress.

#### (4) Definition of Miller indices

The definition of Miller indices in the *Online Dictionary* has been modified to point out that the Miller indices for planes in centred unit cells are not necessarily relatively prime if the plane includes points related by a centring translation. The author, U. Shmueli, of Section 1.1 of Volume B of *International Tables*, proposed a minor change that was made in March 2017 to the online version of Volume B and will be incorporated in the print version of any revision.

#### (5) Nomenclature for arithmetic crystal classes

In mid-2015 Howard Flack proposed that the nomenclature of arithmetic crystal classes be changed so that the symbol of each class would start with the symbol for the Bravais-lattice type and conclude with the symbol for the crystal class (oriented point group). Thus space group No. 45, *Iba*2, for which the current symbol is *mm2I*, would have the new symbol *oImm*2. The proposal did not generate much enthusiasm, and lost its impetus with the untimely passing of its sponsor. An important

consideration is the amount of work that would be required to change all occurrences of affected symbols in the various volumes of *International Tables* and in the *Online Dictionary*.

## *II. The Online Dictionary of Crystallography (or, ODC)*

The CCN is responsible for maintaining this dictionary, which was established in 2006. A snapshot view was published in paperback in time for the Montreal Congress.

While many crystallographers believe the dictionary to be important, the number of contributed definitions is still below 300. Furthermore, important questions have been raised about how authoritative the included definitions should be considered to be, especially since the *ODC* is being cited in the scientific literature (*ca* 8 times in 2015–2016). During 2016 it was decided that these matters would be discussed informally before the Hyderabad Congress and then in Hyderabad. One plan would be to ask the various Commissions to be more formally involved in contributing and reviewing definitions.

*C.P. Brock, Chair*

## **A6.9. Commission on Crystallographic Teaching**

### *Overview of activities*

The Commission has been a large and enthusiastic group (nine members and nine consultants) in the triennium. We have worked together to develop and refine rubrics for review of applications that request IUCr support for workshops and summer schools. In addition, working with our representative to the International Programme Committee, Manfred Weiss, we assisted with the planning of several exciting Microsymposia relevant to teaching and education for the Hyderabad Congress. While our discussions have largely been via e-mail, we held our Commission meeting in March 2017 synchronously online using Zoom. This enabled our membership to engage in fruitful face-to-face discussion across 14 time zones. We intend to continue this practice moving forward.

### *Community outreach*

Social media. Since the Montreal Congress, the Commission (CCT) has continued its efforts to reach out to the crystallographic community, the scientific community, and the community at large using social media. The Commission Facebook page has been the most active (<http://www.facebook.com/IuCrCommissionOnCrystallographicTeaching>), with 1,120 ‘likes’ (an increase of 700% since the last triennial report). Our Twitter feed (@IUCrTeach) has 146 followers (up 500% since the last triennial report). The CCT attempts to post items and subscribe to other relevant social media feeds in parallel on both sites. Facebook, however, tends to stimulate more discussion among followers, and we receive messages asking for information and help with certain topics. Twitter seems to serve the purpose of disseminating announcements and interesting findings. The CCT will strive to post on both social media outlets more regularly, to stimulate interest and to disseminate better exciting findings and important information. To achieve this goal, we will designate a subset of the Commission membership to share in this task.

Web resource pages. We are also reviewing our web pages on the IUCr web site, examining resources for utility and audience, reorganizing content as appropriate, and updating information. We intend to designate a subset of the Commission membership to share in this task. In addition, we hope to reactivate a quarterly Newsletter with a global outlook. Our objective is to make our electronic communication channels and information targeted and relevant to specific audiences worldwide.

**Action item:** Reorganization and updating of web resources will be a high priority for the next triennium.

**Action item:** Commission members will be tasked to assist with contributing to and monitoring social media feed, as well as moderating discussion boards and managing the resource page contents.

### Sponsorship of professional programming

Manfred Weiss (Germany), a member of the CCT, has represented the CCT on the International Programming Committee for the Hyderabad Congress. The CCT is sponsoring/co-sponsoring the following Microsymposia:

New Approaches in Crystallographic Teaching (MS16); Chairs: Louise Dawe, Peter Moeck; Speakers: Gemma de la Flor Martin, Helen Maynard-Casely, Robert Hanson.

Crystallography Courses Around the World (MS32); Chairs: Annalisa Guerri, Juan Manuel Garcia Ruiz; Speakers: Not yet announced.

Structural Databases as Teaching Tools – Part A (Macromolecules) (MS44) Chairs: Christine Zardecki, Joel Sussman; Speakers: Urmila Kulkarni-Kale, Jaime Prilusky, Shuchismita Dutta, Sameer Velanka.

Structural Databases as Teaching Tools – Part B (Organics, Minerals) (MS45); Chairs: Amy Sarjeant, Graciela Delgado; Speakers: Simon J. Coles, Miguel Delgado, Louise Dawe.

How Does Crystallography Help You in Your Career? (MS87); Chairs: Ashwini Nangia, Soorya N. Kabekkodu; Speakers: Soorya N. Kabekkodu, Sudhir Nambiar, Sriram Subramaniam, Anant Paradkar, Miguel Delgado.

As these MS are intended, they will provide a platform for speakers to present on a wide variety of topics, from technology, to K-16 education and outreach, to community engagement, to teaching innovations. The CCT will encourage the MS Chairs to disseminate the content of their sessions in manuscripts to the *Journal of Applied Crystallography*, which showcases effective teaching and education.

At the Montreal Congress, Saulius Grazulis (Lithuania) and Amy Sarjeant (USA) co-Chaired Crystallography Education and Training in the 21st Century: New Pedagogies, New Paradigms, MS92. The content of this session has been nicely presented in the publication *Crystallography Education in the 21st Century* [Grazulis, S., Sarjeant, A.A., Moeck, P., Stone-Sundberg, J., Snyder, T.J., Kaminsky, W., Oliver, A.G., Stern, C.L., Dawe, L.N., Rychkov, D.A., Losev, E.A., Boldyreva, E.V., Tanski, J.M., Bernstein, J., Rabeh, W.M. & Kantardjieff, K.A. (2015). *J. Appl. Cryst.* **48**, 1964–1975] (<https://doi.org/10.1107/S1600576715016830>).

**Action item:** The CCT will work with the MS co-Chairs from Hyderabad to coordinate transactions manuscripts on content from the upcoming MS. Publications will also highlight the CCT's efforts to revitalize the web teaching resource pages and solicit contributors to this repository. The CCT will coordinate with the IUCr editorial office to add contributions to the resource pages from peer-reviewed materials in the *Journal of Applied Crystallography* that have demonstrated assessment of successful learning outcomes.

**Action item:** Manuscripts that are not suitable as full research manuscripts for *Journal of Applied Crystallography* may still be redirected to the CCT for evaluation and possible reposting on the web as teaching materials. The CCT will work with the editorial office to capture these sorts of efforts and devise a means to evaluate them.

### IYCr2014

Since the Montreal Congress, the CCT has attempted to follow up on activities linked to the International Year of Crystallography. One example is the complete restoration of an original Kendrew model at California State University San Marcos. Under the guidance of faculty, a team of science and art students has completely refurbished the model, as well as created an identical 3D-printed replica. The student team was led by Sharon Patray, a refugee from Liberia, who is the first in her family to complete undergraduate studies and to seek higher education. A veteran of the marine corps, Sergeant Patray will graduate in May with a BS in Biochemistry, and she will begin graduate studies at Johns Hopkins University in virology in August 2017 (<http://news.csusm.edu/refugee-to-marine-to-graduate/>).

**Action item:** The CCT will follow up with recipients of IYCr funding for education and outreach and report on the outcomes of activities in upcoming Newsletters, as well as highlight outcomes on social media.

### *Review of workshop and summer school proposals*

Since the Montreal Congress, the CCT now reviews and writes recommendation letters for all workshop and summer school proposals, and the CCT has been very pleased to do this. We have developed a set of internal rubrics, which must now be articulated in the form of guidelines or a ‘tip sheet’ for applicants to follow prior to submitting an application. Rubrics will enable the CCT to determine more easily whether the proposals meet the mission and goals of the IUCr, to compare and contrast the proposals better, and to provide more useful feedback to the Executive Committee so that precious funds can be invested wisely and with maximum return.

The CCT has reviewed and written 27 supporting letters for workshops and summer schools, which have largely been of exceptional quality. Issues that have arisen during the course of evaluation have mainly concerned incomplete applications, missing information, whether the activity constitutes a truly international event, and constraints imposed by funding sources other than the IUCr. We wish to thank Wulf Depmeier (Germany) for his efforts to help streamline the evaluation process by sending applications in bundles for evaluation by the CCT. This has helped the CCT members manage time and effort and engage in fruitful discussion. Still, proposers often send in documents at the last minute, which are vague in details, missing supporting data, and/or do not justify the funds requested. The expectation on the part of proposers for immediate response by the CCT and an automatic endorsement at full funding levels is unrealistic. Through its forthcoming guidelines and ‘tip sheet’, the CCT will coach the crystallographic community about IUCr funding mechanisms and expectations. Guidelines will enable proposers to make the best possible case in their request.

We also still experience e-mails with important attachments becoming caught up in e-mail spam filters. Professor Depmeier has been exceptionally nimble to keep the evaluation process moving forward. In the next triennium, the CCT will work with the IUCr to establish a share point in the cloud for files to expedite review and processing of applications for financial support. This is preferred over using a member’s personal Dropbox or Google Drive account.

Better still, the CCT will explore with the IUCr office establishing an online submission system for workshop and summer school applications. Ideally, the content of the applications would be streamlined such that review could be accomplished similarly as is done for manuscripts. CCT members would have access to files and could provide comments. This could also be extended to other IUCr Commissions as needed. An exemplar recommended by the CCT Chair is submittable (<https://www.submittable.com/>).

**Action item:** To facilitate best practices and high impact educational experiences, the CCT encourages the Executive Committee to continue the practice that a letter of support from the CCT should be required for all school and workshop proposals, along with additional letter(s) from the appropriate subject matter Commission(s).

**Action Item:** The CCT will work with the IUCr to streamline the application process, either by establishing a share point in the cloud or launching an online submission system.

**Action Item:** The CCT will formally articulate its evaluation rubrics on its web site and provide a ‘tip sheet’ to prospective applicants seeking financial support for workshops and summer schools.

**Action item:** The CCT will explore ways for the IUCr to incentivize nations to host workshops and summer schools.

**Action Item:** The CCT will explore ways to capture lecture content from workshops and summer schools in ways that will enhance students’ ability to master scientific English.

### *Future meetings*

As noted earlier in our report, the CCT regularly ‘meets’ in cyberspace via email discussion. While this has worked generally well, given differences in time zones, we believe it is beneficial to have face-to-face meetings during the triennium. We held our Commission meeting in March 2017 synchronously online using Zoom. This enabled our membership to engage in fruitful face-to-face discussion across 14 time zones. We intend to continue this practice moving forward.

*K.A. Kantardjieff, Chair*

## A6.10. Commission on Crystallography in Art and Cultural Heritage

The Commission continued to pursue the aim of diffusing crystallographic knowledge related to artworks and ancient materials. The aim was especially important during IYCr2014, to show to the general public the link between crystallographic symmetry and art, and the role of crystallographic techniques in archaeometry and conservation.

2014

The following IYCr2014 actions were completed through the effort of Commission members:

Preparation of calendars for IYCr2014. The official calendar printed by the IUCr and distributed during the Opening Ceremony of IYCr2014 was an initiative of the Commission (CrysAC) (Alicja Rafalska-Lasocha, Bernardo Cesare). This calendar and other calendars prepared by the Commission can be downloaded from <http://crysac.visual-chemistry.net/downloads.html>.

Public exhibitions. October 2013 – March 2014: Padova, Italy – Exhibition *CRISTALLI* (organized by Gilberto Artioli) (more at <http://147.162.183.151/cristalli/welcome.html>; <http://www.iycr2014.org/photos/italy/cristalli>). The panels, the text and the iconographic part of the exhibition travelled through Italy as part of other events <http://www.iycr2014.it/eventi>).

May 2014 – August 2015: Krakow, Poland – Exhibition *In The Unusual World of Crystals* (organized by Alicja Rafalska-Lasocha in cooperation with the Faculty of Chemistry, Jagiellonian University) was shown 14 times in various places in Poland ([http://www2.chemia.uj.edu.pl/krysztaly\\_wystawa/](http://www2.chemia.uj.edu.pl/krysztaly_wystawa/)).

Juan Manuel García-Ruiz & Fermín Otálora, from the Laboratorio de Estudios Cristalográficos (IACT, CSIC/UGr), developed the exhibition *CRISTALES* to increase the awareness of students and the general public about crystallography. All materials are available at the web site <http://cristales2014.org>.

Special conferences, sessions, lectures. During the Opening Ceremony of IYCr2014 (Paris, France, 20–21 January 2014), two members of CrysAC delivered lectures: Abdelmalek Thalal – *Symmetry in Art and Architecture of the Western Islamic Golden Age*; Emil Makovicky – *Highlights of Eastern Islamic Ornamental Art As Seen Through Crystallographers' Eyes*.

Organization of the international scientific conference: 5th Meeting of X-ray and Other Techniques in Investigations of the Objects of Cultural Heritage Celebrating the International Year of Crystallography and the 650th Anniversary of Jagiellonian University, Krakow, Poland, 14–17 May 2014 (organized by A. Rafalska-Lasocha; G. Artioli and P. Bezdicke lectured) (<http://www.chemia.uj.edu.pl/nauka-i-badania/konferencje/X-ray>).

Organization of the scientific session Role of Crystallography in Science, Art and Everyday Life in cooperation with the Faculty of Chemistry, Jagiellonian University, Krakow, Poland, 14 May 2014 (A. Rafalska-Lasocha).

5th ALMA interdisciplinary conference 2014: Interpretation of the Fine Art Analysis in Various Contexts, Dominican Monastery of St Giles, Prague, Czech Republic, 20–21 November 2014 (P. Bezdicke, David and Janka Hradil, ALMA Laboratory).

294th edition of the one-day Rozhovory seminar: Discussions on Problems of X-ray and Neutron Structure Analysis, 23 April 2014 ([http://www.xray.cz/xray/csca/r294\\_en.htm](http://www.xray.cz/xray/csca/r294_en.htm)) (P. Bezdicke, R. Kuzel, S. Svarcova).

Colloquium Struktura 2014 of the Czech and Slovak Crystallographic Association and Regional Committee of the IUCr, Kutna Hora, Czech Republic, 9–12 June 2014 (P. Bezdicke).

Presentation at Montreal Congress: Crystallography on Stage: Presenting the Concepts and History Dramatically (C. Abad-Zapatero).

Lecture *Diagnostics in Art and Archaeology: Concepts and Case Studies*, GABEC-GNM International School on Innovative Methodologies for Characterization, Diagnosis and Conservation of the Cultural Heritage, Catania-Siracusa, Italy, 1–4 July 2014 (G. Artioli).

Lectures on Crystallography and the International Year of Crystallography delivered in Krakow, Madrid, Warsaw etc. (A. Rafalska-Lasocha).

IYCr2014 OpenLab Ghana, University of Ghana, Accra, 9–12 June 2014 (G. Artioli, PANalytical).

IYCr2014 OpenLab Turkey, Bilkent University, Ankara, 19–22 January 2015 (G. Artioli, PANalytical), contained a full day on cultural heritage.

Crystallography contest. The Commission, in cooperation with the Faculty of Chemistry of Jagiellonian University, organized a contest entitled The Role of Crystals in Human Life for secondary-school, high-school and University students in Poland (A. Rafalska-Lasocha). More about the contest and most of the contributions (in Polish) can be found at [http://www2.chemia.uj.edu.pl/konkurs\\_krysztaly/](http://www2.chemia.uj.edu.pl/konkurs_krysztaly/). A photo gallery is available at [http://www2.chemia.uj.edu.pl/konkurs\\_krysztaly/?page\\_id=525](http://www2.chemia.uj.edu.pl/konkurs_krysztaly/?page_id=525).

Participants in the contest were asked to prepare a poster, a presentation or a video clip. Prepared contributions were sent to the organizers by e-mail. The deadline was 28 February 2014. We received 99 contributions (61 from secondary-school students, 33 from high-school students, and 5 from University students). The judging was carried out in two stages: online voting and, after that, experts' evaluation. In online voting, 8,819 votes were received.

Continuing project. C. Abad-Zapatero continued collaboration with Mr Painton Cowen throughout the triennium to incorporate scientific content into the Rose Window web site (<http://therosewindow.com/TheRoseWindow2/Rose-numbers.htm>).

## 2015

The Exhibition In The Unusual World of Crystals was organized by A. Rafalska-Lasocha and shown in: January – in the Institute of Physical Chemistry PAS, Warsaw; February – in the Institute of Physics PAS, Warsaw; March–August – at Warsaw University of Technology (shown in several places).

Conferences, sessions, lectures. Organization of the Microsymposium Cultural and Historical Aspects of Crystallography, ECM29, Rovinj, Croatia (Chair: P. Bezdička; invited lecturer G. Artioli) (<http://ecm29.ecanews.org/programme/microsymposia/#ms50>)

The meeting Tilings and Tessellations at Isfahan University of Technology, Isfahan, Iran (invited lecturers J.-M. Castera, E. Makovicky (<http://isfahan.sciencesconf.org/>)).

Lectures on Crystallography and International Year of Crystallography were delivered in Warsaw and Paris (A. Rafalska-Lasocha).

## 2016

Conferences, sessions, lectures. The Commission has started to organize CrysAC workshops. The first CrysAC workshop on Cultural Heritage Authentication and Forensic Science was organized in Krakow, Poland, 18 May 2016 (A. Rafalska-Lasocha, G. Artioli, P. Bezdička).

CrysAC was a co-organizer of the scientific international conference 6th Meeting of X-ray and Other Techniques in Investigations of the Objects of Cultural Heritage, Krakow, Poland, 19–21 May 2016 (A. Rafalska-Lasocha, G. Artioli and P. Bezdička) (<http://www.biurokarier.chemia.uj.edu.pl/conf/x-ray16>).

Organization of Microsymposium MS48 Crystallography in Art and Cultural Heritage at ECM30 Basel, Switzerland (Chair A. Rafalska-Lasocha).

CrysAC actively participated in organization of the Hyderabad Congress.

The Commission is also a co-organizer of the 6th Interdisciplinary ALMA Conference to be held in Brno, Czech Republic, in 2016 (P. Bezdička as Chair of the Organizing Committee; G. Artioli and A. Rafalska-Lasocha as members of the IPC).

G. Artioli is contributing the article *Powder Diffraction in Art and Archaeology* to the new Volume H of *International Tables*.

CrysAC Website. A new CrysAC web site has been prepared: <https://www.iucr.org/resources/commissions/crysac>.

*G. Artioli, Chair*

*A. Rafalska-Lasocha, Secretary*

#### **A6.11. Commission on Electron Crystallography**

During the last the years the most progressive achievements in electron microscopy and crystallography were due to usage of direct electron detectors (DE) and software developments irrespective of the application area: *in situ* TEM, STEM (scanning), DTEM (dynamic), ETEM (environmental), HRTEM (high-resolution), and others. Several type of cameras are commercially available on the market: K2 (Gatan), Falcon II (FEI), and DE20 (Direct Electron). The Gatan K2-IS direct detector (*in situ* camera to resolve dynamic details in heating, catalysis, mechanical deformation, STEM diffraction, electrical testing, and chemical reaction experiments) was used for 4D-STEM probe diffraction patterns. Cs correctors continue to be improved, finding more implementations in high-resolution biological microscopy. The development and application of new electron microscopy techniques provided a foundation for the significant progress in structural and functional studies of properties of materials.

The CEC Gjønnes Medal Sub-committee (an international committee of five scientists from Japan, China, USA, and UK) considered four nominations. Any of them would be suitable to be a recipient of the Medal. Criteria for selection of a person to be awarded were based on whether the research concerned opened a new field, and how significant was its impact and influence to the crystallographic community. After thorough consideration, the CEC Gjønnes Medal Sub-committee awarded the 2017 Gjønnes Medal in Electron Crystallography jointly to Richard Henderson and Nigel Unwin for their development and powerful application of structural determination methods for biological complexes at near-atomic resolution using electron crystallography. The numerous results of the last five years in cryoEM with structures at  $\sim 3.5 \text{ \AA}$  would be impossible without the first steps in electron crystallography made by Richard Henderson and Nigel Unwin. The recommendation for the award has been approved by all members of the Commission.

Participation in organizing the programme for the Hyderabad Congress. Professor Van Dyck represented the Commission on the International Programme Committee (IPC) of the Hyderabad Congress. A Sub-committee of the Commission (E.V. Orlova, D. Van Dyck and L. Marks) followed proposals of members of the Commission and suggested the list of Microsymposia to the IPC. Professor Van Dyck was very successful in representing scientific directions and new developments suggested as the most advanced topics to the IPC. Professor Van Dyck has discussed with FEI options for financial support and obtained this for students from India, so they have a chance to participate in the impressive Congress.

The Commission was fully committed to use all opportunities to take a leadership role in training the young generation of scientists in electron crystallography and diffraction, including imaging; various workshops, summer schools and symposia on electron crystallography and microscopy were organized around the world, and the Commission was directly involved in the following events.

Electron Crystallography School – Introduction to Electron Diffraction Tomography, Darmstadt, Germany, April 2014 (Professor Ute Kolb).

Advanced Imaging Techniques For Scanning Electron Microscopy, Westmont, IL, USA, July 2014; the major topics covered were very high resolution imaging and low voltage imaging.

ESTEEM2 Electron Crystallography Workshop, UK, July 2014 (Alexander Eggeman).

Kuo Symposium on 3D Cryo-EM Molecular Imaging and 7th K.H. Kuo Summer School of Electron Microscopy and Crystallography, Shanghai, People's Republic of China, July 2014 (Professor H. Li).

International Workshop on Advanced and *In-Situ* Microscopies of Functional Nanomaterials and Devices (IAMNano 2014), Rio de Janeiro, Rio de Janeiro, Brazil, July 2014.

Cryo-Electron Microscopy and 3D Image Processing: EMBO Practical Course, Heidelberg, Germany, August 2014 (J. Briggs).

International Symposium on Crystallography, Fortaleza, Ceará, Brazil, October 2014; the symposium will be the first scientific event on crystallography to be held in the Northeast of Brazil.

Ano Internacional da Cristalografia na UFMG, Universidade Federal de Minas Gerais, Belo Horizonte, Minas Gerais, Brazil, November 2014; the UFMG has had research groups engaged in crystallography since 1980 and were involved in the celebration of the International Year of Crystallography in Brazil.

Electron Diffraction for Quantitative Surface Structure Determination: ICSOS Workshop-3 on Surface Structures, Łódź, Poland, July 2015 (D.I. Zasada was an organizer).

Electron Crystallography School, Poreč, Croatia, August 2015 (Organizer T. Gorelik); this school was a satellite meeting of ECM29.

Second European Crystallography School (ECS2), Oviedo, Spain, August 2015 (Organizer D. García-Granda).

XLIV Annual Meeting of the AIC, Vercelli, Italy, September 2015; Plenary Lectures by Lukas Palatinus (Institute of Physics of the AS CR, Prague, Czech Republic), Bartolomeo Civalleri (University of Torino, Italy), Jan Pieter Abrahams (Universiteit Leiden, The Netherlands).

International Conference on Electron Spectroscopy and Structure (ICESS-15), Stony Brook, USA, 28 September – 2 October 2015.

22nd Meeting of the Brazilian Crystallographic Association and First Meeting of the Latin-American Crystallographic Association (LACA), São Paulo, Brazil, September 2015.

Cristallographie Electronique, Lille, France, November 2015 [Organizers: D. Jacob (Université de Lille, France), P. Roussel (Ecole Nationale Supérieure de Chimie de Lille, France), P. Boullay (CNRS, CRISMAT, France)].

Micro Electron Diffraction Workshop, Ashburn, USA, February 2016 (Organizer T. Gonon); a hands-on workshop on structure determination from sub-micron-sized crystals.

Course on Cryo Techniques in Electron Microscopy, Harpenden, UK, April 2016; an intensive five-day residential course on sample preparation and cryo-microscopy techniques for both scanning and transmission electron microscopy.

International Conference on Nanoscopy (ICON 2016), Basel, Switzerland, June 2016; focus on super-resolution imaging methods that provide spatial resolution well below the diffraction limit.

9th K.H. Kuo Summer School of Electron Microscopy and Crystallography and Symposium, Beijing, People's Republic of China, June 2016.

ED-XPD Workshop, Combining Electron and X-ray Powder Diffraction Techniques for Structural Characterization, Stockholm, Sweden, June 2016.

International School on Fundamental Crystallography with Applications to Electron Crystallography, Antwerp, Belgium, July 2016.

Cryo-Electron Microscopy and 3D Image Processing of Macromolecular Assemblies and Cellular Tomography, Kerala, India, July 2016; a practical course on single particle cryo-electron microscopy of biological macromolecular assemblies and cryo-electron tomography of cellular structures.

American Crystallographic Association Annual Meeting, Denver, USA, July 2016; sessions on cryo-electron microscopy and electron diffraction, and molecular machines.

Fifth 2DX Workshop on Electron Crystallography of Membrane Proteins, Basel, Switzerland, August 2016; theoretical foundations and practical image processing of 2D crystal cryo-EM images with the 2DX software package.

MicroED Workshop, Ashburn, USA, November 2016; a hands-on workshop on structure determination using micro-electron diffraction from sub-micron-sized crystals.

The Commission continues to play a leadership role in promoting methods of electron crystallography and microscopy. Electron crystallography has progressed tremendously and has found successful implementations in studies of biological microcrystals. The progress of scientific studies in the field of electron crystallography is reflected in the huge number of publications, the high level of citations, and the organization of both small local and international meetings.

*E. Orlova, Chair*

#### A6.12. Commission on High Pressure

This report covers the triennial period between the IUCr Congresses in Montreal (August 2014) and in Hyderabad (August 2017). The Commission on High Pressure (CHP) in this term initially consisted of the following members: Andrzej Katrusiak (Poland) (Chair), Haozhe Liu (China) (Secretary), Ross Angel (USA), Elena Boldyreva (Russia), Simon Clark (Australia), Wilson Crichton (France), Francesca Fabbiani (Germany), Yasuo Ohishi (Japan), Chrystele Sanloup (France) and Guoyin Shen (USA). Consultants: Kamil Dziubek (Italy) (Treasurer), John Loveday (UK), Richard Nelles (UK), Ingo Loa (UK) (web site), Przemek Dera (USA) and Boris Zakharov (Russia).

After about a year, Wilson Crichton (France) resigned from the Commission owing to the new commitments at work. Thus the CHP continued with nine members.

The main tasks of the CHP were to organize annual workshops, schools and other conferences and to undertake the task of preparing guidelines for high-pressure metadata and high-pressure data deposition, as well as other tasks, such as preparation for the systematic recording of historical contributions to high-pressure research.

*IUCr High-Pressure Workshop.* The 2015 IUCr workshop was held at the Brazilian Synchrotron Light Laboratory (LNLS) in Campinas, Brazil. It was attended by 61 participants from 14 countries. The workshop primarily focused on recent advances in high-pressure techniques and research. Lectures and posters covered various aspects of high-pressure crystallography, structural phase transitions and their kinetics, new materials synthesis, Earth and planetary science, soft and biological matter, physical and chemical properties, theory and computation, as well as technique developments for high-pressure studies at synchrotron, neutron and laboratory-based facilities.

Nearly 30 lecturers presented their results: K. Dziubek, M. Zaworotko, L. Miyagi, S. Hunt, H. Marquardt, J. Haines, N. Brooks, D. Paliwoda, R. Wentzcovitch, K.-M. Ho, K. Umemoto, V. Solozhenko, A. Cairns, S. Deemyard, M. Pravica, M. Probert, R. Miletich, Y. Le Godec, S. Redfern, R. Conceicao, J. A. Lima Jr, J. Smith, R. Bini, C. Murli, A. Gomes, G. Finkelstein, M. Marcondes and O. Kurakevych.

Best-poster awards went to Zuzana Konopkova (Towards Time-Resolved Studies Using X-Ray Diffraction at Synchrotrons) and Marcelo Nobrega (High Pressure Study and Oligomerization of 2-Aminoterephthalate/Ni-Al Layered Double Hydroxide Composites).

The workshop was held just after the 1st Latin American Crystallographic Association (LACA) Meeting in São Paulo, promoted by LACA jointly with the 22nd Sociedade Brasileira de Cristalografia (SBC Meeting), and before the 25th RAU (LNLS Annual Users Meeting), promoted by LNLS, from September 16–17. This allowed those interested to participate in all these events. A few companies sponsored the workshop, namely: Agilent Technologies, Quantum Design, MCI/Princeton Instruments, Dectris, Almax-EasyLab and Huber. In addition to the support from the IUCr, the Brazilian funding agencies FAPESP and CAPES also supported the event.

*IUCr High-Pressure Workshop 2016 at PAL in Pohang, South Korea.* The 14th IUCr High-Pressure Commission (CHP) Workshop was held at the Pohang Advanced Laboratory in South Korea, 20–24 September 2016, with the Organizing Committee chaired by Professor Yongjae Lee (Yonsei University, Seoul). The workshop was primarily focused on recent

advances in high-pressure techniques and research. Lectures and posters covered various aspects of high-pressure crystallography, structural phase transitions and their kinetics, new materials synthesis, Earth and planetary science, soft and biological matter, physical and chemical properties, theory and computation, as well as technique developments for high-pressure studies at synchrotron, neutron and laboratory-based facilities. The workshop was attended by 120 participants from 19 countries.

The workshop started with a welcoming speech by Professor Kibong Lee, the Director of PAL. Plenary talks were given by Dr Ho-Kwang Mao, the Director of HPSTAR, China, on Pressure and X-Radiation; Dr Chi-Chang Kao, the Director of SLAC, National Accelerator Laboratory, USA, on The Potential of X-ray Free Electron Lasers for High Pressure Research; and by Professor Takehiko Yagi, University of Tokyo, Japan, on Synchrotron Facilities and High Pressure Science in Japan. Invited and contributing lecturers included Tomoo Katsura, Sang-Heon Shim, Vladimir Solozhenko, Timothy Strobel, Naoki Noguchi, Barbara Lavina, Byeongchan Lee, Kamil Dziubek, Takamitsu Yamanaka, Lin Wang, Keizo Murata, Wenge Yang, Hyunchae Cynn, Bin Chen, Stanislav Sinogeikin, Olivier Mathon, Yanbin Wang, Alfred Baron; Naohisa Hirao, Catalin Popescu, Cindy Bolme, Hae Ja Lee, Yanming Ma, Toshiaki Iitaka, John Tse, Garry McIntyre, Jack Binns, Boris Zakharov, Andrzej Katrusiak, Sung Keun Lee, Simon Clark and Luhong Wang.

Two special sessions were held to highlight PAL and High Pressure Research in Korea. Before an excursion to the PLSII and PAL-XFEL facilities, Jae-Young Kim (PAL) discussed the current status of PLS-II beamlines, and an introduction to PAL-XFEL was presented by its Director, In Soo Ko. Highpressure research in Korea was reviewed by Young-Ho Kim (Gyeongsang National University), and current high-pressure research and activities were introduced by a number of researchers from Korea; Young-Ho Ko (Agency for Defense Development, Korea), Research on Materials Under High Pressure or Temperature; Sung Keun Lee (Seoul National University), Glasses and Melts Under Compression and Extreme Confinement; Kee Hoon Kim (Seoul National University), Critical Behavior in Quasi-One-Dimensional Organic Conductors as Investigated by a Cubic Anvil Cell up to 8.5 GPa; Jaeyong Kim (Hanyang University), HYUHPSTAR-CIS High Pressure Research Center; Geun Woo Lee (KRISS), Study of High Pressure and High Temperature in KRISS; Yongjae Lee (Yonsei University), Construction of Max-X (Matter in eXtreme conditions X-ray) Beamline at Pohang Accelerator Laboratory. Six young scientists were distinguished by a diploma and IUCr awards, and presented short talks. Four Young Scientist posters were awarded.

Following the positive experience from the previous IUCr CHP Workshop in Campinas (2015), we fully implemented a scheme of standby lecturers filling any gaps caused by lastminute cancellations. Consequently, no session suffered from missing lectures at all, as several scientists selected according to their contributed posters and all the CHP members were asked to step in with prepared lectures that replaced the missing ones. Only these presented lecturers are listed above. The workshop was sponsored by a number of institutions including YONSEI-SLAC-USC Global Research Laboratory and HYU-HPSTAR-CIS High Pressure Center, funded by the Korean Ministry of Science, ICT, and Planning (MSIP) and the BK21Plus Institute at Yonsei University, funded by the Korean Ministry of Education. In particular, support from the IUCr, HPSTAR and PAL are gratefully acknowledged.

Detailed reports of the two workshops were given in the *IUCr Newsletter*.

*Course on High-Pressure Crystallography: Status Artis and Emerging Opportunities*, 27 May 27 – 5 June 2016. This third high-pressure course was held in Erice, Italy, and it continued the tradition of high-pressure crystallographic courses aimed at the dissemination of high-pressure techniques. The course directors were Dr Francesca Fabbiani (CHP member), Professor J. B. Parise and Dr M. Guthrie. The course attracted about 100 participants and was an occasion for several CHP members to meet. During the course several meetings of the Subcommission on High-Pressure (Meta)data Deposition were held.

*High-Pressure Magic* at Wits, Johannesburg, 19–23 October 2015. One of the main aims of the IUCr High Pressure Commission is the dissemination of high-pressure techniques in crystallographic laboratories, and in this spirit the High-Pressure Magic Workshop was organized at the Jan Boeyens' Structural Chemistry Department of the Witwatersrand University in Johannesburg. To our knowledge, this was the first high-pressure crystallographic event in South Africa. The programme of the workshop included five working days, Monday to Friday, each morning starting with a two-hour lecture, followed by a coffee break, practical exercises in the laboratory, lunch and practical exercises. The workshop was sponsored by the National Research Foundation of South Africa, Research and Innovation Support and Advancement (RISA) grant, and by Bruker South Africa.

*CHP Subcommission on (Meta)data deposition (SMDD)*. One of the main tasks of the CHP was the preparation of guidelines for metadata deposition. For this purpose a CHP Subcommission was established with the following members: Kamil Dziubek

(Italy) (Subcommission Chair), Ross Angel (USA), Andrzej Katrusiak (Poland), Guoyin Shen (USA) and Boris Zakharov (Russia). The SMDD has met several times during conferences and has also corresponded throughout the term. We have established that guidelines for the deposition of both crystallographic data for high-pressure experiments and of the metadata have to be prepared. A report on the deposition of high-pressure data and metadata has been prepared and will be published soon.

A. Katrusiak, Chair

#### A6.13. Commission on Inorganic and Mineral Structures

This report summarizes the activities of the Commission (CIMS) during its fifth triennium of existence, after its establishment at the Geneva Congress in 2002.

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

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

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

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

Strong links exist between CIMS and the European Crystallographic Association: O. Yakubovich was a member of the Executive Committee; the Secretary of the Special Interest Group SIG-5 is O. Siidra, the Chair S. Krivovichev and F. Hatert is Vice-Chair (ECA - SIG5, <http://sig5.ecanews.org/>).

There are very good relationships between CIMS and the European Mineralogical Union (EMU, <http://eurominunion.org/>); R. Oberti (EMU Past-President) is a member of CIMS and also Commissioning Editor of the EMU *Notes in Mineralogy* and Co-Editor of the Volume *The Contribution of Mineralogy to Cultural Heritage* to be printed in 2017. The Volume *Mineralogical Crystallography*, co-edited by J. Majzlan, Sergey Krivovichev and J. Plasil, will also be published in 2017.

Sergey Krivovichev served as President of the IMA in 2015–2016. M. Nespolo is Book Review Editor for the IUCr journals. C. Ling is the Vice-President of the Society of Crystallographers in Australia and New Zealand (SCANZ) and the Secretary of the Asia–Oceania Neutron Scattering Association (AONSA). P. Mercier has been Chair of the Canadian National Committee for Crystallography since August 2015. R. Oberti is Chair of the Committee on the participation of CNR (Consiglio Nazionale delle Ricerche) in the IUCr.

#### *Co-organization of scientific meetings*

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

(1) The main activity of CIMS in 2014 was the preparation and running of the following events at the Montreal Congress:

(i) MS1 Phase Transitions in Functional Inorganic Materials and Minerals (Chairs P. Thomas and K. Sugiyama);

(ii) MS 15 The Role of Defects in Crystal Structure Formation, Organization and Stability (Chairs O. Yakubovich and S. Pereira);

(iii) MS74 Mineralogical Crystallography (Chairs P. Mercier and R. Peterson). Moreover, D. Pandey delivered a Keynote Lecture entitled *The World of Perovskites: Phase Transitions and Exotic Properties*.

(2) R. Oberti co-Chaired the Organizing Committee of the first European Crystallographic School (ECS) held in Pavia, Italy, 26 August – 6 September 2014, to celebrate the International Year of Crystallography. Some 120 students from 30 countries (selected from among 200 applications) and more than 20 internationally renowned teachers (including the Nobel laureate V. Ramakrishnan) contributed to the success of a 10-day school for Masters and PhD students and a 6-day school designed for students with expertise. The school was supported by an Erasmus Intensive Programme grant to a consortium of 9 European Universities and provided students with 3 ECTS credits. The successful request of sponsorship to the IUCr was supported by CIMS.

(3) M. Nespolo and S. Krivovichev represented CIMS on the International Advisory Board of the 2014 Meeting of the International Mineralogical Association, Gauteng, South Africa, 1–5 September 2014, where CIMS was in charge of the session Modular Aspects of Mineral Structures in the theme Mineralogical Crystallography.

(4) J. Rocha was a member of the Organizing Committee of SMARTER4, Durham University, UK, 1–4 September 2014 (<http://www CCPNC.ac.uk/smarter4/>).

(5) Joint IUCr MaThCryst–CIMS Workshop: D. Pandey was workshop coordinator, M. Nespolo and J. Rocha were members of the International Programme Committee of the Workshop on Symmetry Relationships Between Crystal Structures with Application to Structural Phase Transitions, Varanasi, India, 27–31 October, 2014 (Dhananjai Pandey, Massimo Nespolo, Mois Aroyo and Juan Carvazal were lecturers) (<http://iitbhu.ac.in/conferences/mst/IUCr/>).

(6) G. Ferraris and R. Oberti were members of the Scientific Committees for the organization of two meetings celebrating IYCr2014 in Italy: (i) Impact of Crystallography on Modern Science was organized by the Accademia delle Scienze di Torino and held in Torino, Italy, 25 June 2014; a talk was given by Robert Hubert, Nobel laureate 1988 (*Beauty and Fitness for Purpose, the Architecture of Proteins, the Building Blocks of Life*). R. Oberti gave a talk on the impact of crystallography and crystal-chemistry on petrology and geochemistry. (ii) Challenges in Crystallography was organized by the Accademia Nazionale dei Lincei, and held in Rome, Italy, 13–14 October 2014. The CIMS Chair, J. Rocha, gave an invited talk.

(7) O. Yakubovich was a member of the Organizing Committee of the XVIII International Conference on Crystal Chemistry, X-ray Diffraction and Spectroscopic Studies of Minerals, Ekaterinburg, Russia, 2014.

(8) R. Oberti was a member of the Scientific Committee of the 8th European Conference on Mineralogy and Spectroscopy, Rome, Italy, 9–11 September 2015, at the headquarters of CNR, the National Research Council ([www.ecms2015.eu](http://www.ecms2015.eu)). There were 120 attendees and Plenary talks by Frank C. Hawthorne (University of Manitoba, Canada), Laurence Galois (Université Pierre et Marie Curie, Paris, France), Robert D. Shannon (University of Colorado, USA), Giancarlo Della Ventura (Università Roma TRE, Rome, Italy), Bjorn Winkler (University of Frankfurt, Germany) and Catherine McCammon (University of Bayreuth, Germany). The scientific programme focused on the interplay between short-range and long-range information to account for the stability and physical properties of crystalline and amorphous materials.

(9) O. Yakubovich was a member of the Programme Committee of the 29th European Crystallographic Meeting held in Rovinj, Croatia, August 2015. J. Rocha and O. Yakubovich gave invited talks at this event.

(10) C. Ling was Chair of the Organizing Committee of the 2nd Asia–Oceania Conference on Neutron Scattering (AOCNS-2015), Sydney, Australia, 19–23 July 2015 (<http://aocns-2015.com>).

(11) C. Ling was a member of the Organizing Committee for Crystal-30 (<http://crystal30.com>), the 30th meeting of the Society of Crystallographers in Australia and New Zealand, Hobart, Australia, 29 March – 1 April 2016.

(12) G. Ferraris organized the international meeting Mineral Phases and Synthetic Analogues in Earth and Materials Science at the Accademia dei Lincei, Rome, 13–14 June 2016, and João Rocha delivered one of the 12 invited lectures.

(13) R. Oberti was a member of the Scientific Committee of the 2nd European Mineralogical Conference, Rimini, Italy, 11–15 September 2016 (<http://emc2016.socminpet.it/>). Sergey Krivovichev was also a member of the Scientific Committee. 28 scientific sessions discussed cutting-edge aspects of mineral sciences, and structure-based approaches played a major role. One of the six Plenary Lectures was delivered by Karen Appel (European XFEL Hamburg) and was dedicated to the exciting perspectives provided to Earth sciences, and in particular to the study of mineral reactions, by XFEL techniques. The 2016

school of the Associazione Italiana di Cristallografia on Polymorphism, Stability and Phase Transitions in Crystals: Theory, Experiments, Applications (with international audience and lecturers) was held as a satellite meeting (Rimini, Italy, 7–11 September) and received support from the IUCr (via CIMS sponsorship).

(14) J. Rocha was on the Organizing Committee of the 5th SMARTER 5 meeting in Bayreuth, Germany, for the first time a satellite meeting of the (30th) Meeting of the European Crystallographic Association (<http://www.smarter5.uni-bayreuth.de/de/index.html>). This event is now promoted jointly by CIMS and the Commission on NMR Crystallography and Related Methods.

(15) O. Yakubovich was an invited speaker at the VII Russian school for young scientists: Experimental Mineralogy, Petrology and Geochemistry, Chernogolovka, Russia, 20–21 October, 2016. She also gave an oral presentation at the 1st Russian Crystallographic Congress, Moscow, Russia, 21–26 November 2016.

#### *Co-organization of 2017 meetings*

(1) CIMS has been involved in the preparation of the Hyderabad Congress. In particular, CIMS members and consultants are chairing the Microsymposia: (i) MS7 Topology and Symmetry of Modular Structures (I. Pignatelli, S. V. Krivovichev); (ii) MS52 Minerals/Gems in Industrial Applications (P. Mercier). M. Nespolo will give the Keynote Lecture *Crystal Rationale for the Formation of Twinned Crystals*.

(2) P. Mercier is a member of the Programme Committee for the 2017 IUCr Crystallographic Computing School, Bangalore, India, 15–20 August 2017.

(3) R. Oberti is a member of the Scientific Committee of the 2017 EMU School on Mineral Fibers: Crystal-Chemistry, Chemical-Physical Properties, Biological Interactions and Toxicity, Modena, Italy, 19–23 June 2017 (<http://emu2017.unimore.it>). Among the different aspects relevant to the topic, lessons and tutorials will also discuss both the present knowledge on the relations between structure, surface properties and activity of mineral fibers, and the advantages and limits of the most suitable experimental methods, among which are crystallography and spectroscopies. The school received support from the IUCr after CIMS sponsorship.

#### *CIMS support of applications for financial funding by the IUCr, or ‘moral’ support*

(1) First European Crystallographic School (ECS), Pavia, Italy, 26 August – 6 September 2014, to celebrate the International Year of Crystallography.

(2) 8th USPEX Workshop – Computational Materials Discovery Using the USPEX Code, Shiv Nadar University, India, 20–24 January 2015, promoted by Artem O. Oganov; D. Pandey gave the opening lecture.

(3) 8th European Conference on Mineralogy and Spectroscopy, Rome, Italy, 9 September 2015, promoted by R. Oberti (Scientific Committee).

(4) 11th USPEX Workshop – Evolutionary and Interpretation Methods for Discovering the Structures and Rationalizing the Properties of Crystalline, Surface and Nanoparticles Materials, Varenna, Lake Como, Italy, 5–9 June 2016.

(5) Workshop on Crystallography for Space Sciences, Instituto Nacional de Astrofísica Óptica y Electrónica, Puebla, Mexico, 17–30 April 2016.

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

(7) First Pan-African Meeting on Crystallography, Dschang, Cameroon, 6–11 October 2016.

*J. Rocha, Chair*

#### A6.14. Commission on Magnetic Structures

At the Commission meeting in Montreal, it was decided that in the coming term, Wieslawa Sikora would serve as Secretary of the Commission, Danny Litvin would serve as liaison to the Commission on Crystallographic Nomenclature, Maria-Teresa Fernandez-Diaz would continue to serve as liaison to the Commission on Neutron Scattering, Taku Sato would manage the Commission web resources, and Alexander Pirogov would lead the effort to contribute entries relevant to magnetic structure to the IUCr's online *Dictionary of Crystallography*. We congratulate Wieslawa Sikora for her recent retirement and Vaclav Petricek for receiving the European Crystallographic Association's Perutz Prize in 2016.

In addition to the in-person Commission meeting in Montreal, Canada, 9 August 2014 annual or biennial meetings of the Commission spanning 16 time zones have been conducted once or twice each year via internet-video: 11 February 2014, 24 November 2015, 8 February 2016, 13 October 2016.

The extensive efforts of Commission members and consultants to plan, organize, advertise, attend, and present at the Montreal Congress made it a hugely successful venue for the magnetic-structure community. Wieslawa Sikora (AGH University of Science and Technology, Poland), the Commission's representative to the Congress IPC, helped to secure a scientific programme that included 14 directly relevant Keynote addresses and Microsymposia, 8 of which were co-sponsored by the Commission, and nearly all of which were supported in some way (e.g. organizer, Chair, presenter, etc.) by Commission members. These sessions were well attended (completely full in some cases), and the presentation quality was generally very high:

*Multiferroics*, Keynote Lecture by Tsuyoshi Kimura.

Small-Angle Scattering for Magnetism and Magnetic Structures, chaired by Joachim Kohlbrecher and Andreas Michels.

Magneto-Structural Relationships in Molecular Compounds, chaired by Andrea Cornea and Barbara Sieklucka.

Commensurate and Incommensurate Multiferroics and Magnetoelectrics: Structure and Properties, chaired by Radoslaw Przenioslo and Hiroyuki Kimura.

*Commensurate and Incommensurate Multiferroics: Structure and Properties*, Keynote Lecture by Laurent Chapon.

Symmetry Constraints in Magnetic Structure Determination: Experiment and Theory, chaired by Branton Campbell and Mois Aroyo.

Electronic and Magnetic Phenomena at Extreme Conditions, chaired by Karen Friese and Karel Prokes.

*The Expanding Scope of Crystallographic Representation Analysis*, Keynote Lecture by Branton Campbell.

*Sixty-Five Years of Magnetic Structures: Present and Future of Magnetic Crystallography*, Keynote Lecture by Juan Rodriguez-Carvajal.

Cross-Disciplinary Investigations of Structural and Magnetic Properties of Materials by Solid-State NMR and Diffraction Techniques, chaired by J. M. Gillet and Francis Taulelle.

Pushing the Boundaries of Aperiodic Magnetic and Crystal Structure Solution, chaired by Vaclav Petricek and Walter Steurer.

Structural, Electronic and Magnetic Ordering: From Fundamental Physics to Functionality, chaired by Yuichi Shimakawa and Paul Attfield.

X-ray, Muon and Neutron Studies of Magnetic Structure in Materials, chaired by Youichi Murakami and Oksana Zaharko.

Frustration, Topology and Chirality in Metals and Complex Oxides, chaired by Taku Sato and Laurent Chapon.

Taku Sato (Tohoku University, Japan), the Commission representative to the Hyderabad Congress IPC, travelled to Hyderabad in March 2016 to negotiate the programme for the upcoming Congress, and was similarly successful. We anticipate 13

sessions at the Hyderabad Congress with strong magnetic-structure themes, 9 of which were either sponsored or co-sponsored by the Commission.

The Commission continues actively to discuss three common methods of describing a magnetic structure: the commensurate-supercell description, the incommensurate-wave description (also known as the propagation-vector description), and the representational (group-theoretical) description. Each description type has a distinct parameter set, which if treated in a fully general way can be converted into any of the other descriptions. And each description can be executed with or without taking magnetic symmetry into account. The new magCIF dictionary developed primarily by Commission members has been the principle arena for forging consensus on magnetic-structure descriptions since the Commission was formed in 2011.

During the past three years, Commission members in the magCIF working group (Branton, Manu, Vaclav, Juan, Wieslawa) generated numerous revisions to the prototype dictionary, including (1) the addition of support for incommensurate structures, which had been negotiated during the previous year, (2) improvements to entries involving Opechowski-Guccione (OG) and Belov-Neronova-Smirnova (BNS) settings of commensurate magnetic space groups, (3) changes to entries that describe commensurate and incommensurate setting transformations, (4) the use of magnetic propagation vectors within descriptions that employ OG-settings, (5) entries supporting the definition of a parent-structure, (6) symmetry constraints on structural parameters, and (7) many more minor changes. Some of these issues involved lengthy debates and discussions. The collaboration with the COMCIFS Chair, James Hester, to convert our custom-markup version of magCIF into a proper DDLm dictionary began in earnest in March 2016. This process required some significant and even painful changes to the planned tag structures in the dictionary, as a prototype tag set was already in use by several widely used software packages. The new dictionary was submitted to COMCIFS for review in September and was approved on 31 October 2016. Preparations to take the dictionary online require some infrastructure development, but will hopefully be complete before the upcoming Hyderabad Congress. The magCIF format is already employed by a number of software packages and tools, including *FullProf*, *JANA*, the Bilbao Crystallographic Server, the *ISOTROPY* suite, *Vesta*, *JMol*, and others. Ideally, all magnetism-capable structural-analysis packages should be able to exchange final-version magCIF files. Assignments to coordinate with a variety of software developers were delegated to working-group members.

The MAGNDATA database of magnetic structures hosted by the Bilbao Crystallographic Server team now contains over 400 published commensurate and incommensurate structures, each of which is unambiguously presented with magnetic space-group or superspace-group symmetry in the magCIF format, and ready to be visualized immediately and/or exported to a variety of other software packages. This effort builds upon the well known work of Sikora and Oles. See Gallego *et al.* [(2016), *J. Appl. Cryst.* **49**, 1750–1776 and 1941–956] for recent articles on the progress of the MAGNDATA project.

To celebrate the International Year of Crystallography, the Commission conducted a three-day workshop on The Role of Magnetic Symmetry in the Description and Determination of Magnetic Structures (<http://magcryst.org/meetings/cmsworkshop2014>) at the Brockhouse Institute for Materials Research at McMaster University, Hamilton, Canada, 14–16 August 2014. This satellite meeting of the Montreal Congress had 46 participants (including 8 presenters) from 29 institutions from 15 countries and 6 continents (Argentina, Australia, Belgium, Canada, Czech Republic, France, Germany, India, Norway, South Korea, Spain, Sweden, Switzerland, UK, USA). The workshop combined the practical aspects of magnetic structural analysis (e.g. analytical software tools and neutron scattering instruments) with the theoretical foundations of magnetic crystallography (e.g. magnetic symmetry groups, tensor properties, and matrix representations). Hands-on tutorials emphasized new magnetic-structure capabilities of the *JANA*, *FullProf*, *TOPAS*, Bilbao Crystallographic Server, and *ISOTROPY* Suite tools and resources. Lectures demonstrated the application of these novel capabilities to a variety of interesting structures.

A one-week workshop on New Trends in Magnetic Structure Determination at the Institute Laue–Langevin, Grenoble, France, 12–16 December 2016 (<https://indico.ill.fr/indico/event/53/overview>) was sponsored by the Commission, which highlighted the magCIF format and other new infrastructure for magnetic-structure descriptions developed by the Commission during the past five years. The meeting was organized by Juan Rodriguez Carvajal and Oscar Fabelo, and generously supported by the ILL. Lectures and tutorials were given by Laurent Chapon and Juan Rodriguez-Carvajal (*FullProf*), Vaclav Petricek (*JANA*), J. Manuel Perez Mato (Bilbao Crystallographic Server), and Harold Stokes and Branton Campbell (*ISOTROPY* Suite). Of the 60 applicants, 40 were selected to attend. Most participants were accomplished magnetic neutron scatterers aiming to stay abreast of recent developments. The focus of the meeting was on new software capabilities for treating magnetic space-group and superspace-group symmetry, magnetic representation analysis, fully general magnetic structures, and incommensurate magnetic modulations. An underlying theme throughout the workshop was the use of the new magCIF format for

communicating magnetic-structure information between a variety of structure-analysis programs, visualization packages, and data resources.

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

Tentative future plans and interests of the Commission include the following:

- (1) Expand efforts to educate the crystallographic and broader structural-science communities in the art of unambiguously and concisely describing a magnetic structure.
- (2) Promote the widespread adoption of the magCIF standard amongst crystallographic software developers.
- (3) Extend magCIF to support magnetic structure factors, magnetic reflection conditions, low-dimensional magnetic order, short-range magnetic order, etc. Possibly support rotational moments in parallel with magnetic moments, both of which are axial vectors.
- (4) Support the development of tools that convert between OG and BNS presentations of a commensurate magnetic-structure (in magCIF format), and between commensurate-supercell and incommensurate-wave descriptions of a commensurate magnetic structure.
- (5) Explore the possibility of a new standard for magnetic-space-group symbols.
- (6) Develop a representation-analysis CIF dictionary that provides for the complete description of a magnetic or non-magnetic structure in terms of basis functions of irreducible representations of a relevant higher-symmetry parent structure.
- (7) Debate long-term strategies for supporting and preserving computational tools and data resources relevant to the determination and communication of magnetic structures.
- (8) Prepare a new volume of the *International Tables for Crystallography* that focuses on magnetic symmetry, magnetic diffraction, and magnetic structures.

B. Campbell, Chair

#### A6.15. Commission on Mathematical and Theoretical Crystallography

Following the recommendation of the Executive Committee and to encourage greater participation of individual members within Commissions, members were assigned to different aspects of the work of the Commission: M.L. De Las Peñas accepted to serve as a Secretary of MaThCryst; M. Aroyo as liaison to the Commissions on International Tables, Crystallographic Nomenclature, and Magnetic Structures; J. Hadermann as liaison to the Commissions on Electron Crystallography and Aperiodic Crystals, and also to the ECA (being a member of its Executive Committee); L. Suescun as liaison to the Commission on Crystallographic Teaching and LACA; E. Esteves as liaison to LACA; K. Momma as liaison to AsCA; G. McColm as liaison to AMS and SIAM; M. Nespolo as liaison to the Commission on Inorganic and Mineral Structures; D. Litvin as liaison to the Commission on Magnetic Structures.

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

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

## (I) Educational and scientific activities

## (A) International schools

During the triennium MaThCryst continued with the support and organization of international schools following the idea of the importance of improving the teaching of fundamental aspects of crystallography, especially to graduate students and young researchers in countries where nowadays the subject is overlooked in common University courses. This mission is accomplished through a series of schools and meetings in a wide range of regions. We should greatly acknowledge the constant IUCr financial support (as grants for young participants and Visiting Professorships) that was essential for the successful organization of the events. Details on the programmes of the different educational events, didactic material, photos, etc. are available at the web site of the Commission.

(1) MaThCryst Schools in Latin America. The series of MaThCryst schools in Latin America (International School on Fundamental Crystallography) started ten years ago at the University of Havana, Cuba (2007), followed by Montevideo, Uruguay (2010) and Uberlandia, Brazil (2012), and over the years these biennial schools have turned into an essential educational event for students interested in crystallography from all over Latin America. Two such schools took place during the triennial period:

(i) The IV MaThCryst School in Latin America was held in La Plata, Argentina, 27 April – 3 May 2014 (MaThCryst coordinators: E. Esteves and L. Suescun). The 37 selected participants (from more than 80 applications) including post-docs, PhD and MSc students, came from Universities and research centres in Argentina, Bolivia, Brazil, Colombia, Costa Rica, Mexico, Peru, Uruguay and USA.

(ii) The V MaThCryst School in Latin America, was held in Havana, Cuba, 30 October – 5 November 2016: MaThCryst coordinator and local organizer E. Esteves. The school was held at the University of Havana and gathered around 35 students from Cuba, Uruguay, Argentina, Costa Rica, Mexico, Puerto Rico, Brazil, Colombia and Ecuador. On the last day, a workshop on nanocrystallography took place.

(2) Series of International Scientific Schools in Samara (Russia) on topological methods in material science. The schools have been organized since 2008 on a yearly basis by the Samara State University, Samara Center for Theoretical Materials Science and MaThCryst with MaThCryst Coordinators D. Proserpio and V. Blatov.

(i) The School on Topological Methods for Expert Systems in Materials Science was held in Samara, 12–16 August 2014. Twenty young researchers and professors from Russia, Poland, Brazil, India, China and Saudi Arabia participated in the school. The school programme included lectures and practical training applying the *TOPOS* software package.

(ii) The 2015 School on Combined Topological and DFT Methods for Prediction of New Materials was held 15–20 September. The school gathered together 20 postgraduate students and young researchers from Russia, Germany, Italy, UK, India, South Korea and Vietnam. Materials from the meeting may be found at [http://english.sctms.ru/novosti\\_centra/nc\\_20151005\\_01/](http://english.sctms.ru/novosti_centra/nc_20151005_01/).

(iii) The 2016 school (held 4–10 July) continued the series of educational activities of the Samara Center for Theoretical Materials Science started in 2008. It was an intensive training course on the computer package *ToposPro* and related topological and quantum methods. Among the 45 participants (16 were from Brazil, Switzerland, Germany, Spain, UK, Italy, India, Nepal, Vietnam, etc.), there were graduate and postgraduate students, as well as scientists – active users of *ToposPro*.

(3) Training courses on symmetry and group theory in Japan. On the occasion of the International Year of Crystallography, the initiative of proposing a training course in symmetry and group theory in Japan was launched in August 2014 by the Photon Factory, co-sponsored by the Crystallographic Society of Japan; the MaThCryst coordinator and lecturer was M. Nespolo. The unexpected success (the maximal number of participants was reached in a few hours after the opening of the registration), has prompted the organizers and sponsors to repeat it and eventually transform it into a regular event, running twice a year, with the Crystallographic Society of Japan as one of the main organizers. Since 2017 the training courses have formed part of the curriculum of the Graduate University for Advanced Studies in Japan, and participants could receive the corresponding credits after passing a written examination.

In 2015 the training course was held twice, in March in Tsukuba, and in August in Osaka. Both events were again sold out in a few hours. Despite a very intensive programme (lectures from 9 a.m. to 7 p.m., with additional question and answer sessions

after dinner), participants enthusiastically took part in all the lectures and practical exercises. At the end of the course, they received a certificate of attendance. Photographs are available at the IUCr gallery web site.

The fourth training course on symmetry and group theory was held 7–11 March 2016 (Tsukuba), and the First Advanced training course on symmetry and group theory, 1–5 August 2016 (Tsukuba). The fourth basic course was attended by 43 participants coming from various places in Japan while the first advanced training course, restricted to those who had attended and completed the basic course, was attended by 30 participants. The lectures were given in Japanese by M. Nespolo. A series of articles is now being published by the *Journal of the Crystallographic Society of Japan* based on the content of the basic course.

(4) The second South African School on Fundamental Crystallography was held in Bloemfontein, South Africa, 25–29 August 2014 (MaThCryst coordinators: M. Nespolo and M.I. Aroyo). The second school organized by the Commission in Bloemfontein was also run as a satellite meeting of the 21st Congress of the International Mineralogical Union. The school was attended by 36 participants from 9 different institutions and six countries.

(5) The Second International PhD School on Geometry and Topology of Liquid Crystals and Related Ordered Materials was held at RMIT University in Melbourne, Australia, 12–16 August 2014 (MaThCryst Coordinator: S. Hyde). The school was an intense five-day immersion in newer aspects of (mainly) two-dimensional (generalized) crystallography and structure, focusing on nets and tilings, surface topology and differential geometry, orbifolds, and point, plane (wallpaper) and hyperbolic discrete groups. Eleven students, mainly materials scientists, ranging from PhD students to mature researchers from Australia and Europe, attended the school.

(6) The Second Balkan School on Fundamental Crystallography and Workshop on Magnetic Symmetry and its Application in Magnetic Structure Descriptions was held at the Institute of Theoretical and Applied Physics, Istanbul, Turkey, 13–19 July 2015 (MaThCryst Coordinator: M. I. Aroyo) and organized as a follow-up to the International School on Fundamental Crystallography held in Gjulechitza, Bulgaria, in 2013. There were a total of 32 applicants coming from Turkey, Bulgaria, People's Republic of China, Spain, Romania, Switzerland, Russia and Japan.

(7) The International School on Fundamental Crystallography with Applications to Electron Crystallography was held at the University of Antwerp, Belgium, 27 June – 2 July 2016 (MaThCryst coordinator and local organizer: J. Hadermann). The school was attended by 38 participants from 21 nations, of which 30 were under the age of 30. Apart from MaThCryst, the school was also supported by the ECA Special Interest Group on Electron Crystallography. Material and organizational support was also provided by the University of Antwerp and, in particular, the Antwerp Summer University.

(8) The School on Polymorphism, Stability and Phase Transitions in Crystals: Theory, Experiments and Applications, was held in Rimini, Italy, 7–11 September 2016 (MaThCryst coordinator: Mois I. Aroyo). The school was organized by the Commission on Crystallographic Teaching of the Italian Crystallographic Association (AIC) in partnership with MaThCryst and the Italian Society for Mineralogy and Petrology (SIMP). It was organized as a satellite event of the European Mineralogical Conference 2016. The school was attended by 42 students from 14 countries (Albania, Algeria, Brazil, France, Germany, Israel, Italy, Netherlands, Russia, Spain, Tunisia, Turkey, Uzbekistan, USA; over 60% from outside Italy) with different scientific backgrounds (chemistry, mineralogy, material sciences, biology, pharmaceutical sciences). The scientific programme of the school addressed various aspects of crystallographic analysis of polymorphism and structural phase transitions in inorganic, organic and hybrid compounds, with molecular or extended structures.

#### (B) Workshops, courses and meetings

In the triennium the Commission continued actively to promote mathematical and theoretical crystallography by organizing, supporting and promoting worldwide scientific events as workshops and meetings. The main scientific activities can be summarized as follows:

(1) Montreal Congress. All the activities of MathCryst during 2014 were dedicated to the celebration and promotion of the International Year of Crystallography with our active participation in the Montreal Congress as a central event. M. Nespolo was the representative of MaThCryst in the International Programme Committee. MaThCryst organized one Keynote Lecture (KN13 *Mathematical Crystallography in the 21st Century*, M. Senechal, Smith College, USA), suggested two Microsymposia [MS72 Methods, Algorithms and Software for Powder Diffraction (co-Chairs R. Oishi-Tomiya, J. Wright) and MS95

Symmetry and its Generalizations in Science and Art (co-Chairs M.L. De las Peñas, E. Makovicky)] and co-organized four Microsymposia proposed by other Commissions [MS1 Phase Transitions in Functional Inorganic Materials and Minerals (co-Chairs P. Thomas, K. Sugiyama); MS33 Symmetry Constraints in Magnetic Structure Determination: Experiment and Theory (co-Chairs B. Campbell, M.I. Aroyo); MS34 Crystals and Beyond (co-Chairs S.I. Ben-Abraham, J.-Y. Lee) and MS42 Diffuse Scattering and Partial Disorder in Complex Structures (co-Chairs R. Welberry, M. de Boissieu)].

Together with the Commission on Magnetic Structures, MaThCryst co-organized a satellite workshop of the Montreal Congress on The Role of Magnetic Symmetry in the Description and Determination of Magnetic Structures at the Brockhouse Institute for Materials Research at McMaster University, Hamilton, Canada, 14–16 August 2014. The workshop was attended by 46 participants (including 8 presenters) from 29 institutions in 15 countries (Argentina, Australia, Belgium, Canada, Czech Republic, France, Germany, India, Norway, South Korea, Spain, Sweden, Switzerland, UK, USA). The main subjects of the workshop programme include practical aspects of magnetic structural analysis combined with the theoretical foundations of magnetic crystallography. Hands-on tutorials emphasized new magnetic-structure capabilities of the *JANA*, *Fullprof*, *TOPAS*, Bilbao Crystallographic Server and *ISOTROPY* Suite computer tools and resources.

(2) Workshop on Symmetry Relationships Between Crystal Structures with Application to Structural Phase Transitions, Varanasi, India, 27–31 October 2014. The workshop was successfully organized in cooperation with the Commission on Inorganic and Mineral Structures. D. Pandey was the main local organizer and also the MaThCryst Coordinator. About 40 participants (apart from the lecturers and organizers) attended the workshop. The lectures, which included topics on crystallographic groups and applications in structural and magnetic phase transitions, were accompanied by online training using the Bilbao Crystallographic Server and practical exercises on refinement of magnetic and nuclear structures using the *FullProf* Suite.

(3) Spring Eastern Sectional Meeting of the American Mathematical Society, University of Maryland, Baltimore, USA, 29–30 March 2014 (MaThCryst Coordinator: G. McColm). Three special sessions on Discrete Geometry in Crystallography were co-organized by the Commission. Among the different lectures treating various aspects of mathematical crystallography, one should highlight the excellent contributions of three members of MaThCryst: M. Nespolo – on pseudosymmetry analysis and its applications in twin studies; B. Souvignier – on relations between icosahedral polytypes induced by group ring elements; and G. McColm – on generation of crystal nets in Euclidean space.

(4) The Samara Center for Theoretical Materials Science held the IUPAC project meeting and workshop Topology Representations in Coordination Networks, Metal-Organic Frameworks and Other Crystalline Materials, Samara, Russia, 21–23 May 2015 (MaThCryst coordinators: D. Proserpio and V. Blatov). Co-organizers of the meeting were the International Union of Pure and Applied Chemistry (IUPAC), the International Union of Crystallography, Samara State University and Chalmers University of Technology (Sweden). Task-group members of IUPAC from all over the world (Sweden, Italy, Russia, USA, Brazil, Australia, Republic of Korea, Republic of South Africa) took part in the meeting. Apart from the main organizers of the event, D. Proserpio and V. Blatov, MaThCryst was represented by S. Hyde and J.-G. Eon.

(5) SIAM Conference on Mathematical Aspects of Material Science, Philadelphia, USA, 8–12 May 2016; G. McColm was MaThCryst coordinator and local co-organizer (together with J.-G. Eon, M. Krajcevski and M. Senechal). The four MaThCryst Minisymposia on Tilings, Packings, Graphs, and Other Discrete Models, on Polyhedra, Cluster Models, and Assembly, on Groups, Lattices, Spaces and Superspaces, and Beyond Crystallography had sixteen speakers from seven nations.

## (II) Publishing activities

(1) Members and consultants of the Commission have contributed actively to different IUCr publishing activities:

(i) Special Issue of *Acta A* (published in December 2014 with Guest Editors M. Nespolo and G. McColm): this is the second Special Issue on mathematical crystallography whose articles form a wide but necessarily incomplete selection from the panorama of research activities in the field. Some of the articles are based on work that was reported at the 2013 SIAM Conference on Mathematical Aspects of Materials Science in Philadelphia.

(ii) The 6th Edition of *International Tables for Crystallography*, Volume A, *Space-Group Symmetry*, published in 2016 (print and online): M.I. Aroyo (Editor); B. Souvignier (chapters on general introduction to group theory, on space-group symmetry, on space groups and their descriptions); K. Momma (generation of the general-position diagrams for cubic space groups,

chapter on computer preparation of Volume A); E. Koch (chapters on lattice complexes of space groups and space-group normalizers); D. Litvin (chapters on special topics of space groups, and magnetic subperiodic groups and magnetic space groups).

(iii) Editors of IUCr journals: M. Nespolo (Book Review Editor for all IUCr journals); J.-G. Eon (Co-editor of *Acta A*), D. Pandey (Co-editor of *JAC*).

(2) Special Issue of *Zeitschrift für Kristallographie* (published in December 2015 with Guest Editors: M. Nespolo and M.I. Aroyo) devoted to the recent developments and the current state of art in the field of mathematical and theoretical crystallography. The issue includes articles by members and consultants of the Commission: G. McColm's contribution focuses on the generation of periodic graphs for crystal design, M. Tanemura and T. Matsumoto disclose the fascinating world of ellipses and their closest packing while in the contribution by M. Loquias and P. Zeiner the idea of colour symmetry, originally defined for symmetry of lattices, is extended to the analysis of coincidence site lattices. The Special Issue was dedicated to the memory of H. Wondratschek.

### *(III) Near-future activities*

The planned activities of MaThCryst for 2017 include:

(i) active participation of the Commission in the Hyderabad Congress. Thanks to the hard work and very successful and efficient negotiations of L. Suescun, as our MaThCryst representative at the International Programme Committee, the Commission is responsible for a Keynote Lecture and two Microsymposia (MS35 Crystal-Structure Relationships and Their Applications and MS26 A Bridge Between Two Worlds: Graphs as Standard Descriptors), and will co-share the organization with other Commissions of five Microsymposia. Further, the Commission is the organizer of a satellite event of the Congress, namely the International School on Fundamental Crystallography and Workshop on Structural Phase Transitions, Rourkela, India, 30 August – 4 September 2017 (MaThCryst coordinator: M.I. Aroyo, local organizer: D. Pradhan);

(ii) The Second Philippine Workshop on Mathematical Crystallography will take place in Manila, Philippines, 20–25 May 2017; L. de la Peñas will act as the main local organizer and MathCryst coordinator;

(iii) Shanghai International Crystallographic School working with Bilbao Crystallographic Server, Shanghai University, 11–17 June 2017 (MaThCryst coordinator M.I. Aroyo; local organizers: A. Stroppa and Wei Ren);

(iv) International Autumn School on Fundamental and Electron Crystallography, Sofia, Bulgaria, 8–13 October 2017 (MaThCryst coordinators: J. Hadermann and M.I. Aroyo; local organizer: D. Karashanova);

(v) Training Course on Symmetry and Group Theory (ongoing series in Japan); fifth course 6–10 March 2017, sixth course 31 July – 4 August 2017, both at KEK Tsukuba (MaThCryst coordinator and lecturer: M. Nespolo).

*M. I. Aroyo, Chair*

## A6.16. Commission on Neutron Scattering

The Commission 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. Notable developments in these areas over the period 2014–2016 include: ongoing construction of

the European Spallation Source in Sweden, which is projected to produce the first neutrons in 2019, and the Chinese Spallation Neutron Source, which is expected to be operational in 2018; operation of the Spallation Neutron Source in the USA at a world-record level of 1.4 MW and progress toward a major upgrade of the power capability of the accelerator complex to 2.8 MW; the continued progress at the spallation neutron source at the Japan Proton Accelerator Research Complex (J-PARC) toward operation at 1 MW and progress toward obtaining the authorization to restart the Japan Research Reactor, perhaps as early as 2018. Further, several new neutron scattering instruments were brought into user programmes at facilities across the world.

One major event in Australasia in 2016 was the ‘Bragg Institute’ at the Australian Nuclear Science and Technology Organization (ANSTO) being renamed the ‘Australian Centre for Neutron Scattering’. As part of an ongoing restructure of the research side of ANSTO, emphasis has moved away from the former institute model to a structure that distinguishes the rich instrumental capability on the one side and the internally driven research with a nuclear focus on the other. This research should make considerable use of the extensive ANSTO research infrastructure. It was with mixed feelings that the neutron scattering group relinquished the Bragg name, but the new titles of the infrastructure ‘platforms’ do reflect more explicitly their capabilities on a global scale, and plans are afoot for the Bragg name to be associated with another entity at ANSTO that is equally worthy of the title. A major event in the USA was a reduction in the scope of the user programme at the Lujan Center for Neutron Scattering, which has been highly productive over the past couple of decades.

Commission members were also involved in organizing several meetings, including the Montreal Congress and various annual meetings of regional crystallographic associations. Notable neutron conferences include: the American Conference on Neutron Scattering which was held in Knoxville (USA) in 2014 and Long Beach (USA) in 2016, and which is sponsored by the Neutron Scattering Society of America; the Asia–Oceania Conference on Neutron Scattering, which was held in Sydney (Australia) in 2015, and which was hosted by the Asia–Oceania Neutron Scattering Association (AONSA) and sponsored by ANSTO; the European Conference on Neutron Scattering which was held in Zaragoza (Spain) in 2015 (the International Union of Crystallography provided partial financial support for students who attended the conference working in neutron crystallography); the inaugural Gordon Research Conference on Neutron Scattering, which is a new series featuring several world-leading neutron scattering scientists, took place in Hong Kong in 2016; the triennial International Symposium on Diffraction Structural Biology, which was held in Knoxville (USA) in 2016; a conference on Neutron Scattering organized at Bhabha Atomic Research Centre at Mumbai (India) in 2016. Neutron scattering was well represented in various regional meetings and conferences.

Several neutron schools were supported by Commission members, including: the AONSA Neutron School held in Japan, Indonesia and India (this school was canceled in 2011 and in 2013 owing to the accident at the Hadron Experimental Hall in J-PARC); the Oxford School on Neutron Scattering in the UK; the Paul Scherrer Institute (PSI) Summer School on Condensed Matter Research at PSI in Switzerland; the Inelastic Neutron Scattering School at ANSTO, Australia; the National School on Neutron and X-ray Scattering, jointly organized by Argonne and Oak Ridge National Laboratories, USA; the annual Center for High Resolution Neutron Scattering Summer School on Neutron Scattering, NIST Center for Neutron Research, USA; the Biennial Meeting of the Spanish Neutron Society held in Pamplona (2014) and Bilbao (2016), Spain; the annual Berlin School on Neutron Scattering at Helmholtz-Zentrum Berlin, Germany; the Canadian Neutron Scattering Summer School; and the Neutron and Muon School at J-PARC, Japan.

In addition to schools, numerous workshops were organized by Commission members across a broad range of neutron scattering topics. For example, a Workshop on New Trends in Magnetic Structure Determination was co-organized with the Commission on Magnetic Structures at the Institute Laue–Langevin (France) in 2016. The aim of this workshop was to contribute to training scientists in the treatment of neutron diffraction data for magnetic structure determination with new and improved methods and tools. Dozens of similar workshops hosted by neutron user facilities across the world continue to

engage the research community in identifying emerging scientific challenges and needs that can be best addressed using the unique capabilities of neutron scattering.

P. Langan, Chair

#### A6.17. Commission on NMR Crystallography and Related Methods

The proposal to establish the Commission was formally presented by Professor Francis Taulelle (with support from Rod Wasylishen and Manish Mehta) to the Executive Committee of the IUCr on 1 August 2014, at its meeting in Montreal prior to the triennial Congress. Following a brief discussion, the Executive Committee gave a warm formal approval to the existence of the Commission with an amended title: Commission on NMR Crystallography and Related Methods, to emphasize the inclusion of such techniques as EPS/ESR.

Details of the objectives and activities of the Commission can be found on the IUCr web site at <http://www.iucr.org/iucr/commissions/nmr-crystallography>.

In its first year, the Commission was finding its feet and trying to make its existence known to the general crystallographic and NMR/ESR communities. We had ongoing discussions with *Acta Crystallographica* about the appropriate way to encourage the submission of research papers involving NMR/ESR. The journal has, of course, been reconsidering the contents of its various sections. NMR is now mentioned specifically in the remit of *Acta Crystallographica Section D (Structural Biology)* and is implicitly included for the other IUCr journals (except *Journal of Synchrotron Radiation*). A Special Issue of *Acta Crystallographica Section C* was published in March 2017. We anticipate that several of the journals will appoint a magnetic resonance expert to their editorial boards and the Commission has submitted names of suitable people to the Commission on Journals.

The Commission is encouraging the planning of conferences that address NMR crystallography as a topic. In consequence, the British Radiofrequency Spectroscopy Group devoted its traditional one-day Christmas-time meeting in London on 14 December 2015 to the topic NMR and Crystallography, as discussed with the British Crystallographic Association. The ideas and intentions of the Commission have been presented in talks at several conferences, including some in Poland and the USA. An article on NMR crystallography has been published in *Chemical and Engineering News*.

A series of SMARTER conferences has been instituted on the topic of NMR crystallography, with participants from both the NMR and the diffraction communities. The fourth of this type was held in Durham (UK) in September 2014; these meetings are now sponsored (*inter alia*) by the IUCr. The 5th SMARTER conference was held in Bayreuth, Germany, and was designated as a satellite meeting of the European Crystallographic Meeting. Paul Hodgkinson and Gareth Lloyd organized a session on NMR crystallography at the annual spring meeting of the British Crystallographic Association, held in Nottingham in April 2016. NMR crystallography talks have been included in a number of conferences, for instance in the IX Symposium on NMR in Chemistry, Physics and Biological Sciences, held in Warsaw, Poland, in September 2016, in the meeting of the Canadian Society for Chemistry in Halifax in June 2016, and in the 2016 Rocky Mountain Conference. Solid-state NMR was also involved in a national training course on Modern Methods of Structure Elucidation held in Lisbon, Portugal, in September 2016.

F. Taulelle, Chair

#### A6.18. Commission on Powder Diffraction

The steady stream of requests for meetings sponsorship kept coming in the triennium. Some of these were for the latest in a series, such as the Durham Powder Diffraction School, but a number of other meetings in developing countries, notably in Africa, requested support. It is gratifying to say that support was forthcoming from the Commission (CPD) membership in the majority of cases.

Financial travel restrictions did not permit a CPD meeting in 2015, but the European Powder Diffraction conference in Bari, Italy, in 2016 brought together the majority of the Commission membership. The EPDIC conference is the premier powder

diffraction conference and the standard of the scientific content was very high as always. In a more sombre vein, 2016 also was notable for the passing of Hugo Rietveld shortly before the EPDIC meeting where he was due to give the opening Plenary Lecture. As the pioneer of the technique that bears his name he has impacted powder diffraction and materials analysis immensely, and he will be greatly missed.

As one of the principal EPDIC organizers, CPD member Angela Altomare is to be commended for finding time to attend the CPD meeting in a hectic schedule. A variety of topics were covered at the meeting, ranging from the Hyderabad Congress to desired future activities. A discussion regarding the Rietveld guidelines led to additional time brainstorming a possible extension to PDF analysis with a number of people from central facilities.

There are indications that the long-delayed Volume H of *International Tables* will finally be published in the not-to-distant future. The continuing delays to the Volume have been an ongoing irritant to the powder diffraction community and I shall be relieved to see the labours of many in the community at long last come to fruition.

Unfortunately, ongoing health issues adversely impacted my ability to carry out many of the tasks I wished to accomplish, even medical leave during a recovery period ended up being much less productive than I had hoped. I relinquish the position of CPD chair after three terms at the Hyderabad Congress (unfortunately I am unable to attend myself) and sincerely hope that whoever succeeds me can take the Commission forward with renewed energy.

*P. Whitfield, Chair*

#### A6.19. Commission on Small-Angle Scattering

##### *Meetings and communication*

The majority of Commission (CSAS) members and consultants contribute to each of the various activity categories described below on an ongoing basis. Upon learning the sad news of the passing of our colleague Ritva Serimaa on 12 July 2016, we prepared as a tribute an obituary that was published in the *Journal of Applied Crystallography* (<http://journals.iucr.org/j/issues/2017/01/00/es0424/es0424.pdf>), noting her contributions to science, to small-angle scattering in particular, and as a valued colleague to many.

The work of the Commission members was largely accomplished via e-mail communications, during personal meetings at national and international conferences, and importantly at the triennial Small-Angle Scattering meeting (SAS2015, September 2015, Berlin, Germany), which provided a special opportunity for face-to-face discussions and an open meeting where Jill Trehewella, as CSAS Chair, presented a brief overview of recent CSAS activities. She went on to describe recent developments with regard to structural biology modelling with hybrid data. Dmitri Svergun then presented developments of the extended sasCIF for easy structural biology data exchange, followed by U-Ser Jeng with an update on canSAS activities (canSAS: collective action for nomadic Small Angle Scatterers: an ongoing activity to provide the small-angle scattering user community with shared tools and information, <http://www.cansas.org/>), and Andrew Allen on the NIST SAXS intensity standard. The meeting concluded with a discussion regarding encouraging bids for the 2021 triennial SAS meeting (SAS2021).

We wish to recognize and thank those retiring from the CSAS this year for their many contributions: Vladimir Volkov, Toshiji Kanaya, Jan Skov Pedersen, Yoshiyuki Amemiya, Gernot Kostorz, Bente Vestergaard, and Naoto Yagi. The voluntary work done by the members and consultants of CSAS is very important for the continued growth and health of our science community and a significant pull on an individual's time and effort in what is a very busy professional life.

##### *Commission activities*

CSAS activities in the last triennial period focused on support for the International Year of Crystallography, IYCr2014, the Montreal and Hyderabad Congresses, and the triennial SAS meetings and associated publications. The CSAS also recommended IUCr support for a number of SAS-related meetings.

### IYCr2014 celebrations

CSAS members were active in marking the celebration of IYCr2014 through active involvement in symposia and sessions at conferences held around the world during 2014. For example, Andrew Allen took part in IYCr2014-themed symposia at both the The Metallurgy Society (TMS) Annual meeting in San Diego, CA, USA, in February 2014, and the Materials Research Society (MRS) Fall meeting in Boston, MA, USA, November 2014. Toshiji Kanaya was co-organizer of a Special Seminar on Polymer Crystals in the annual meeting of the Fiber Society, Japan, celebrating IYCr2014 in Tokyo, June 2014, and also gave an invited lecture on SAS dedicated to IYCr2014 at the International Union of Materials Research Societies International Conference in Asia 2014 meeting in Fukuoka, August 2014. Iris Torriani was a co-organizer of a Latin-American Summit Meeting in Brazil on Biological Crystallography and Complementary Methods (<http://pages.cnpem.br/iycr2014-lasummit/organizing-committee/>) and presented a talk on the Latin-American Crystallographic Association (LACA). Additionally, David Babonneau acted as regional representative to serve as a bridge with the French steering committee of IYCr2014.

### IUCr Congress related activities

CSAS members and consultants worked with Elliot Gilbert, the CSAS nominated member of the Montreal Congress International Programme Committee (IPC), to develop a programme that included a Keynote speaker (Takeji Hashimoto) and an unprecedented number of SAS-related Microsymposia, including six dedicated Microsymposia plus three further Microsymposia jointly organized with other Commissions. The Microsymposia ranged over broad areas of interest: SAS of biological macromolecules; SAS for magnetism and magnetic structures; grazing incidence surface techniques; simultaneous methods with SAS; *in operando* and structure evolution – from atomic to micrometre scale; industrial and technological applications of SAS (organized by CSAS members U-Ser Jeng and Ritva Serimaa); and applications of anomalous SAXS. Andrew Allen chaired an open meeting of the Commission to report on CSAS activities over the previous three years and, with incoming Chair Jill Trewella, met the IUCr Executive Committee to provide a verbal report on CSAS activities and recommendations for CSAS membership and consultants.

For the Hyderabad Congress the Commission nominated Kristina Djinovic Carugo for the IPC and she worked collaboratively to recommend a Keynote speaker (Dmitri Svergun), two CSAS-sponsored Microsymposia (SAS data formats, standards and repositories; SAS studies of biomacromolecular kinetics), four shared Microsymposia with other Commissions [Macromolecular Structures by Hybrid Methods (CSAS, CBM, CEM); New Challenges in Interpretation of Structural Data (CSAS, CBM, CEM); Expression of Macromolecular Complexes (CBM, CSAS, CEC); Functional Materials on the Nanoscale (CCM, CAC, CSAS)] and a Joint Workshop (Validation Including Data From MX, SAS, XAFS, EM (CM, CSAS, CAC)].

### Triennial SAS meetings (SAS2012, SAS2015 and SAS2021)

A major event for the international SAS community is the triennial SAS meeting [recently held in Oxford, UK (SAS2009), Sydney, Australia (SAS2012) and Berlin, Germany (SAS2015)], with the next meeting in Traverse City Michigan, USA (SAS2018). The IUCr sponsors the Guinier Prize that is awarded at this meeting and the CSAS is formerly engaged in a number of roles, such as evaluation of bids to host future meetings. Members and consultants also broadly provide strong support for these meetings and associated activities.

The 16th meeting of Small-Angle Scattering, SAS2015, was held in Berlin, October 2015, with Conference co-Chairs Michael Gradzielski and Matthias Ballauff, with Peter Fratzl as Programme Chair ([https://www.helmholtz-berlin.de/events/sas/index\\_en.html](https://www.helmholtz-berlin.de/events/sas/index_en.html)). Daniel Clemens from the Organizing Committee acted as the principle liaison for CSAS and ensured excellent communication and coordination of joint activities. Andrew Allen, Duncan McGillivray, Elliot Gilbert, Jan Skov Pedersen and Jill Trewella served on the International Advisory Board and Dmitri Svergun served on the Scientific Programme Committee. The conference attracted 424 delegates from Europe, Eurasia, Asia and the Americas who submitted 514 abstracts for oral presentations, posters and flash talks across a broad range of topics including the most recent progress in instrumentation and data analysis and their applications in biology and materials science. A special initiative of the CSAS at SAS2015 was led by Elliot Gilbert and U-Ser Jeng who organized a forum on Stimulating Industrial Interactions: Challenges, Barriers and Opportunities for Application of Small-Angle Scattering to Industry.

Following initial publication of papers associated with the SAS2012 Conference (Sydney, Australia) in the *Journal of Applied Crystallography*, 24 were selected for a fully open-access virtual Special Issue edited by Elliot Gilbert and Andrew Allen

(<http://scripts.iucr.org/cgi-bin/paper?me0538>) that was published in Spring 2014, representing the state-of-the-art in the broad SAS field for IYCr2014. This selected publication model was followed for SAS2015 with Andrew Allen and Michael Gradzielski as Guest Main Editors. This Special Issue appeared in November 2016 ([http://journals.iucr.org/special\\_issues/2016/sas2015/](http://journals.iucr.org/special_issues/2016/sas2015/)) and highlighted developments in the field of neutron and X-ray SAS, covering different areas of fundamental and applied research.

The IUCr co-sponsored Guinier Prize was awarded at the SAS2015, on recommendation from a joint CSAS/SAS2015 Committee, to Professor Sow-Hsin Chen for his many contributions to the field of small-angle scattering methods development and applications in fundamental studies of soft condensed matter (see announcements at [https://www.helmholtz-berlin.de/events/sas/awards/index\\_en.html](https://www.helmholtz-berlin.de/events/sas/awards/index_en.html) and [http://www.iucr.org/news/notices/archived/announcements/2014/2015\\_guinier\\_award](http://www.iucr.org/news/notices/archived/announcements/2014/2015_guinier_award)).

The location for successive triennial SAS meetings is chosen by first inviting bids from all interested parties with a set of criteria specified. Bids for SAS2021 were received during 2016 from Campinas (Brazil), Gyeongju (Korea), and Taipei (Taiwan) and were posted on line ([https://www.helmholtz-berlin.de/events/sas/bid/index\\_en.html](https://www.helmholtz-berlin.de/events/sas/bid/index_en.html)) for review by attendees of the conferences who were then polled for their preference. A Bid Evaluation Committee (BEC) of the past and present Meeting Chairs and IUCr CSAS Chairs then considered all bids in the context of the vote of the community and in this case the community preference for SAS2021 to be hosted in Campinas (Brazil) was endorsed by the BEC, who also asked that the bid teams from Gyeongju (Korea) and Taipei (Taiwan) update and re-submit their bids for SAS2024 for a vote at SAS2018, Traverse City, USA. The SAS2021 Conference BEC included: Andrew Allen, Jill Trewella, Elliot Gilbert (SAS2012), Randall E. Winans, Pete Jemian, and Jan Ilavsky (SAS2018), Stephen King and Nick Terrill (SAS2009), Matthias Ballauff and Michael Gradzielski (SAS2015), with Daniel Clemens (SAS2015) coordinating.

#### *Recommendations for IUCr support for SAS-related meetings*

The CSAS evaluated applications and recommended support for a number of SAS-related meetings, including: the 9th AOFSRR Cheiron School, Hyogo, Japan, September 2015; the 4th International Soft Matter Conference, Alpexpo, Grenoble, France, September 2016; the International Summer School To.sca.lake 2017, Como, Italy, May–June, 2017; the 50th Course of the International School of Crystallography, Erice, Italy, 2017, with Integrative Structural Biology a theme for which SAS is highly relevant; the 12th International Conference on Biology and Synchrotron Radiation (BSR12), Stanford, CA, USA, August 2016.

#### *Educational activities*

CSAS members and consultants contributed to and organized a large number of courses, tutorials and lectures to improve awareness of SAS methods and applications, and also to increase the expertise in SAS and its applications broadly.

The European Molecular Biology Organization (EMBO) supported Global Exchange Lecture and Practical Courses are growing in popularity among those aspiring to learn about SAS applications in structural biology. A feature of these is that they generally do not focus exclusively on SAS, rather they put SAS in the context of what have been traditionally more mainstream techniques, including crystallography, NMR and EM, and thus are able to emphasize the complementarity of SAS among the suite of modern structural biology tools. In the last triennial period the following courses have been supported by EMBO with strong input and participation from CSAS members and consultants.

EMBO Global Exchange Lecture Courses; typically with ~15 international lecturers for 50–60 students selected from ~150 applicants:

Structural and Biophysical Methods for Biological Macromolecules in Solution, São Paulo, Brazil, January 2014 (main organizer Dmitri Svergun and main local co-organizer C. Oliveira; Jill Trewella and Bente Vestergaard contributing lecturers).

Structural and Biophysical Methods for Biological Macromolecules in Solution, Taipei, Taiwan, May 2015 (main organizer Dmitri Svergun and U-Ser Jeng one of the main local organizers; Jill Trewella and Bente Vestergaard contributing lecturers).

Structural and Biophysical Methods for Biological Macromolecules in Solution, Suwon, Korea, June 2016 (main organizer Dmitri Svergun with local organizer Sangho Lee and participants Jill Trehewella and Bente Vestergaard).

EMBO Practical Courses, typically with ~15 tutors and lecturers attracting 200–300 applicants for just 20–30 available spaces:

Solution Scattering from Biological Macromolecules, October 2014 and 2016, organizer Dmitri Svergun with Jill Trehewella and Bente Vestergaard participants.

Small-Angle Neutron and X-ray Scattering from Proteins in Solution, Grenoble, France, May 2015; Jill Trehewella and Dmitri Svergun contributing Keynote talks.

Structural Characterization of Macromolecular Complexes, Grenoble, France, May, 2016; Keynotes with a focus on SAS by Jill Trehewella and Rob Rambo (ISIS).

Additionally, a special EMBO Conference on Molecular Machines: Integrative Structure and Molecular Biology, was held in Heidelberg, Germany, November 2016. Organizers included Dmitri Svergun, with Bente Vestergaard and Jill Trehewella invited speakers; special EMBL Advanced Training Centre Corporate Partnership Programme travel grants for European participants and EMBO travel grants were provided for researchers working in laboratories in India, Taiwan, South Africa and Singapore.

CSAS members from the Asia-Pacific region were very active promoting SAS methods and teaching the required skills to students and researchers in the region. For example:

U-Ser Jeng gave invited lectures on SAS applications with a focus on soft materials at the Taiwan Neutron Science Society (TWNSS) Annual Meeting and Summer School and International Neutron Conference, October 2014, Kaohsiung, Taiwan; the annual meeting of the Biophysical Society of ROC, Tainan, Taiwan, May 2014; and International Symposium on Frontier Technology for the Future, Hsinchu, Taiwan, June 2014. He organized SAS courses for the 2015 Asia-Pacific Edition of HERCULES at the National Synchrotron Research Center (NSRRC), Taiwan, July 2015, and gave an invited talk at the workshop canSAS-VIII J-PARC, Tokai, Japan, April 2016.

Toshiji Kanaya acted as an advisor to the AONSA Neutron School, Indonesia, October 2014, and gave a number of tutorial lectures on SAS applications including at the annual meeting of the Chemical Society in Japan, Nagoya, March 2014, Nanjing (People's Republic of China) in June, 2014, and Hsinchu (Taiwan), in September 2014. He gave invited lectures: on neutron scattering including SANS at the annual meeting of the Chemical Society of Japan, March 2015; on polymer thin films by neutron scattering at the Gordon Conference on Neutron Scattering held in Hong Kong, June 2015; at the Asia-Oceania Conference on Neutron Scattering (AOCNS2015) in Sydney, Australia, July 2015; at the 5th Asian Symposium on Advanced Materials: Chemistry, Physics and Biomedicine of Functional and Novel Materials, Korea, November 2015; and in Jülich for Soft Matter Days 2015, in Germany, November 2015. He was principle organizer of the 1st Neutron and Muon School held in J-PARC MLF in November 2016, where he presented a seminar on polymer thin films. He also gave tutorial talks on SANS and neutron reflectivity for soft matter at IIT in Hyderabad, Mumbai and Bangalore, India, in March 2016 to introduce the activities at J-PARC MLF. Again he travelled to India to deliver an invited lecture at the 8th Asia-Oceania Neutron Scattering Association (AONSA) Neutron School Held in Mumbai in November 2016.

Elliot Gilbert gave an invited talk at the International Union of Food Science and Technology, Montreal, August 2014, to describe how SAS methods may be applied to study food-based systems, and lectured in the Croucher neutron school in Hong Kong and at Universitat Politècnica de València.

Expanding our Educational activities to Turkey, U-Ser Jeng also presented SAS talks at two workshops in Denizli and Ankara (Pamukkale University and Hacettepe University) on Nanoscopic Analyses on Industrial Materials in November 2015.

For the Russian research community, Vladimir Volkov was very active in contributing SAS expertise to training courses and providing specialist lectures, with a number focused on condensed matter applications and nanoscience, including topics such as: Supra-Atomic Structures in Nanomaterials; Mathematical Methods in SAS Data Treatment; SAS Methods in X-ray Methods for Investigation of Matter; and Investigation of Structure of Nanoscale Disperse Systems by Small-Angle Scattering Methods. A number of these courses are included in the curriculum of Moscow State University and its physics Institutes.

With a focus on the growing SAS community in Scandinavia, Bente Vestergaard gave lectures at the Applications of X-ray and Neutron Scattering in Biology, Chemistry and Physics course for students in the Øresund region [primarily Copenhagen (Denmark) and Lund (Sweden) Universities] and Jill Trewhella delivered an 8 lecture course with practical tutorials in Biomolecular SAS at Lund, Uppsala, and Linköping Universities in Sweden during 2016.

#### Community-building activities

CSAS members and consultants served on various SAS-related committees, panels and editorial boards in 2015:

Andrew Allen serves as one of the Main Editors of *Journal of Applied Crystallography* with Elliot Gilbert, Gernot Kostorz and Dmitri Svergun as Co-editors.

Elliot Gilbert joined the editorial board of *Food Structure* (Elsevier).

Dmitri Svergun is a member of the Associate Editorial Board of *Frontiers in Molecular Biosciences*, section Structural Biology.

Jill Trewhella serves as a Co-editor (biology and medicine) for *IUCrJ*, and is an editorial board member of the Cell Press journals *Biophysical Journal* (Proteins) and *Structure*.

Iris Torriani serves as Treasurer and Counsellor of the Teaching Commission of the Brazilian Crystallographic Association (ABC) and is the Provisional Treasurer of the Latin-American Crystallographic Association (LACA); also responsible for home page and networking.

Toshiji Kanaya chairs the steering committee of the Advanced Soft Material Beamline Consortium (FSBL) for 2016, and organized a sub-research group dedicated to GISAS and educational meetings for industry researchers. He was also co-organizer of the annual FSBL meetings in Kyushu, January 2014, Kyoto, January 2015, and Nagoya, January 2016.

Vladimir Volkov served on the committee for Small-Angle Scattering in Biopolymers, St Petersburg State University, Russia, 2015 and 2016.

Members and consultants of CSAS were prominent contributors to scientific meetings around the world supporting the dissemination of research using small-angle scattering: Iris Torriani gave a Plenary Lecture on X-ray Scattering of Macromolecular Biological Structures: Dealing with Intrinsic Disorder at the VIII Mexican Crystallography Congress and LACA II Meeting – 2016; Toshiji Kanaya organized a Bioscience Seminar in J-PARC MLF in May 2016, gave an invited talk at the International Symposium on Polymer Physics in Guizhou, People's Republic of China, June, 2016, and another invited talk at the International Conference of Molecular Engineering of Polymers in Shanghai, People's Republic of China, November 2016; U-Ser Jeng has delivered invited talks for BioSAXS promotion at the workshop of the 7th Japan–Taiwan Joint Meeting on Neutron and X-ray Scattering, Kumatori, Osaka, Japan, March 2016, and at the Grand Challenges in Small-Angle Scattering meeting in Okazaki, Japan, March 2017.

#### Consultant activities

CSAS members and consultants served on SAS-related proposal and design evaluation committees, and consult on the development of standards for SAS:

CSAS members and consultants provide strong support to the Worldwide Protein Data Bank (wwPDB) initiatives to establish a federated system of interconnected databases similar to what exists presently for the PDB (RSCB, PDBe, PDBj) but extended to include SAS data and models. The wwPDB SAS Task Force continues its work on requirements for validation of biomolecular SAS data and modelling (chaired by Jill Trewhella with Dmitri Svergun), and additional members have recently been recruited including Masaaki Sugiyama.

Andrew Allen served as a technical consultant for the new ISO 17867:2015 SAXS (best practice) international standard: Particle Size Analysis — Small-Angle X-ray Scattering, developed in connection with particle size measurements by ISO/TC 24/SC 4 Particle Characterization. Standard issued 1 May 2015; see [http://www.iso.org/iso/iso\\_catalogue/catalogue\\_tc/catalogue\\_detail.htm?csnumber=45820](http://www.iso.org/iso/iso_catalogue/catalogue_tc/catalogue_detail.htm?csnumber=45820). He also continues to interact with

the canSAS effort – acting as liaison with canSAS on SAS publication issues (i.e. IUCr journals), data and metadata requirements for SAS, NIST Standards Reference Materials, and ISO standards activity. This work included a presentation by video link from NIST directly to the canSAS meeting in Tokai, Japan, entitled: *Data Deposition, Metadata, ISO Standards, Calibration Standards, Publication Standards for Small-Angle Scattering*, April, 2015.

Naoto Yagi was advisor for design of the proposed LIX (High Brightness X-ray Scattering for Life Sciences) beamline at NSLS-II, Brookhaven Laboratory, NY, USA, and attended a Beamline Advisory Team meeting (April 2014). He was also adviser for the Advanced Soft Material Beamline, SPring-8 (a dedicated SAXS beamline for industry-oriented polymer and soft materials science).

David Babonneau serves on Peer Review Committee 3: Matter and Material Properties: Structure, Organization, Characterization, Elaboration for beam-time allocation at SOLEIL synchrotron, France.

Vladimir Volkov is a consultant for studies of nanosystems by small-angle scattering, giving lectures to staff of several research Institutes throughout Russia. This activity was performed in the framework of the Shared Research Center IC RAS. He is also a referee providing expertise for SAS-oriented projects submitted to the Russian scientific funds.

Bente Vestergaard serves as a member of the priority and evaluation committee (SAXS and crystallography beamtime) at EMBL-Hamburg (Germany).

#### *Organizational activities*

SAS Commission members and consultants served on a broad range of programme or organization committees for SAS-related conferences and workshops in the period 2014–2016. For example:

David Babonneau planned and co-Chaired the 3rd International GISAS Conference (satellite meeting of the SAS2015 conference) held in Nice, France, September 2015.

Elliot Gilbert represented SAS interests for the Polarized Neutrons for Condensed Matter Investigations Conference, Sydney, Australia, September 2014, and served on the Organizing Committee for the Australia–Oceania Neutron Scattering Association Conference, held in Manly, Australia, July 2015.

U-Ser Jeng organized the National Synchrotron Radiation Research Center (NSRRC) SAXS interest group meeting, Hsinchu, Taiwan, September 2014. Naoto Yagi presented a Plenary talk at the meeting. U-Ser Jeng also organized an international BioSAXS workshop at the meeting. He worked with the SAS community in Taiwan to prepare a proposal to host SAS2021 and was a co-organizer of the workshop Synchrotron for Industry: SAS for Polymer Industrials, Taiwan, September 2016.

Toshiji Kanaya was co-organizer and invited lecturer at the 6th Taiwan–Japan Joint Meeting on X-ray and Neutron Scattering, Tokai, March 2104; co-organizer of the Special Session on Flow-Induced Polymer Crystallization at the International Conference on Fibre Science and Technology, Tokyo, Japan, September/October, 2014; co-organizer of the 7th Asia–Oceania Neutron Scattering Association (AONSA) Neutron School, Tokai, Japan, November–December 2015 as a President of the school. He also organized a seminar on recent developments of scattering methods and the electron microscope at the Polymer Society in Japan in Tokyo, May 2015.

Dmitri Svergun served on the Programme Advisory Committee for the International Biology and Synchrotron Radiation Conference (BSR2016, Stanford, USA, August 2016) that was well attended by the SAS community, with multiple talks highlighting the contributions of SAS and an invited talk by Jill Trewella.

Iris Torriani served as Chair for the organization of the First Latin-American Crystallographic Association (LACA) Meeting that took place in São Paulo, Brazil, jointly with the Brazilian Crystallographic Association, in September 2015. Work began on Statutes and By-Laws to establish the Regional Association with the aim of having them approved for the LACA meeting held in Mexico in October 2016. She was also Counsellor for the elaboration of By-Laws and Statutes of the Latin-American Regional Associate of the IUCr.

Bente Vestergaard and Dmitri Svergun co-organized the 61st Benson Symposium Structural Biology on the Move, Copenhagen, Denmark, August 2015, where the achievements within structural biology were highlighted, covering magnitudes of length scales, from high-resolution analysis to whole-cell imaging, with a prominent role of SAXS and SANS. Jill Trewella and Bente Vestergaard gave invited talks.

Vladimir Volkov served on the Organizing Committees of: the Conference of the National Union of Crystallographers (to be held in Russia in 2016); the III International Conference on Small-Angle Neutron Scattering (SANS-YuMO, Dubna, Russia, 2016); and the Conference of the National Union of Crystallographers Russia, 2016.

#### Technical activities

A major initiative supported by CSAS members relates to the continued work of the Worldwide Protein Data Bank (wwPDB) SAS Task Force (SASTf) on data requirements for biomolecular modelling. The SASTf is chaired by Jill Trewella with Dmitri Svergun and Masaaki Sugiyama as members. In accordance with the recommendations of the SASTf [Trewella *et al.* (2013). *Structure* **21**, 875–881, <http://www.sciencedirect.com/science/article/pii/S0969212613001500>], D. Svergun's group developed and made publicly available a Small-Angle Scattering Biological Data Bank (SASBDB) ([www.sasbdb.org](http://www.sasbdb.org)) [Valentini *et al.* (2015). *Nucleic Acids Res.* **28**(43) (Database issue), D357–363], a curated repository for SAS data and models made public in October 2014 and now containing 527 models and 323 experimental data sets, with 261 models and 134 experimental data sets on hold. The wwPDB foresees a future with a federated system of interconnected databases similar to what exists presently for the PDB (RSCB, PDBe, PDBj) but extended to support the deposition of the hybrid modelling results, as recommended by the new wwPDB Hybrid Methods task force (HMtf) that had its inaugural meeting at the European Bioinformatics Institute, Hinxton, UK, October 2014. The meeting was co-chaired by Andrej Sali, Torsten Schwede and Jill Trewella with Dmitri Svergun as one of a select group of 35 leaders in structural biology methods invited to consider the future direction and needs for hybrid modeling; a report from the meeting has been published [Sali *et al.* (2015). *Structure* **23**(11), 56–67] (<http://www.sciencedirect.com/science/article/pii/S096921261500194X>).

To facilitate data exchange between data bases, a requirement for the envisioned federated system of interconnected databases supporting hybrid data and model validation, Dmitri Svergun with John Westbrook (Protein Data Bank, Rutgers) led an effort to provide a universal data exchange format for the bio-SAS community, based on the use of the widely adopted crystallographic information framework (CIF) [for full description see Kachala *et al.* (2016). *J. Appl. Cryst.* **49**, 302–310 (<http://journals.iucr.org/j/issues/2016/01/00/aj5271/>)]. In this work, an earlier version of the sasCIF format implemented as an extension of the core CIF dictionary, available since 2000, has been extended to describe comprehensively the necessary experimental information, results and models, including relevant metadata for SAS data analysis and for deposition into a database. Processing tools for these files (sasCIFtools) have been developed, and these are available both as stand-alone open-source programs and integrated into the SAS Biological Data Bank (SASBDB), allowing the export and import of data entries as sasCIF files. Software modules to save the relevant information directly from beamline data-processing pipelines in sasCIF format are also developed. This update of sasCIF with the relevant tools is an important step in the standardization of the way SAS data are presented and exchanged, to make the results easily accessible to users and to promote further the application of SAS in the structural biology community.

Other technical activities CSAS members and consultants took part in include:

Andrew Allen completed development of NIST standard reference material (SRM 3600) for SAXS intensity calibration, based on glassy carbon (in collaboration with others at NIST and at the Advanced Photon Source, Argonne National Laboratory). The new NIST SRM 3600 became available in July 2016 and can be ordered via the following web site: [https://www-s.nist.gov/srmors/view\\_detail.cfm?srn=3600](https://www-s.nist.gov/srmors/view_detail.cfm?srn=3600). An open-access paper detailing the measurements that underlie the new SRM has been published by Allen *et al.* [(2017). *J. Appl. Cryst.* **50**(2), 462–474] (<https://doi.org/10.1107/S1600576717001972>).

Andrew Allen completed a chapter on heterogeneous materials for the new IUCr *International Tables for Crystallography* Volume H.

U-Ser Jeng is leading the construction of a new, dedicated, high brilliance, biological SAXS/WAXS beamline at the new 3GeV synchrotron of NSRRC, Taiwan, planned to be operational in 2018.

David Babonneau continued development of *FitGISAXS* (software package for modelling and analysis of GISAXS data using *Igor Pro*).

In summary, it is fair to say that the CSAS sustained a busy and productive agenda for the three years 2014–2016, and with new leadership and refreshed membership the CSAS will continue supporting and promoting the application of SAS techniques in a broad range of scientific fields.

On a personal note, it has been a pleasure to serve as a member of CSAS for the past twelve years, as Chair for the past three, and I look forward to continuing my association with CSAS as a consultant and representative to the IUCr Commission on Journals.

*J. Trewella, Chair*

#### **A6.20. Commission on Structural Chemistry**

The Commission met in Montreal and had robust discussions on a number of matters, including increasing support from chemical crystallographers for IUCr journals and direction and strategy of these journals, and the need for the Commission actively to encourage and support crystallography schools and regional meetings, particularly in developing countries.

Since Montreal, the Commission supported the following meetings:

The SAGAMORE XVIII Conference on Charge, Spin and Momentum Densities, Sardinia, Italy, June 2015; organized by the Commission on Charge, Spin and Momentum Densities; Chairs C. Gatti, P. Macchi ([www.sagamorexviii.org](http://www.sagamorexviii.org)).

The 22nd International Conference on the Chemistry of the Organic Solid State (ICCOSS XXII), Niigata, Japan, July 2015; Chairs K. Ogawa, H. Uekusa ([www.iccoss2015.org](http://www.iccoss2015.org)).

The 2015 meeting of the Zürich School of Crystallography held in June 2015; Chair A. Linden.

Indaba 8, an interdisciplinary workshop organized by the South African Crystallographic Society, and with the theme Serendipity vs Prediction, Skukuza, South Africa, August 2015; Chair A. Roodt ([www.sacrs.org.za/indaba](http://www.sacrs.org.za/indaba)).

The 2nd North African Crystallography Conference (NACC2), Tunisia, November 2015; Chair H. Boughzala ([www.nacc2.com](http://www.nacc2.com)).

A Workshop on Powder Diffraction of Organic Compounds, Frankfurt, Germany, October 2015; Chair M.U. Schmidt ([www.anorg.chemie.uni-frankfurt.de/AK\\_Schmidt/chemkrist2015](http://www.anorg.chemie.uni-frankfurt.de/AK_Schmidt/chemkrist2015)).

Looking forward to the Hyderabad Congress, it is important that chemical crystallography is well represented and supported. To this end, an extensive list of potential advisory committee members was provided to the organizers, with the aim of having a good chemical crystallography programme at the meeting, and thus good support for the meeting from the chemical crystallography community. Four of these nominees were appointed to the International Programme Committee, and a very strong scientific programme of interest to structural chemists has resulted, including 14 Microsymposia on the Crystal Engineering of MOFs and Open Framework Compounds, 13 Microsymposia on the Crystal Engineering of Organic and Pharmaceutical Compounds, and 12 Microsymposia in the Materials and Minerals theme.

*S.R. Batten, Chair*

#### **A6.21. Commission on Synchrotron and XFEL Radiation**

The aim of the Commission is to promote access and awareness of crystallographers worldwide to the world's synchrotron radiation (SR) facilities. To this end, the Commission broadly promotes the development of crystallographic instrumentation, technology and standards, and the synergies between storage-ring-based and LINAC-based next-generation sources such as X-

ray Free Electron Lasers (XFELs). The bulk of the Commission's work is carried out via e-mail, with occasional face-to-face meetings held at selected conferences attended by sufficient of the Commission members.

#### *Synchrotron radiation and free electron laser facilities*

The progress of synchrotron radiation and FEL-based user facilities and science continued at a rapid pace during the triennium. The two operating XFEL light sources, LCLS and SACLAC, are highly oversubscribed, and rapid progress was made on several new XFEL facilities. The Pohang Accelerator Laboratory XFEL in South Korea achieved hard X-ray laser light in November 2016 and user operation is scheduled to begin in March 2017. Construction of the European XFEL in Hamburg, Germany, is complete and commissioning began in October 2016 with user operation expected in the second half of 2017. The Swiss FEL facility, at the Paul Scherrer Institute, is also in an advanced stage of commissioning. Soft X-ray FEL facilities are also continuing to produce high impact science, at facilities such as FLASH in Hamburg and FERMI in Trieste, Italy, and a new soft X-ray FEL is under construction at the Shanghai Synchrotron Radiation Facility, People's Republic of China.

The triennium also saw continued development of storage-ring-based light sources, with both new facilities and planned upgrades to existing light sources pushing to ever-higher brightness. Two new high-brightness storage-ring light sources, NSLS II at Brookhaven National Laboratory, USA, and the Taiwan Photon Source in Hsinchu, Taiwan, entered user operation. Newer designs, featuring new magnetic lattice designs, are allowing the brightness of synchrotron X-rays to be increased still further. The first such '4th Generation' storage ring, MAX IV in Sweden, features 7 bending magnets per 'cell', compared with 2 or 3 in current light sources. MAX IV is currently accepting proposals from expert user groups for its first four beamlines. Most existing facilities, including the three original third-generation hard X-ray facilities (ESRF, APS and SPring-8) are either undertaking or planning significant upgrade programmes based on these new designs. For example, the upgraded SPring8-II will be more than an order of magnitude brighter than the current ring (its 'natural emittance is calculated to be ~100 picometre.radian compared with 2.8 nm.radian currently'). New facilities, such as the 6 GeV High Energy Photon Source to be built near Beijing, People's Republic of China, and the 3 GeV facilities SLiT-J (Tohoku, Japan) and SIRIUS (Campinas, Brazil) will also use the new high brightness designs. The ultimate extrapolation of these 4th generation storage rings is a diffraction limited hard X-ray synchrotron storage ring light source, which would have obvious and far reaching applications in many areas, including potential crystallographic applications.

Advances in synchrotron and XFEL research and technology are not limited to the light source facilities. The advent of the XFEL sources and the push to higher brightness in general is being matched by developments in all areas. Detector performance in particular is rapidly advancing, with new hybrid pixel area detectors replacing CCD based detectors and offering nearly 10 times higher throughput from current crystallography beamlines. X-ray focusing optics are also advancing allowing smaller foci, and consequently smaller crystals to be measured. On the technique side, serial crystallography, pioneered at XFEL sources, is now being introduced at storage ring synchrotron facilities.

#### *Commission name change*

In recognition of the increasing significance of free electron laser sources to crystallography, at the Montreal General Assembly the Commission proposed that its name should be changed to Commission on Synchrotron and XFEL Radiation. This change was approved.

#### *International Year of Crystallography*

The international synchrotron community embraced the IYCr in a number of capacities, with 15 facilities directly sponsoring IYCr2014 and all hosting special events, including dedicated sessions at their user meetings and events aimed at furthering public understanding of the impacts and benefits of crystallography. Examples include:

the one-day symposium Celebrating 100 Years – A Journey Through the World of Crystallography, held by the Canadian Light Source on 14 September and co-organized by Commission member Pavel Gochulski. This symposium combined a hands-on introduction workshop for local high-school students, and a general public session featuring the role of crystallography in HIV/AIDS research.

SOLEIL and LLB jointly hosted a satellite symposium composed of four Plenary Lectures dedicated to crystallography on 23 January, before their 2014 Users' Meeting. Commission member Jean-Louis Hodeau was involved in the organization.

Additional activities associated with Commission members included collaboration between the Polish Synchrotron Radiation Society (Commission consultant Maciej Kozak is President of the Society) and Polish Mail to issue a limited set of four postal stamps to mark IYCr2014 ([http://www.iy-cr2014.org/events/postage\\_stamps/postage-stamp-issue2](http://www.iy-cr2014.org/events/postage_stamps/postage-stamp-issue2)).

Commission member Jean-Louis Hodeau was particularly active, planning a number of European activities to celebrate IYCr2014 and the associated centenary of the Laue–Bragg discoveries. This included the development of the travelling exhibition *Journey into the Crystal*, which takes visitors on a journey of the discovery of matter – but also on a journey through time to the beginnings of crystallography. An important contribution was made by several large light source facilities (such as ESRF, ILL, SOLEIL and ALBA) to its translation into English and Spanish, to allow an international distribution of this travelling exhibition during 2014. A condensed version (12 panels) was subsequently produced in additional languages: Arabic, English, Spanish, Dutch–Flemish, French, Russian, Slovakian, Portuguese–Brazilian, German, Catalan, Finnish, Swedish, Turkish.

#### *Commission involvement in the Montreal Congress*

The Commission was represented by Richard Garrett on the International Programme Committee for the Montreal Congress.

The Commission organized the following Microsymposia:

Advances in X-ray FEL Coherent Scattering and Diffraction (MS-CSR-2);

Advances in X-ray, Neutron and Electron Detectors (MS-CSR-3).

The Commission also successfully proposed two Keynote presentations: *Future Light Sources and Their Impact on Structure Studies* by Edgar Weckert (DESY) and *Use of Two Colour XFEL Modes for SAD/MAD Phasing and Improved Intensity Measurements for de novo Macromolecular Structure Determination* by Commission consultant Soichi Wakatsuki (SLAC).

Participants at the Open Commission meeting held at the Madrid Congress suggested that more joint symposia be proposed for future Congresses, given that synchrotron and XFEL light sources underpin the research of many other Commissions. Consequently the Commission worked with a number of relevant Commissions to propose the following symposia for the Montreal Congress:

High-Resolution Charge Density using SR, jointly proposed with the Commission on Charge, Spin and Momentum Densities (MS-CCSMD-7);

Advances in Experimental Techniques and Data Analysis for Science at Extreme Conditions at Synchrotron and Neutron Sources jointly with the Commission on High Pressure (MS-CHP-5);

Applications of Anomalous Small-Angle X-ray Scattering to Soft Materials and Bimolecular Systems jointly with the Commission on Small-Angle Scattering (MS-CSAS-2);

Time-Resolved Spectroscopic Studies with Synchrotron Radiation and Free Electron Laser Sources jointly with the Commission on XAFS (MS-CXAFS-1);

XFEL Macromolecular Crystallography jointly with the Commission on Biological Macromolecules (MS-CSR-1);

X-ray, Muon and Neutron Studies of Magnetic Structure in Materials jointly with the Commission on Neutron Scattering (MS-CNS-5).

The Commission organized a one-day Workshop on Crystallography at XFEL Sources at the Montreal Congress in recognition of the increasing impact of the XFEL facilities in crystallography. The aim of the workshop was to introduce Congress participants to the new capabilities of the XFEL sources, and to provide information and advice on how best to carry out a successful XFEL experiment. While crystallography was the main focus of the workshop, other applications of these new sources were introduced in the opening presentations.

The Commission held an Open Meeting at the Congress, attended by 10 members and consultants. It was noted that, as synchrotron facilities are indispensable to much of the science encompassed by the IUCr, we have a broad mission but it is multi-disciplinary and therefore somewhat ill-defined compared with most other Commissions. The Commission will continue to work with appropriate conferences, both to bring synchrotron expertise to crystallography conferences and crystallography input to synchrotron meetings.

Commission members, responding to a request from the IUCr Executive Committee, provided feedback on an article published in *Nature* by Paolo Radaelli addressing concerns on user input into large-scale facilities (the European Spallation Source in particular). The advice of the Commission members was included in the presentation to the Executive by the Chair at the Montreal Congress.

#### *Supported meetings, schools and workshops*

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

The RapiData course on automated data collection to support participation of Latin-American students. The Commission has endorsed this annual event for many years, and did so again for each year of the triennium, for schools held in April 2014, 2015 and 2016. It is worth noting that from 2015 the school moved to the SLAC National Accelerator Laboratory, after being hosted at Brookhaven National Laboratory since its inception in 1999.

The International School on Structural Basis of Pharmacology: Deeper Understanding of Drug Discovery Through Crystallography, Erice, Italy, May/June 2014.

Symposium on the Applications of *In-Situ* Synchrotron Radiation Techniques in Nanomaterials Research, held as part of the Materials Research Society spring meeting in San Francisco, USA, April 2014.

Funding for a Visiting Professor for Atomic Pair Distribution Functions Technique: Fundamentals and Applications, Mar del Plata, Argentina, beginning 31 October 2014.

The Sixth School of the Argentinian Crystallography Association, Universidad Nacional de Mar del Plata, Mar del Plata, Argentina, November 2014.

13th School on Synchrotron Radiation, 14–25 September 2015, organized by the Italian Synchrotron Radiation Society in collaboration with Elettra–Sincrotrone Trieste, to support the attendance of young scientists from Africa and the Middle East.

9th AOFSSR Cheiron School, organized by the Asia–Oceania Forum for Synchrotron Radiation Research and held at SPring-8 in September 2015, to support the attendance of two students from Africa and the Middle East (see AOFSSR section below).

The 12th International Conference on Biology and Synchrotron Radiation (BSR), SLAC, USA, 21–24 August 2016.

The Commission noted a significant increase in the number and variety of events requesting its endorsement in our last triennium report. This trend continued in 2014, but the subsequent two years of this triennium have seen a sharp fall in endorsement requests. In general, the Commission has strongly supported IUCr sponsorship for the purpose of assisting attendance by young researchers and scientists from developing countries.

#### *Activities of Commission members*

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

Three Commission members played an active role in the 2015 Synchrotron Radiation Instrumentation Conference, hosted by the NSLS, Brookhaven National Laboratory, USA: Youichi Murakami was a member of the International Advisory Committee, and Miguel Angel Garcia Aranda and Thomas Tschentscher served on the Scientific Programme Committee.

Soichi Wakatsuki chaired the 12th International Conference on Biology and Synchrotron Radiation (SLAC, USA, 2016) and Paweł Grochulski served on the Organizing Committee.

Richard Garrett co-Chaired synchrotron Microsymposia at the AsCA 2015 (Kolkata, India) and 2016 (Hanoi, Vietnam) crystallography conferences.

Maciej Kozak is President of the Polish Synchrotron Radiation Society and a member of ‘Polish Synchrotron’ – a council supporting the construction of the Polish synchrotron SOLARIS.

Pawel Gochulski represented the Commission on the International Programme Committee of the Hyderabad Congress.

#### *Asia–Oceania Forum for Synchrotron Radiation Research (AOFSRR)*

The Asia–Oceania Forum for Synchrotron Radiation Research is an international network whose mission is to foster collaboration among synchrotron radiation facilities and user communities in Asia and Oceania, as well as promoting collaborations with facilities and communities in America and Europe. The eight facility operating nations in the region are full members of the AOFSRR, and the Forum’s mission includes promotion of synchrotron-based science throughout the region. To this end, Malaysia, New Zealand and Vietnam are associate members of the AOFSRR. Two members of the Commission play active roles in the organization, including Youichi Murakami (AOFSRR President, 2015–2016) and Richard Garrett (Executive Committee member and Treasurer). The AOFSRR holds an annual conference/workshop, hosted by each full member nation in turn. The workshops in the 2014–2016 triennium were hosted by Taiwan (2014), Australia (2015) and People’s Republic of China (2016).

One of the core activities of the AOFSRR has been the Cheiron School, a two-week international synchrotron school, which has been held annually at SPring-8 since 2007. The curriculum is very broad, covering both the fundamentals of synchrotron radiation generation and the various applications, including all the common crystallography applications. Between 50 and 60 young students and post-docs from countries in Asia and Oceania attend the school each year. In 2015 the IUCr supported the attendance of two students, one each from the Middle-East and Africa, to the Cheiron School. The IUCr attendees were Dr Areej Abuhammad, an Assistant Professor at the School of Pharmacy, University of Jordan, and Mr Boudraa Issam, a PhD student from the University Mentouri Constantine, Algeria. This followed the attendance of three African students in 2014, supported as part of the International Year of Crystallography. Lecturers at the 2015 Cheiron School included IUCr Executive Committee members Mitchell Guss and Masaki Takata, and Commission Chair Richard Garrett.

The 2015 Cheiron School was the 9th and final year that SPring-8 hosted this event. Following a review it was decided to change the format of the SPring-8 school to a shorter higher level workshop aimed more specifically at staff members of the AOFSRR synchrotron light source facilities. At its 2016 Council Meeting the AOFSRR decided to establish the AOF Synchrotron Radiation School as an annual school rotating between the member countries. An initial rotation has been decided, with Australia hosting the first AOF school in 2017, to be followed by South Korea in 2018 and Thailand in 2019.

*R.F. Garrett, Chair*

#### **A6.22. Commission on XAFS**

Commission members were assigned the following responsibilities: liaison with the International Programme Committee for the Hyderabad Congress – Farideh Jalilehvand; responsibility for the web site – Giuliana Aquilanti and Masao Tabuchi; IXAS liaison – Peter Glatzel; IUCr dictionary of XAFS terminology – Jesus Chaboy; coordinators for new editions of the Q2XAFS workshop – Steven M. Heald and Sofia Diaz-Moreno; working group on databases – Bruce Ravel and Steven M. Heald.

2014 involved consolidation of the achievements of the Commission with the Montreal Congress.

#### *Tutorial workshop at Montreal Congress*

The CXAFS tutorial Workshop on XAFS organized by the Commission and held 5 August had a record number of attendees with 165 registrants from 28 countries (compared to 56 in Madrid). Key discussions about the XAFS tutorial workshop led to the suggestion that the ‘hands-on’ aspect should be emphasized next time. This should be considered by C. Chantler and B. Bunker as co-Chairs and an additional co-Chair from India acting as local coordinator. This should be a ‘zero-cost’ workshop that encourages and emphasizes the outreach nature of the activity.

*Microsymposia at Montreal Congress*

A record number of 6 MS were organized or co-organized by CXAFS:

MS6 Time Resolved Spectroscopic Studies with Synchrotron Radiation and Free Electrons (co-Chairs: Federico Boscherini, Christian Bressler). The symposium covered time-resolved spectroscopic techniques at storage rings and FELs. Time-resolved XAFS experiments have taken up momentum at SRs and FELs and now offer time resolution in the 100 fs time frame, which is of high relevance for many chemical systems.

MS14 Electronic Structure and Chemical Bond Information by High Energy Resolution X-ray Spectroscopy (co-Chairs: Richard Strange, Pieter Glatzel). The symposium was devoted to RIXS and hard X-ray emission spectroscopy (XES) that provide information on electronic structure that is complementary to X-ray diffraction. They can identify ligands, determine the chemical state of the metal site and some ligands and are very sensitive to X-ray damage. XES unlike XAS does not require a monochromatic X-ray beam and is thus compatible with a diffraction setup. This property is particularly interesting for crystallography at X-ray free-electron lasers. The MS reviewed the state of the art, introduced the technique, presented recent experiments (also at LCLS) and discussed future applications.

MS38 X-ray Techniques for Innovation in Industry (co-Chairs: Krystyna Jablonska, Jeffrey Cutler) (attendance 85). Utilization of various X-ray techniques in material characterization is becoming increasingly important in science and technology development, leading to innovation and commercialization efforts for industry, and this was highlighted in the Microsymposium. Topics ranged from life science to material science and included how industry engagement is being facilitated by dedicated industry support programmes at various lightsources

MS46 XAS of Hydrated Metal Ions and Protein Active Centres in Aqueous Solutions (co-Chairs Ingmar Persson, Ritimukta Sarangi) (attendance 40–50). The symposium presented the real possibilities and limits of XAS analysis (combined with molecular dynamics, for example) in the study of the solvation structure of metals. This includes inorganic and organometallic metal ions, solvation effects on metalloproteins and high-pressure interactions.

MS64 EXAFS Analysis at the Nanoscale and in Highly Disordered Materials (co-Chairs Sofia Diaz-Moreno, Jesús Chaboy, Alexei Kuzmin). The symposium presented the real possibilities and limits of EXAFS analysis at the nanoscale. To date, different papers have mainly addressed the existence of surface effects in terms of the reduction of the number of coordination. This is a controversial issue that needs clarification coupled with the analysis of disorder effects. Finally, what EXAFS (XANES) can really say regarding the existence of vacancies should be also an interesting topic.

MS103 Spectroscopic Approaches (XAFS, XANES, NMR, ...) in Crystallography (co-Chairs: M. Tabuchi, Carlo Lamberti). The symposium presented the spectroscopic approach to crystallography. Many spectroscopic techniques are naturally complementary with crystallographic methods. Multiple wavelength anomalous dispersion is intrinsically a combined XRD/XAS technique, for example. XAFS and XANES combine to give detailed information on dynamical bonding, dynamical versus static disorder, oxidation and coordination number of active or intermediate states, which complement other techniques extremely well. Further, XAFS and XANES combine well with IR to probe detailed molecular dynamics.

*International Tables for Crystallography, Volume I – XAS and editorial activities*

Procedures for a new volume of *International Tables for Crystallography* dedicated to XAFS (Volume I) have been progressed. C.T. Chantler, F. Boscherini and B. Bunker have been appointed as Editors. The current draft *Outline* was revised and final approval of the Volume should occur soon. The three Editors encouraged CXAFS members to provide input for the contents of this volume. A preliminary *Contents* has been circulated. The aim is for this to be a stand-alone Volume, but it will necessarily have some overlap with Volume C, and possibly also Volumes H and F. One possible way to market Volume I would be to offer delegates at relevant meetings the chance to preorder the volume when registering for the conference.

Chantler and Boscherini are heavily involved in the preparation as two of the three Main Editors, with Bruce Bunker ex-Chair of IXAS. All Commission members are involved in this extensive activity. Currently some 100–150 experts have accepted invitations to write specific advanced chapters and many have completed their drafts using the IUCr template. Many of these have been sent to expert referee panels for review. All chapters will be fully reviewed in a normal journal peer-review process.

A good number of the chapters have been accepted. The interest across the world experts in different sections and topics augurs very well for an excellent outcome, though much more work will be needed over the next 6–12 months.

#### *IXAS Newsletter and links to IUCr journals*

Richard Strange and Steve Heald act as a link to *JSR* and *Acta*. The Commission (CXAES) encourages the application of the IXAS conference organizers for the Proceedings to be in a Special Issue of *JSR*. CXAES also encourages high-quality submissions related to XAFS.

#### *Joint CXAES IUCr / IXAS Database Working Group*

Progress was made on the format and content of the Database and it was agreed that a report (status or otherwise) would be presented regularly every six months. The current Chairs of the Commission (Bruce Ravel and Steven M. Heald) and IXAS will work together to define the Chair and membership of the new Working Group, and to appoint jointly and to clarify the outcomes of the past cycle.

#### *Conference support and proposals*

An application for support of XAFS16 to be held in Karlsruhe, Germany, August 2015, was submitted to the IUCr. The Commission endorsed the application.

#### *Development of data overlap and format with Japanese XAFS Society*

The report/summary of the status of the Japanese XAFS Society and their current initiatives, especially including those relating to a database, in collaboration with H. Oyanagi, K. Asakura and many others was prepared by M. Tabuchi.

#### *CXAES Commission meeting at the XAFS16 conference, Karlsruhe, 25 August 2015*

Chris Chantler, Krystyna Jablonska, Giuliana Aquilanti, Farideh Jalilehvand, Pieter Glatzel, Masao Tabuchi, Bruce Ravel, Bruce Bunker and Federico Boscherini were present.

The CXAES members present reported on performed and planned activities. In particular, the activity regarding Volume I of *International Tables for Crystallography* was discussed in detail. C.T. Chantler, B. Bunker and F. Boscherini are the Editors. They completed the plan of the volume and invitations to submit chapters had been sent to many scientists. The planned activity regarding the preparation for the scientific programme for the Hyderabad Congress was also discussed and approved.

#### *CXAES web page*

G. Aquilanti and M. Tabuchi had the responsibility for the web site. The lectures of the XAS workshop held in Montreal have been uploaded to the web page. The information about the new members of the Commission had been updated and photographs of most of the members were uploaded. Updates in the XAFS beamlines section are being implemented. At the meeting during XAFS16 the possibility of mirroring the site [www.wayforlight.eu](http://www.wayforlight.eu) for the list of European EXAFS beamline users was discussed. G. Aquilanti has decided to update the existing list as a careful analysis of the web site shows some discrepancies between the information given and the actual situation at synchrotrons. The information about forthcoming events is continuously updated.

#### *Conference support and proposals*

An application for support of the conference Biology and Synchrotron Radiation to be held 21–24 August 2016, and hosted by SLAC National Accelerator Laboratory, was submitted to the IUCr.

The activity of CXAES in 2016 was concentrated on preparation for the Hyderabad Congress.

F. Jalilehvand is the CXAES liaison with the International Programme Committee of the Congress and is coordinating the activity – the outcome for our Commission and XAFS is outstanding. We will co-Chair or Chair 8 MS, including all

previously proposed MS + High Resolution Spectroscopy with SSRL Dimosthenis Sokaras as suggested Chair from CXAFS + Porous Framework for Catalysis and Renewable Energy with Christian Doonan as proposed Chair from CXAFS.

The following CXAFS Microsymposia have been accepted:

Two unshared Microsymposia:

MS90 Spectroscopy Applications in Biologically Relevant Systems (co-Chairs: Sofia Diaz-Moreno, Bhoopesh Mishra).

MS51 Recent Developments in XAFS Spectroscopy: Theory, Instrumentation and Data analysis (co-Chairs: Hiroyuki Oyanagi, Konstantin Klementiev).

Six shared Microsymposia:

MS107 Synchrotron Measurement in Conservation and Cultural Heritage (co-Chairs: Bruce Ravel, Eric Dooryhée); shared with Commission on Crystallography in Art and Cultural Heritage.

MS60 XAS at Extreme Conditions (co-Chairs: Giuliana Aquilanti, Daniel Haskel); shared with Commission on High Pressure.

MS96 XAFS of Materials for Clean Energy (co-Chairs: Pieter Glatzer, Steven M. Heald); shared with Commission on Crystallography of Materials.

MS121 Synchrotron-Based X-ray Techniques and the Environment (co-Chairs: Richard Garrett, Hugh Harris); shared with Commission on Synchrotron and XFEL Radiation.

MS42 High Resolution Spectroscopy (co-Chairs: Dimosthenis Sokaras, Hamid Reza Khavasi).

MS74 Porous Framework for Catalysis and Renewable Energy (co-Chairs: Christian Doonan, Gustav Van Tendeloo).

Most excitingly, our Commission put forward several names as possible Keynote Invited Speakers. The Commission has never proposed Keynote or Plenary Speakers in past Congresses but instead have worked towards strengthening the visibility of XAFS in MS. That this has been welcome and useful is seen by the outcome that two of our Keynote proposals have been accepted – a great demonstration of the recognition of new, advanced, and complementary techniques in the wider community. Sakura Pascarelli and Vittal Yachandra are both accepted. Ingrid Pickering's name is also on the waiting list. These three cover widely different areas and are all excellent speakers and choices, and are well known for incisive and relevant talks. Congratulations to all for all suggestions and contributions towards this success.

#### *IUCr XAFS Workshop*

The next Workshop dedicated to XAFS for crystallographers will also be organized for the day before the Congress. W1 X-Ray Absorption Spectroscopy for the Crystallographer, Hyderabad, 21 August 2017. This one-day, free tutorial workshop will provide an overview of the physics and chemistry of X-ray absorption spectroscopy with a particular emphasis on its complementarity with diffraction techniques. The curriculum will include introductions to beamline instrumentation, measurement methods, and methods of data processing and analysis. This workshop, which is organized by the IUCr Commission on XAFS and the International X-ray Absorption Society, with local support from the Board of Research in Nuclear Science (India), will be held in HICC.

#### *IUCr Congress Satellite with IXAS: Database Standards and Structures*

The organization of the second workshop on data standardization (Q2XAFS) to be held at Diamond, UK, 14–15 August 2017, as a satellite of the Hyderabad Congress, was started by Sofia Diaz-Moreno, C.T. Chantler, Matt Newville as co-Chairs. Q2XAFS2017: International Workshop on Improving Data Quality in XAFS Spectroscopy includes a strong presence by members of the Commission and by members of the IXAS Executive. It aims to increase the recognition of the importance of combined techniques for crystallography and for structure–function investigations.

*C.T. Chantler, Chair, K. Jablonska (Secretary) and G. Aquilanti, Secretary*

## A7. Committee for the Maintenance of the CIF Standard (COMCIFS)

### *Introduction*

COMCIFS is responsible for maintaining and developing the Crystallographic Information Framework (CIF) on behalf of the IUCr. COMCIFS activities include assistance and approval for new CIF dictionaries as well as development and support of associated standards for syntax and dictionary construction. The new set of standards underpinning CIF was essentially finalized in the previous triennium, which also saw the beginning of collaborations with other standards bodies and moves towards widespread CIF adoption among the macromolecular community.

### *Dictionaries*

A key aspect of the CIF project over the last two decades has been codification of crystallographic knowledge into machine-readable dictionaries. The current triennium has seen the publication of (i) a dictionary for describing twinning, authored by V. Young, and (ii) the magCIF dictionary for describing magnetic structures, the result of several years' careful work by the Commission on Magnetic Structures led by B. Campbell.

### *DDLm*

At the 2014 Montreal meeting, COMCIFS resolved that all dictionaries currently written in the original DDL1 language would be converted to the new DDLm language [Spadaccini, N. & Hall, S.R. (2012). *J. Chem. Inf. Model.* **52**(8), 1907–1916]. DDLm versions of two of the largest legacy dictionaries, covering single crystal and powder diffraction, have now been accepted, and draft versions of the remaining dictionaries are in an advanced state. Efforts in the coming triennium will focus on converting the remaining legacy dictionaries to DDLm, and disseminating dictionary-writing knowledge and tools to the wider community.

### *Syntax*

The CIF2 syntax is an enhanced version of the original CIF syntax, including support for Unicode and complex data structures. Final adjustments to CIF2 were approved at the Montreal IUCr meeting. The full syntax specification was subsequently published in the *Journal of Applied Crystallography* [Bernstein, H. *et al.* (2016). *J. Appl. Cryst.* **49**, 277–284].

### *Software*

In an effort to ease the burden of implementing the CIF syntax specifications, COMCIFS supported the work of J. Bollinger to produce a high-quality programming library for reading and writing CIF files in either CIF1 or CIF2 formats. The library has been made available under an open-source licence (see [https://github.com/COMCIFS/cif\\_api](https://github.com/COMCIFS/cif_api)) and described in a companion article to the CIF2 syntax publication [Bollinger, J. (2016). *J. Appl. Cryst.* **49**, 285–291]. In other software developments, the new magnetic CIF definitions have been rapidly incorporated into leading packages for magnetic powder diffraction and structure visualization.

### *Macromolecular developments*

The worldwide Protein Data Bank (wwPDB) manages the combined PDBx/mmCIF dictionary for macromolecular crystallography, which is by far the largest CIF dictionary with over 7,000 definitions. The coverage of this dictionary has been expanded over the recent triennium to include small-angle scattering [Kachala, M. *et al.* (2016). *J. Appl. Cryst.* **49**, 302–310] and hybrid methods. These additions were accompanied by expansion of the PDBx/mmCIF-based deposition system to include both NMR and 3DEM measurements. The homology modeling dictionary was also enhanced to support initiatives for public deposition of theoretical macromolecular models.

### *Interaction with other data management initiatives*

There is increasing pressure for scientific data to be made widely available and accessible. This is leading a number of scientific disciplines to initiate data description projects, some of which overlap with CIF dictionary coverage. One of these projects, NeXus, which defines raw data standards widely used at neutron and X-ray facilities, has an ongoing collaboration with COMCIFS, via H. Bernstein's membership of the NeXus International Advisory Committee (NIAC) and joint work on

managing data from the next generation of imaging detectors. NIAC are working to harmonize their data descriptions with those found in CIF dictionaries – for example, adopting the goniometer axis descriptions used in the macromolecular mmCIF files.

Several COMCIFS members were involved with the IUCr's Diffraction Data Deposition Working Group (DDDWG) over the triennium, including strong representation at an ECM satellite workshop in 2015. This close relationship has been formalized with the inclusion of the COMCIFS Chair in the DDDWG's successor, the Committee on Data.

#### *Future concerns*

The collaboration with NeXus has underscored the advantages of having different file formats available for different contexts. The CIF1 and CIF2 formats are excellent as widely accessible, long-term archival and interchange formats, but are less suitable as, for example, containers for working access to the gigabytes of image data produced by the current generation of X-ray detectors. Fortunately, the contents of arbitrary file formats can be aligned using datanames defined in CIF dictionaries [Hester, J. (2016). *Data Science Journal* **15**, 1–17]. This broad applicability of CIF dictionaries and increasing pressure properly to codify data may lie behind increased requests for CIF dictionaries from communities that are sometimes only peripherally related to the IUCr. In order to meet this rising demand, dictionary-writing techniques need to be documented and spread to avoid bottlenecks in the dictionary creation process. A planned dictionary-writing workshop at the Hyderabad Congress is a first step in this programme, and the second edition of Volume G of *International Tables* will provide further high-quality material. The topic areas to which the IUCr and COMCIFS will provide active, long-term support must also be resolved; for example, is a spectroscopy dictionary suitable for inclusion in the core IUCr stable of dictionaries?

#### *Membership*

COMCIFS participants include a large number of advisers/observers and a small number of voting members. The current voting members are J. Hester (Chair), B. McMahon (Secretary), H. Bernstein, J. Westbrook and J. Bollinger. A further notional voting position remains unfilled. No decisions in the last triennium have required a vote.

#### *J. Hester, Chair*

### **A8. IUCr Newsletter**

The *IUCr Newsletter* continues to be a vehicle for broadcasting and promoting the interests and activities of the IUCr and its Commissions. It also strives to enhance communication within the global community of crystallographers. Special effort is made to promote meetings and publications sponsored by the IUCr.

This report covers 12 issues (22#1–4, 23#1–4 and 24#1–4). Volume 24, Issues 3 and 4 were published in 2017. In the first two issues of 2014, the President's column was written by G.R. Desiraju and all subsequent columns were written by M.L. Hackert. All three Volumes were edited by Bill Duax.

Each issue contained articles highlighting articles from each of the IUCr journals and news of various IUCr Commissions, a column by Jonathan Agbenyega, notices of elections, awards to crystallographers, and information on web sites, resources and other activities of interest to crystallographic practitioners. The reports covered topics such as high-throughput protein crystallography, materials microstructure, radiation damage, crystals in art and science, crystal growth, synchrotron updates, structural genomics, methods, supramolecular chemistry, small molecules, biomaterials, electron crystallography, applied crystallography, high-pressure studies, new materials and aperiodic crystals. Contributions are received from crystallographers in many countries and other materials are gathered from the Newsletters of crystallographic associations and science news magazines. Almost all submitted contributions are published and all material is edited to varying degrees.

With the celebration of the International Year of Crystallography in 2014, a new category was created and each issue contained at least two pages highlighting crystallographic efforts around the world. With Volume 24, we created the new feature 'Products' to give our advertisers an incentive to advertise with us. Each advertiser that contracted for all 4 issues of the Volume received a free products article equal to the advertisement size. Three advertisers took advantage of this offer.

The meeting reports covered meetings of IUCr Regional Associates and national crystallographic associations as well as extensive coverage of the Montreal Congress. Reports were published covering meetings in Australia (2), Brazil (2), Cameroon, Costa Rica, Croatia (6), Cuba (2), Czech Republic, France, Germany, Italy (2), Japan (4), Korea, Mexico, Poland (5), Russia, Slovenia, Spain, Switzerland (2), UK and USA (2).

A series of articles on crystallography in countries adhering to the Union began in 2003. In the last triennium issues appeared on North America (Volume 22#1, Bill Duax, Editor) and Norway (Volume 23#1, Bjørn Pedersen, Editor).

The Hyderabad Congress and the Regional Associates took advantage of the *Newsletter* to advertise their upcoming meetings as well as other meetings in Canada, Germany (2), Italy, Switzerland and USA. In addition, a calendar of future meetings throughout the world was published in every issue and, sadly, obituaries of 11 prominent crystallographers were reported during the triennium. There were five cover/feature articles: *XXIII IUCr Congress and General Assembly; Development of Superspace Crystallography and its Application to the Analysis of Aperiodic Crystals; How Lawrence Bragg Shortened World War I; War, Peace and Crystallographers; and First Pan-African Conference on Crystallography*. Covers highlighted IYCr2014, IUCr journals, the 2014 Ewald Prize, Regional Associate and other meetings, Crystallography in Norway and the Montreal and Hyderabad Congresses.

All twelve issues published in the triennium contained 24 pages, to give a total of 288 pages.

A significant portion of the support for the publication and distribution of the *Newsletter* comes from advertising revenue. We experienced a decrease of revenue over the triennium with Volume 22 averaging 7.75 advertisements per issue, Volume 23 averaging 6.25 and Volume 24 averaging 5.75. There were a total of 29 advertisements on the electronic issue web site.

The electronic version had an average distribution of 12,602. We continue to send print copies to 560 libraries and individuals and various crystallographic meetings.

Patti Potter is responsible for the desktop preparation of all copy, all negotiations with the printer, postal authorities, and distribution houses, maintenance and production of the mailing list, and solicitation and handling of all advertising. She is working remotely from Alaska.

*W.L. Duax, Editor*

#### **A9. Diffraction Data Deposition Working Group (DDDWG)**

The DDDWG was established in 2011 and approved to continue in 2014. It has achieved a global coverage, an excellent range of specialist consultants and good links to the IUCr Commissions. Furthermore, it has been very active as measured, for example, by organizing the following events: a launch meeting at the Madrid Congress; a meeting at the ACA Boston meeting in 2012; an international Workshop at ECM27 in Bergen, Norway; a lunchtime Forum held at ECM28 in Warwick, UK; a two-day Workshop at the ECM29 meeting in Rovinj, Croatia; and a one-day Workshop at the ACA New Orleans meeting in May 2017. The IUCr Forum on Data (<http://forums.iucr.org/viewforum.php?f=21>) established by the DDDWG has been very actively utilized for community input as well as for sharing the reports and discussion documents of the DDDWG.

The presentations at the Rovinj Workshop entitled Metadata for Raw Data from X-ray Diffraction and Other Structural Techniques can be found at <http://www.iucr.org/resources/data/dddwg/rovinj-workshop>.

An overview article [Kroon-Batenburg, Helliwell, McMahon & Terwilliger (2017). *IUCrJ*, **4**, 87–99] arose from the Rovinj Workshop and is entitled *Raw Diffraction Data Preservation and Reuse: Overview, Update on Practicalities and Metadata Requirements*. A number of other articles arising directly or indirectly from the Rovinj workshop have also been published in IUCr and other journals.

We led the IUCr's response to the ICSU Report *Open Data in a Big Data World*, which can be found at <http://www.iucr.org/news/press-releases/open-data>.

We have taken an active role in International Data Week held in Denver, USA, in September 2016, including organizing a session on Crystallographic Databases that has resulted in a summary overview article submitted to *Data Science Journal*.

We have continued to provide a stimulus to the IUCr Commissions to define their technique's raw data and associated metadata definitions. Most recently, the Research Data Management Workshop at the ACA in New Orleans, USA, in May 2017 included speakers across as many of the IUCr Commissions as possible.

The DDDWG will transform into a wide-ranging Committee on Data for the IUCr from the time of the Hyderabad Congress; known as CommDat, its role and membership is described in detail at <http://www.iucr.org/iucr/governance/advisory-committees/committee-on-data>. Its role basically is as follows: *The Committee on Data (CommDat) will work with the IUCr's Commissions, including the Commission on Journals, having a coordinating and advisory role regarding data. CommDat will report directly to the IUCr's Executive Committee and will subsume the functions of the Diffraction Data Deposition Working Group, which will cease to exist as a separate entity from the time of the IUCr Congress in Hyderabad in August 2017, and will continue the data-related interests of the now discontinued Committee on Crystallographic Databases and of the Committee on Electronic, Publishing, Dissemination and Storage of Information. It will exist alongside, and have a formal relationship with, the Committee for the Maintenance of the CIF Standard (COMCIFS), which will continue with its technical brief to manage the CIF standard, at least during the current period of active development of the CIF specification and dictionaries.*

J.R. Helliwell and B. McMahon

#### A10. IUCr/Oxford University Press Book Series Committee

In the period September 2014 to 2016, the cooperation between Oxford University Press (OUP) and the IUCr/OUP Book Series Selection Committee has been productive. Although no books appeared in 2014 and 2016, this has been an accident of scheduling – there are a good number in the pipeline.

The following were published in 2015:

The history book *Crystal Clear. The Autobiographies of Sir Lawrence and Lady Bragg*, by A. M. Glazer, Patience Thomson, published 23 July 2015.

A new volume in the *Texts on Crystallography* series: *Basics of Crystallography and Diffraction*, Fourth Edition, by Christopher Hammond, published 11 June 2015.

In addition the history book *Early Days of X-ray Crystallography*, by André Authier was republished in paperback 29 October 2015.

At the time of preparing these papers, there are nine forthcoming books in the series.

Sadly, Professor Davide Viterbo, Chair of the Committee, died in May 2017. A new Chair will be appointed by the Executive Committee in due course. In the meantime, the Committee is very interested in proposals for new volumes and encourages prospective authors to contact the Executive Secretary ([execsec@iucr.org](mailto:execsec@iucr.org)). Readers may suggest topics and/or authors, as they know the subjects that are not well covered in the literature. Manuscripts covering important aspects of crystallography and related fields are very welcome.

## A11. Sponsorship of meetings: Sub-committee on the Union Calendar

The present membership of the Sub-committee comprises: H.A. Dabkowska (Canada), R. Baggio (Argentina), D. Billing (South Africa), K. Shankland (UK), P. Spadon (Italy), A. Nakagawa (Japan) and K.A. Kantardjieff (USA; *ex officio* as Chair of the Commission on Crystallographic Teaching), being chaired by W. Depmeier (Germany). The Sub-committee members, including the Chair, for the next triennium will be decided in Hyderabad.

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

The total amount used for sponsoring the participation of young scientists in meetings was CHF 174,268 in 2011, CHF 191,714 in 2015 and CHF 166,691 in 2016.

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

Second South African School on Fundamental Crystallography – satellite meeting of the 21st Meeting of the International Mineralogical Union, Bloemfontein, South Africa, 25–29 August 2014.

Quantum Materials: New Crystals versus Novel Properties, Beijing, People's Republic of China, 26–28 August 2014.

1st European Crystallography School, Pavia, Italy, 28 August – 6 September 2014.

Crystallography in Materials Science: Novel Methods for Novel Materials (EMRS Symposium N), Warsaw, Poland, 15–19 September 2014.

Current Trends in Structural Biology and 7th International Conference of the Hellenic Crystallographic Association, Heraklion, Crete, Greece, 19–21 September 2014.

The 6th AONSA Neutron School 2014, Kawasan Puspitek Serpong, Tangerang, Indonesia, 12–17 October 2014.

XVIII International Conference on Crystal Chemistry, X-ray Diffraction and Spectroscopy of Minerals, Yekaterinburg, Russia, 13–15 October 2014.

2014: Crystal (cl-)Year, Turin, Italy, 16–17 October 2014.

Symmetry Relationships Between Crystal Structures with Application to Structural Phase Transitions, Varanasi, India, 27–31 October 2014.

Atomic Pair Distribution Functions Technique: Fundamentals and Applications, Mar del Plata, Argentina, 31 October – 1 November 2014.

VI School of the Argentinian Crystallography Association, Mar del Plata, Argentina, 3–7 November 2014.

Frontiers of Structural Biology: New Advances in X-ray Diffraction and Cryo-Electron Microscopy, New Delhi, India, 15–17 December 2014.

Structural Biology: Using Synchrotron Radiation to Visualize Biological Molecules, Trieste, Italy, 15–19 December 2014.

Computational Materials Discovery Using the USPEX Code, Shiv Nadar, India, 20–24 January 2015.

- Asian XD Charge Density Workshop, Bangalore, India, 16–18 February 2015.
- Fifth Winter School on Soft X-rays in Macromolecular Crystallography, Athens, GA, USA, 28 February – 3 March 2015.
- XV Intensive Teaching School in X-ray Structure Analysis, Durham, UK, 21–29 March 2015.
- Macromolecular Crystallography School 2015: From Data Processing to Structure Refinement and Beyond, Montevideo, Uruguay, 6–15 April 2015
- 3rd School on Crystal Structure Determination From Diffraction Data: Application to Powder Samples, Sousse, Tunisia, 9–12 April 2015.
- RapiData 2015, Stanford, USA, 26 April – 1 May 2015.
- 5th International School on Biological Crystallization, Granada, Spain, 24–29 May 2015.
- To.Sca.Lake: Total Scattering Analysis of Nanoscaled Materials, Como, Italy, 25–28 May 2015.
- Engineering Crystallography: From Molecules to Crystal to Functional Form, Erice, Italy, 5–14 June 2015.
- Sagamore XVIII Conference on Charge, Spin and Momentum Densities, Sardinia, Italy, 7–12 June 2015.
- Zürich School of Crystallography 2015: Bring Your Own Crystals, Zürich, Switzerland, 7–20 June 2015.
- 22nd International Conference on the Chemistry of the Organic Solid State (ICCOSS XXII), Niigata, Japan, 12–17 July 2015.
- Second Balkan School on Fundamental Crystallography and Workshop on Magnetic Symmetry and Its Application in Magnetic Structure Description, Marmaris, Turkey, 13–19 July 2015.
- 2nd AONSA Asia–Oceania Conference on Neutron Scattering (AOCNS-2015), Sydney, Australia, 19–23 July 2015.
- Electron Diffraction for Quantitative Surface Structure Determination, Lodz, Poland, 19–26 July 2015.
- Annual Meeting of the American Crystallographic Association, Philadelphia, USA, 25–29 July 2015.
- I Peruvian Congress of Crystallography and Course on Methods of Analysis of Polycrystals by X-ray Diffraction, Lima, Peru, 4–6 August 2015.
- Indaba 8, Kruger National Park, South Africa, 16–21 August 2015.
- 16th International Conference on X-ray Absorption Fine Structure (IXAS-16), Karlsruhe, Germany, 23–28 August 2015.
- 29th European Crystallographic Meeting (ECM29), Rovinj, Croatia, 23–28 August 2015.
- Electron Crystallography School (ECS2015), Rovinj, Croatia, 28–31 August 2015.
- ECNS 2015 VI European Conference on Neutron Scattering, Zaragoza, Spain, 30 August – 4 September 2015.
- 2nd European Crystallography School (ECS2), Mieres, Spain, 31 August – 5 September 2015.
- Aperiodic 2015, Prague, Czech Republic, 1–6 September 2015.
- European School on Crystal Growth/Fifth European Conference on Crystal Growth, Bologna, Italy, 5–8 and 9–11 September 2015.

22nd Brazilian Crystallographic Association (ABCr) Meeting and II Latin-American Crystallographic Association (LACA) Meeting, São Paulo, Brazil, 9–11 September 2015.

8th European Conference on Mineralogy and Spectroscopy (ECMS 2015), Rome, Italy, 9–11 September 2015.

9th AOFSSR Cheiron School, Hyogo, Japan, 10–19 September 2015.

2015 High-Pressure Workshop, Campinas, Brazil, 11–15 September 2015.

13th School on Synchrotron Radiation, Grado, Italy, 14–25 September 2015.

XXIII Conference on Applied Crystallography, Krynica Zdroj, Poland, 20–24 September 2015.

Size–Strain VII, Oxford, UK, 21–24 September 2015.

International School on Introduction to the Rietveld Refinement, Sofia, Bulgaria, 28 September – 3 October 2015.

Workshop on Powder Diffraction of Organic Compounds, Frankfurt/Main, Germany, 6–8 October 2015.

VII School of the Argentinian Crystallography Association, La Plata/Buenos Aires, Argentina, 26 October – 3 November 2015.

9th International Conference on Inelastic X-ray Scattering (IXS 2015), Hsinchu, Taiwan, 23–27 November 2015.

13th Conference of the Asian Crystallographic Association, Kolkata, India, 5–8 December 2015.

3rd School on Crystallization and Crystallography for Latin America (ECRISLA 2015), Florianópolis, Brazil, 7–11 and 14–18 December 2015.

BioXFEL STC, San Juan, Puerto Rico, 13–15 January 2016.

Macromolecular Crystallography School 2016: From Data Processing to Structure Refinement and Beyond, São Carlos, Brazil, 3–12 April 2016.

Powder Diffraction and Rietveld Refinement School, Durham, UK, 10–14 April 2016.

Crystallography for Space Sciences, Puebla, Mexico, 17–30 April 2016.

Crystallization Focus on Micro and Nano Crystals and High-Throughput Methods, Stanford, USA, 19–22 April 2016.

RapiData 2016, Stanford, USA, 24–29 April 2016.

6th Meeting on X-ray and Other Techniques in Investigations of the Objects of Cultural Heritage, Krakow, Poland, 19–21 May 2016.

5th International School on Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials, Granada, Spain, 22–27 May 2016.

High-Pressure Crystallography: *Status Artis* and Emerging Opportunities, Erice, Italy, 27 May – 5 June 2016.

11th USPEX Workshop on Evolutionary and Interpretative Methods for Discovering the Structures and Rationalizing the Properties of Crystalline, Surface and Nanoparticle Materials, Lake Como, Italy, 5–9 June 2016.

ED-XPD Workshop – Combining Electron and X-ray Powder Diffraction Techniques for Structural Characterization, Stockholm, Sweden, 6–10 June 2016.

15th European Powder Diffraction Conference (EPDIC15), Bari, Italy, 12–15 June 2016.

2016 Kuo Symposium on 3D Cryo-EM Molecular Imaging and 9th K.H. Kuo Summer School on Electron Microscopy and Crystallography, Beijing, People's Republic of China, 24–29 June 2016.

7th European Charge-Density Meeting (ECDM7): Latest Advances in Methodology and Applications of Charge Densities, Warsaw, Poland, 26 June – 1 July 2016.

International School on Fundamental Crystallography with Applications to Electron Crystallography, Antwerp, Belgium, 27 June – 2 July 2016.

ICCBM16 – 16th International Conference on the Crystallization of Biological Macromolecules, Prague, Czech Republic, 2–7 July 2016.

3rd International School on Aperiodic Crystals, Antwerp, Belgium, 4–9 July 2016.

Annual Meeting of the American Crystallographic Association, Denver, Colorado, 22–26 July 2016.

Serial Crystallography Data Analysis Workshop, Denver, USA, 22 July 2016.

Computational Approaches to the Structural Modelling of Biological Macromolecules using Small-Angle Scattering, Denver, USA, 23 July 2016.

16th International Summer School on Crystal Growth (ISSCG-16), Shiga, Japan, 1–7 August 2016.

18th International Conference on Crystal Growth and Epitaxy (ICCGE-18), Nagoya, Japan, 7–12 August 2016.

12 International Conference on Biology and Synchrotron Radiation, Stanford, USA, 21–24 August 2016.

PSI Powder Diffraction School 2016, Villigen, Switzerland, 22–26 August 2016.

International School on Charge and Spin Density: From Experimental Determination to Interpretation, Nancy, France, 24–27 August 2016.

30th European Crystallography Meeting (ECM30), Basel, Switzerland, 28 August– 1 September 2016.

Fifth SMARTER Crystallography Conference, Bayreuth, Germany, 4–8 September 2016.

AIC International Crystallography School 2016, Rimini, Italy, 7–11 September 2016.

International Soft Matter Conference (ISMC2016), Grenoble, France, 12–16 September 2016.

13th International Conference on Quasicrystals, Kathmandu, Nepal, 18–23 September 2016.

2016 High-Pressure Workshop, Seoul, Republic of Korea, 20–23 September 2016.

3rd European Crystallography School (ECS3), Bol, Croatia, 25 September – 2 October 2016.

First Pan-African Meeting on Crystallography, Dschang, Cameroon, 6–10 October 2016.

2nd International Workshop on X-ray Crsytallography in Structural Biology, Lahore, Pakistan, 15–20 October 2016.

VIII Mexican Crystallographic Meeting (VIII-SMCr) and III Latin-American Crystallography Meeting (III-LACA), Merida, Mexico, 23–27 October 2016.

6th Moroccan School of Crystallography — EMC6, Meknes, Morocco, 22–25 November 2016.

International School on Fundamental Crystallography (Fifth MaThCryst School in Latin America), Havana, Cuba, 30 October – 5 November 2016.

VIII School of the Argentinian Association of Crystallography, San Luis, Argentina, 14–18 November 2016.

14th Conference of the Asian Crystallographic Association, Hanoi, Vietnam, 4–7 December 2016.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

## A12. Reports of Representatives on Regional and Scientific Associates

### A12.1. American Crystallographic Association (ACA)

This triennial report for the activities of the ACA (<http://www.amercrystalassn.org/>) as a Regional Associate of the IUCr is an overview of the more detailed Annual Reports presented each year since the Montreal Congress in 2014, as well as an outline of future activities announced by the ACA.

ACA officers change each year; serving as ACA Presidents during this period were Martha Teeter (2014), Chris Cahill (2015) and Tom Terwilliger (2016). For 2017, Amy Sarjeant is the ACA President and Lisa Keefe is the Vice-President. Michael

James served as the Canadian National Committee for Crystallography (CNCC) representative; he will be replaced by Tomislav Friscic from 2017.

ACA finances rely heavily on individual membership dues, in part to cover expenses for the ACA headquarters office in Buffalo. The membership of the ACA was 1,221 paid members by the end of 2014 compared to under a 1,000 at the end of 2016, a substantial decrease during this triennium.

Most ACA members are from the USA and Canada, although there are some ACA members from countries around the world. ACA activities are primarily focused on its Annual Meetings, support for its summer schools, and the publication of the Newsletter *ACA RefleXions*, which is an excellent source of information about all ACA activities. Past issues of *RefleXions* are available online from the ACA web site.

The 64th ACA Annual Meeting in 2014 (an IUCr Congress Year) was held in Albuquerque, New Mexico, 24–28 May. At this meeting 450 participants presented 128 posters and 221 lectures: thirty-one vendors participated in the Exhibit Show; the Programme Chairs were Christine Beavers and Peter Zwart; Ilia Guzei served as the Poster Chair; Yulia Sevryugina and her fellow young scientists were all responsible for outstanding sessions and great social events. More information about this venue and details about the programme and the three adjacent workshops (Joint Neutron and X-ray Structure Refinement using Joint Refine in *PHENIX* organized by Pavel Afonine, Marat Mustyakimov, Zoe Fisher and Andrey Kovalevsky; Grazing Incidence SAXS Theory and Data Analysis organized by Alex Hexemer and Chenhui Zhu; and Reciprocal Space Visualization *MAX3D* organized by Jim Britten) can be found at <http://www.amercrystalassn.org/2014>.

Three of the ACA's major awards were presented at the meeting in Albuquerque: the Patterson Award to John Helliwell, the Etter Early Career Award to Borden Lacy and the Wood Writing Award to Dan Rabinovich. The 2014 summer school was held from 7–16 July at Notre Dame.

The 65th ACA Annual Meeting in 2015 was held in Sheraton Downtown Hotel, Philadelphia, 25–29 July (<http://www.amercrystalassn.org/2015-mtg-homepage>). It was attended by 656 participants, with many first-time attendees. 448 abstracts were submitted. The educational impact of this and future meetings was hailed as extremely important. The Programme Chairs were Louise Dawe and Kraig Wheeler. Yulia Sevryugina and her fellow young scientists were all responsible for outstanding sessions and great social events. About 40 exhibitors (including the IUCr) participated in the Exhibit Show. The event was sponsored by 24 organizations, including the IUCr and AIP Publishing, and it generated some income.

The 2015 ACA Award Winners were Laurence Marks (Warren Award), Greg Petsko (Buerger Award) and Yan Jessie Zhang (Etter Early Career Award). This year the recipient of the ACA Service Award was Ilia Guzei. Judith Kelly, who is the Council of Scientific Society Presidents (CSSP) Secretary and ACA Representative to CSSP, submitted an extensive report to the ACA Council.

*The 66th ACA Annual Meeting* in 2016 was held in Sheraton Downtown Hotel, Denver, 22–26 July (<http://www.amercrystalassn.org/2016-meeting-homepage>). It was attended by 570 participants, with some first-time attendees. The Programme Chairs were Amy Sarjeant and Eddie Snell; Martin Donakowski and George Lountos were responsible for outstanding YSSIG sessions and great social events. The *Would you Publish This?* session, chaired by Louise Dawe and Danielle Gray, as well as the *Career Development* session, featuring Brad Conrad (AIP), were very well attended and appreciated by young participants.

The 2016 ACA Award winners were Jason Benedict (Etter Award), Axel Brunger (Trueblood Award), Elspeth Garman (Fankuchen Award) and Benno Schoenborn (Bau Award).

The meeting was supported by about 20 sponsors, including the IUCr.

At the General Business Meeting it was voted that the ACA membership renewal rates would slightly increase; these are posted on the web site now. The importance of the educational impact of the Denver meeting was very much applauded.

The ACA 2016 Summer School Course in Chemical Crystallography was hosted at the University of Notre Dame, 12–19 June (<http://acasummercourse.net>).

The 67th ACA Annual Meeting in 2017 (an IUCr Congress Year) will be held at the Hyatt Regency Hotel in New Orleans, Louisiana, 26–30 May. Yulia Sevryugina and Ilia Guzei co-Chair this meeting.

The 68th ACA Annual meeting in 2018 will be held 20–24 July in Toronto, Ontario, Canada.

The 69th ACA Annual Meeting in 2019 is planned in Covington, KY.

International Year of Crystallography (IYCr2014). The ACA strongly and efficiently supported glorifying IYCr2014. Martha Teeter, the head of the *ad hoc* Committee coordinating regional celebrations and activities for IYCr2014, was very pleased with the outcome.

The ACA Council committed USD 12,000 to fund activities related to IYCr2014 in North America. Of this amount, about USD 5,000 was allocated via a call for proposals with the balance used for Task Force projects, including a National Crystal Growth Contest.

The main achievements were:

- (1) US Crystal Growing Competition, organized by Jason Benedict. This served 200–300 students.
- (2) USA/Canada IYCr Facebook Video Contest, organized by Amy Alexis Sarjeant, Louise Dawe, and Christine Beavers. Elementary and high-school students had their teachers submit videos to Facebook. Eight videos were submitted, some of which received more than 2,000 views.
- (3) WI Crystal Growth Contest and Lecture Tour, by Ilia Guzei. 200 students from 18 schools participated in growing crystals of copper sulphate. Very successful venue, the 2015 competition was also very good.
- (4) RCSB PDB's Art if Science Traveling Exhibit, by Christine Zardecki. Two to three thousand high-school and college students have seen the exhibition. This continued into 2015.
- (5) University of Illinois, Chicago, Symposium for IYCr, by Constance Jeffery, Gerd Prehna and Bernard Santarsiero. This served 130 minority-diverse undergraduates and graduate students.
- (6) Crystal Growth Contest for Valley Central High School, by Terri Campbell. 45 students grew crystals and gave poster presentations. 100 attended the poster event.
- (7) NSTA Presentation to Science Teachers in Long Beach Regional Meeting, organized by Martha Teeter. Crystal growth demonstration (borax), crystal packing/properties (fcc and hcp), lego building face-centred cubic (2X), VESTA visualization, diffraction basics with ICE slides. 25 teachers attended.

More information about the IYCr activities can be found at <http://iycr2014.org/countries/usa>.

Cora Lind-Kovacs and Ilia Guzei were the ACA delegates to the IYCr Legacy Meeting Crystallography for the Next Generation organized in Rabat, Morocco, 22–24 April 2015.

ACA Fellows. The ACA Fellows Programme was created to recognize a high level of excellence in scientific research, teaching, and professional duties as well as service, leadership and personal engagement in the ACA and the broader world of crystallography and science. During the past three years 24 Fellows have been inducted. 2014 ACA Fellows were Eddy Arnold, Abe Clearfield, Larry Dahl, George Philips, Ned Seeman, John Spence, Ron Stenkamp and Winnie Wong-Ng. 2015: Zbigniew Dauter, David Eisenberg, John Heliwell, Hakon Hope, Thomas Koetzle, Paul Langan and David Rose. 2016: Gerard Bricogne, I. David Brown, Charles Campana, Bryan Chakoumakos, Yu Sheng Chen, Frank Fronczak, Michael James, Brian Matthews and Arnie Rheingold.

ACA Journal *Structural Dynamics*. The relatively new ACA online journal *Structural Dynamics* ([sd.aip.org](http://sd.aip.org)), with an impact factor of 3.667, is co-published with the AIP. Journal topics include structural dynamics of molecular systems, biological systems, solid materials, liquids and solutions, surfaces and interfaces studies using highly coherent sources. It is not yet bringing any profit to ACA.

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

African Crystallography Initiative. When the IUCr, along with ICSU, UNESCO and other agencies, identified Africa as an area in need of development and support for crystallography research, the ACA started a fund to support students from developing African countries in attending annual ACA meetings, as well as various ACA schools and workshops. Funds will also go to awards for outstanding presentations by African students at conferences within Africa; they will be used to support outreach efforts in developing African countries and to bring African visiting scientists to North America.

The relatively recently created Latin-American Crystallographic Association (LACA) would also probably require some kind of assistance (mostly in the form of short courses and training) from the ACA.

Strategic planning. With the planned retirement of Marcia Colquhoun (Director of Administrative Services) and Bill Duax (CEO), Chris Cahill prepared for the Fall 2016 Council Meeting an impressive overview of the current situation of ACA and of the possible changes that have to be implemented in the near future. Some options were discussed looking for different staffing models. It was decided that Council needed to find a meeting planner to assist in 2017 and to do the complete job in 2018 (outsource the organization of the meeting completely).

Kristina Vitale will be working full time for the ACA Buffalo office from 1 January 2017. Her job title is Membership Secretary.

Marcia Colquhoun will continue to work half time until the end of 2017.

Bill Duax provided recommendations for CEO and Headquarters transition in 2017–2018.

S.N. Rao (CFO) reported to the Council, stressing that 2016 and 2017 budgets project losses. The ways to cut costs were discussed. For the past 10 years the ACA has operated at a loss of about USD 30,000 per year. There are continuous efforts to reduce personnel costs and increase income and membership. Member donations can help carry the ACA through the difficult period. There is a ‘donate’ button on the ACA web site and the ACA is a 501(c)(3) non-profit organization so donations are tax-deductible to the full extent allowed by USA law.

Social Media. The ACA now has a presence on Facebook (American Crystallographic Association) and on Twitter and Instagram (ACAxtal)

In 2017 the *IUCr Newsletter* will be handed over from Bill Duax to the IUCr.

The Canadian National Committee for Crystallography (CNCC). Canada is the largest single country outside the United States to contribute to the goals and purposes of the ACA. The Canadian Division exists therefore to promote the interests of Canadian members and to provide for an elected official to represent these interests on the ACA Council. The main office of the CNCC re-located to the Canadian Light Source (in Saskatoon), the terms of reference agreement between NRC (the group that has been responsible for the CNCC and membership in the IUCr) has been updated and so have the roles of CNCC members in the future. The new CNCC web site is established, <http://xtallography.ca/>. The new Chair of CNCC is Patrick Mercier, the Vice Chair is Tomislav Friscic, the Executive Secretary is Michel Fodje and the Treasurer is Brian Patrick. Their terms will be 3 years.

H.A. Dabkowska, IUCr Representative

## A12.2. Asian Crystallographic Association (AsCA)

AsCA continues to play a leading role in the nurturing of collective crystallographic activities in the Asia–Pacific region with successful scientific meetings being held in those years in which there is no IUCr Congress and General Assembly.

### *AsCA executive officers*

In the period 2013–2016 the office bearers of AsCA were Pinak Chakrabarti (President, India), Jennifer Martin (Vice-President, Australia), J.J. Vittal (Secretary/Treasurer, Singapore) and Se Won Suh (Immediate Past President, Korea). The current executive officers for the term 2016–2019 were elected in Hanoi, Vietnam, and are: Jennifer Martin (President, Australia), Xiao-Dong Su (Vice-President, People's Republic of China), Edward R.T. Tiekkink (Secretary/Treasurer, Malaysia) and Pinak Chakrabarti (Immediate Past President, India).

### *AsCA scientific meetings in the period 2014–2016*

#### (i) AsCA 2015

The 13th Conference of the Asian Crystallographic Association was held at Science City, Kolkata, India, 5–8 December 2015. This is the second time the meeting has been held in India, the earlier occasion being in 2001 (18–21 November) at Bangalore. The meeting had about 393 participants (279 male, 114 female) from 26 countries, with the break-up among different countries being: Australia 36, Bangladesh 19, Brazil 1, People's Republic of China 10, France 2, Germany 4, Hong Kong 2, India 194, Ireland 1, Italy 1, Japan 46, Korea 12, Netherlands 1, New Zealand 3, Nigeria 1, Saudi Arabia 2, Singapore 12, Sri Lanka 2, Switzerland 2, Taiwan 9, Thailand 2, UAE 1, UK 13, USA 13, Uzbekistan 2, Vietnam 2.

The International Programme Committee, led by Alice Vrielink, put up an intensive programme that covered all aspects of crystallography and the latest developments in techniques and software. The scientific session consisted of 4 Plenary talks (by Petra Fromme, Mohaned Eddaoudi, Kenneth Harris and M. Vijayan), 5 Keynote addresses (by Michelle Dunstone, Sue-Lein Wang, Michi Suga, Haitao Li and Parmial Bharadwaj), and 102 oral presentations distributed over 18 Microsymposia (MS1–18), two software sessions (CS1–2) and one General Interest session (GIS) on pharmaceuticals. There were about 180 poster presentations. A special AsCA Rising Star Session was conducted on the last day, where the six best abstracts submitted by young participants (PhD or early post-docs), as selected by a panel of judges, made a 15-minute oral presentation of their work. This gave an opportunity to the promising young scientists to present their work and provide a boost to their scientific career. Besides, there were three IUCr Poster Prizes, three AsCA 2015 Poster Awards and one RCSB PDB Award. About 10 commercial sponsors exhibited at the meeting and Bruker made a worldwide launch of their product D8 Venture – this is the first time that a product has been launched at an AsCA meeting. The IUCr supported the meeting generously, as did many granting agencies from India and academic institutions and bodies.

#### (ii) AsCA 2016

The 14th Conference of AsCA (AsCA 2016) was held in Hanoi, Vietnam (Venue: Hanoi University of Science and Technology, 4–7 December 2016), coinciding with the 60th anniversary of the host Institute. Professor Duong Ngoc Huyen was the LOC Chair, and Professor Masaki Kawano was the Chair of the International Programme Committee. The AsCA 2016 meeting consisted of two parallel satellite meetings, eighteen Microsymposia, an education conference workshop on minerals and gems, crystallographic software sessions, a special section on materials and a 'Rising Star' session by young scientists. The scientific scope of AsCA 2016 covered all important aspects of crystallography-related areas, including synchrotron/neutron, structural biology, chemical crystallography, materials and polymer science, crystal growth/crystallization, electron microscopy, informatics, and much more. 457 participants from 38 different countries attended the conference, the breakup from each country being: Japan 119, Korea 59, Vietnam 42, India 38, People's Republic of China, including Hong Kong 32+9, Australia 24, Thailand 19, Taiwan 18, Singapore 18, UK 17, Malaysia 12, Russia 7, USA 6, New Zealand 5, Germany 5, Nigeria 3, Turkey 2, Sweden 2, Philippines 2, Italy 2, Iran 2, Canada 2, Bangladesh 2, UAE 1, Belgium 1, Côte d'Ivoire 1, Cameroon 1, Czech Republic 1, Spain 1, France 1, Croatia 1, Indonesia 1, Sri Lanka 1, Mongolia 1, Netherlands 1, Tunisia 1, Yemen 1, South Africa 1.

### (iii) AsCA 2018 and beyond

The 15th AsCA Conference (AsCA 2018) will be held in Auckland, New Zealand, 2–5 December 2018. Professors Chris Squire and Kurt Krause will be in charge of the LOC and Professor Ted Baker is the Programme Chair. AsCA 2019 will be held in Singapore, and Professor J.J. Vittal will be the Local Chair. Details of the two meetings will be submitted at the next Council meeting to be held at Hyderabad during IUCr 2017. At the Council meeting held at Hanoi (6 December 2016) a proposal was received from the Malaysian representative to host the 17th AsCA Conference at Sunway University, Petaling Jaya, Malaysia, December 2021.

#### *Sponsoring PCCrI*

AsCA was one of the proud sponsors of the 1st Pan-African Conference on Crystallography, held at the University of Dschang, Cameroon, 6–10 October 2016.

#### *AsCA Regional Committee membership*

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

*M. Takata, IUCr Representative*

### **A12.3. European Crystallographic Association (ECA)**

The ECA is a scientific association among national members and individual members and corporate affiliates. It has 12 SIGs (Special Interest Groups) and 3 GIGs (General Interest Groups). The youngest GIG is GIG3 – Education in Crystallography.

The main ECA event – ECM (European Crystallographic Meeting) – is organized every year except the year of the IUCr Congress. The programmes of ECMs are mainly prepared by SIGs and GIGs and it is usually based on five focus areas: Biological and Macromolecular Crystallography, Materials and Minerals, Physical Including Fundamental Crystallography, Chemical Crystallography, and Experimental and Computational techniques. This way appeared to be quite effective but of course cannot be perfect.

Two conferences in these three years were organized and both were very successful. ECM29 took place in Rovinj, Croatia, 23–25 August 2015. The programme was organized mainly in 50 sessions (6–7 in parallel) with typically five lectures per session. The organizers announced overall 785 scientific contributions and 1,050 participants, which is one of the highest attendances of ECMs in the last 20 years. One third of the participants came from the UK and Germany. There were two Plenary Lectures, 16 Keynote Lectures and quite a large exhibition with 32 exhibitors. The attendance of 55 students was financially supported. Ten satellite meetings were organized mainly close to the start of the conference and mostly focused on crystallographic software. The Electron Crystallography School was in Porec after the conference. In the social programme, the traditional Young Crystallographers Mixer was included (see <http://ecm29.ecanews.org>).

ECM30 took place in Basel, Switzerland, 28 August – 1 September 2016. The programme scheme was as usual and similar to ECM29. There were even more scientific contributions (835), there were 931 delegates from 47 countries, 30 exhibitors, nearly 300 speakers and 467 posters. The organizers have provided more figures: 296 women, 36 retired people from 15 countries, 179 students from 32 countries. The most represented countries were: Switzerland (181), Germany (173), UK (120) and France (71). 8 satellite meetings accompanied the conference (see <http://ecm30.ecanews.org>).

The organization of ECM31 was assigned to the Spanish Crystallographic Association, Oviedo, Spain, 22–27 August 2018 (Chair: Santiago García Granda). It will be organized in the Palace of Exhibitions and Congresses of Oviedo. The organizers also suggested a programme for families and their children in order to attract young crystallographers with families, and also streaming of lectures.

ECM32 will take place at the University of Vienna, Austria, in 2019 (Chair: Klaudia Hradil). France is preparing a bid for the ECM in 2021 in Paris.

The main ECA prizes – Max Perutz Prize and Erwin Felix Bertaut Prize – are awarded during the ECMs.

The Max Perutz Prize is awarded in recognition of meritorious achievements in any branch of crystallography by a crystallographer having a clear affiliation with the ECA region and being an individual member of the ECA. It can be for leadership or scientific contributions or both. It is awarded at each ECM. The 8th Max Perutz Prize was awarded in Rovinj to Professor John R. Helliwell, Emeritus Professor of Chemistry, University of Manchester, UK, for his ‘long, generous and fruitful dedication to developing all aspects of the use of synchrotron radiation for crystallography and for his boosting support to global development of synchrotron and neutron facilities... He also has been constantly engaged in outreach and dissemination of crystallography to the scientific community’. The 9th Prize was awarded in Basel to Dr Václav Petříček from the Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic, for ‘his practical application of the theory of aperiodic structures in his computing system JANA... JANA has made aperiodic structures accessible to a wide community of crystallographers and chemists’.

The Erwin Felix Bertaut Prize is awarded to a young scientist having a clear affiliation with the ECA/ENSA region (up to 5–8 years after finishing PhD thesis) and an individual member of ECA/ENSA (European Neutron Scattering Association), in recognition of notable experimental theoretical or methodological contributions in the field of investigation of matter using crystallographic or neutron scattering methods. ECA and ENSA award the Prize in an alternating sequence. The 7th Prize was awarded to Dr Giorgio Schiro from the Institut de Biologie Structurale of the CNRS Grenoble, France, for his scientific contribution in the innovative science field of protein dynamics and the 8th Prize was given to Dr Linda Reinhard from the Karolinska Institutet at DESY, Hamburg, Germany, for her pioneering contributions to the crystallographic analysis of enzymes and the optimization of protein preparations for diffraction studies.

During ECMs two ECA council meetings are always arranged. The ECA Executive Committee had the following composition until 2015: Andreas Roodt (President), Santiago Garcia-Granda (Past President), Alessia Bacchi (Vice-President), Georgina Rosair (Secretary), Christian Lehmann (Treasurer), Udo Heinemann, Joke Hadermann, Olga Yakubovich (officers) and Fermin Otalora (education coordinator). During ECM29 in Rovinj, a new Executive Committee was elected. Alessia Bacchi became President, Andreas Roodt was Immediate Past President and Udo Heinemann was elected as Vice-President, the Secretary and the Treasurer continued in the new Committee as well as Joke Hadermann and Fermin Otalora. Two new members were elected as officers – Marijana Dakovic and Carl Henrik Görbitz. The next election will be at ECM31 in 2018.

The Committee has regular winter meetings, in a year when there is an ECM this is always in the place of the next ECM and it also checks the corresponding conference venue. This winter meeting is usually scheduled in February and it is always in a very working environment since the whole of the weekend is dedicated to this, unlike the summer one, organized in the busy time of the ECM or IUCr Congress. In 2015, the meeting was in Basel, Switzerland, and in 2016 in Parma, Italy (city of the ECA President because in 2017 there is no ECM).

The ECA is a member of ISE (Initiative for Science in Europe) – an independent platform of European learned societies and scientific organizations whose aim is to promote mechanisms to support all fields of science at a European level. The ISE meetings are attended always by one ECA representative. There is discussion now if the ECA should continue this membership.

The ECA places increasing emphasis on crystallographic education and organizes European Schools of Crystallography. The 2nd European Crystallography School (ECS) was held in Mieres (Asturias), Spain, in 2015 with the title Crystallography: Fundamentals, Online Tools and Applications. It was divided into four different modules: one day Preschool, three days Fundamental Crystallography, two days Specific Subjects and one day Hot Topics (electron diffraction, synchrotron serial crystallography). There were 17 lecturers and 32 students. The students presented 27 posters. The 3rd school was organized by the Croatian Association of Crystallographers (25 September – 2 October 2016, in Bol, Croatia), with 24 lecturers and 77 participants. The programme consisted of three and half days of fundamentals and then two parallel modules: Structure Solution of Small Molecules from Single Crystals, and Structure Solution from Powder Data. The fourth ECS will take place in Warsaw, Poland, 2–7 July 2017, and the fifth ECS in Stellenbosch (South Africa) in 2018. The ECA worked out quite detailed guidelines for organizers/bidders for ECM and ECS meetings.

A European Crystallography Master Programme has been prepared. It is based on four semesters (120 credits). The students should come from widely different fields and have equally different scopes for their future work. So the structure of the Master will include four different modules.

Many activities of the IYCr took place in the region of the ECA. A large contingent of ECA members and representatives of ECA member countries attended the Opening Ceremony of IYCr2014 in Paris, France, 20–21 January 2014. Although the ECA was not formally represented at the ceremony as a Regional Associate, Russia and South Africa as ECA members of the BRICS countries participated formally by invitation. OpenLabs were held twice in Turkey, then Morocco, Ghana, Algeria and Tunisia. A summit meeting hosted in Bloemfontein, South Africa, 12–14 October 2014, brought together government representatives from a large number of countries in sub-Saharan Africa and North Africa.

Some SIGs organize their own events, seminars and schools. The largest is EPDIC – European Powder Diffraction Conference, prepared by SIG8 with a usual participation of more than 300 people. This was held in Aarhus, Denmark, in June 2014 and in Bari, Italy, in June 2016.

There are also activities in the Africa region. After the IYCr Legacy meeting in Rabat, Morocco, there was the Indaba 8 interdisciplinary workshop in South Africa and the First Pan-African Conference on Crystallography in Cameroon (October 2016) with 197 participants, mostly from Cameroon (87) and South Africa (17) but also from nearly 20 other African countries, Europe, America and Asia. An African Crystallography Steering Committee is being prepared.

The ECA has about 300 individual members (annual fee EUR 10), about 20 corporate members (annual fee EUR 250), 37 national members and three observers. The income allows some support of schools and conferences but it is not too high. The main financial contribution usually comes from the ECM. The ECA supports schools or conferences with an amount of EUR 7,000, sometimes more. It was decided to distribute the support for attendance of young crystallographers at ECMs directly (via the ECA scholarship fund) rather than through the bursary committee of the ECM.

The ECA stopped financial support to six countries of the region as the Adhering Body of the IUCr since three of them were accepted as full IUCr members in 2014. It was decided that such groups of countries should be mainly created by them first and not from the top. There are still problems with Russian membership in the ECA. In 2016, two ECA Executive Committee representatives were invited to the first Russian Crystallographic Congress (Moscow, November) – a very successful meeting with a large participation (2,000). There was also a proposal there to establish a Eurasian Crystallographic Association. The ECA has two internet domains – crystallography.eu and ecanews.org and also created links in the main social networks [@social\_eca (twitter) ecanews (facebook)].

A new ECA web site was introduced by Fermin Otaloro. It is using the Buddy Press plug-in and it is still under development. It was suggested that a special area accessible only by ECA individual members should be created. Unfortunately, not all planned features are working yet and there is also the necessity to move the system to another server.

Discussion continues as how to strengthen the position of the ECA as a really European Association, which has some legal issues (now it is registered in the Netherlands according to Dutch law), and the possibility of professional management connected also to the organization of the ECMs.

*R. Kuzel, IUCr Representative*

#### **A12.4. Latin-American Crystallographic Association (LACA)**

At the Montreal Congress, the Latin-American Crystallographic Association (LACA) became the fourth Regional Associate of the IUCr. Also in Montreal, I was appointed the IUCr Representative to LACA and was also a member of the LACA Council. The LACA Provisional Executive Committee in 2014 comprised the following members: Marcia Carvalho de Abreu Fantini, President (Brazil), Diego German Lamas, Vice-President (Argentina), and Lauro Bucio Galindo, Secretary (Mexico).

The countries of the North, Central and South American regions, historically bound by the Luso/Hispanic heritage and language, have constantly made efforts to work together promoting the advance of science and education in all countries. The formation of LACA was approved in Cordoba, Argentina, to gather together all the already consolidated crystallographic groups in the region. The region involved in the LACA initiative includes important scientific communities and well

established crystallographic societies, associations, and consolidated crystallographic groups. The initial groups are Mexico (SBCr), Venezuela (consolidated groups), Brazil (ABCr), Chile (consolidated groups), Argentina (AACr), Colombia (consolidated groups), Peru (consolidated groups) and Uruguay (consolidated groups). New existing groups have started their own national societies, like Costa Rica (UCRC) or the recently established collaborative projects to become a united and active group of countries. The mere existence of this very dedicated and scientifically productive crystallographic community in the Latin-American countries contributed significantly to support the construction of a synchrotron facility in Campinas, Brazil, in operation since 1997, and crystallographers represent the majority of its users. Some LACA countries have been affiliated to the IUCr for more than three decades, and are very aware of the importance of linking the regional scientific community acting in the crystallographic area with the activities and aims of the IUCr.

Through its association with the IUCr as a Regional Associate, LACA expects to increase international interaction among the countries of the LACA region with the rest of the world. As a Regional Associate, LACA will configure the consolidation of the science of crystallography in the LACA countries and acquire an international institutional level that will greatly help the development of new laboratories, student exchange, and financial support from governmental institutions in all countries of the region. A Newsletter dedicated to report all activities related to crystallographic research in Latin America will be published. This will contribute to improving the level of interaction among students and researchers in all areas of science where crystallography plays a key role.

The Statutes and By-Laws of LACA, as a non-profit organization, were discussed in November 2013 at the First LACA Meeting in Cordoba, Argentina. The Statutes will be legally registered in Brazil, under Brazilian laws. There will be versions in Portuguese, Spanish and English. The legalization process of the LACA Statutes is currently under way. The Brazilian National Synchrotron Laboratory (LNLS), in Campinas, Brazil, will be established as the legal address of LACA.

The main objectives of LACA are (i) to contribute to the advancement and the dissemination of crystallography in accordance with the aims of the IUCr, (ii) to promote Latin-American cooperation in crystallography, (iii) to promote the teaching of crystallography in Latin America, (iv) to facilitate the mobility of students and researchers across Latin America and between this region and others, and (v) to promote the formation of national associations or committees of crystallography in all countries of Latin America.

Currently, crystallography in Latin America includes seven countries (Argentina, Brazil, Costa Rica, Chile, Mexico, Uruguay and Venezuela – all members of the IUCr), two countries (Colombia and Peru) are in the process of organization, and two countries (Cuba and Puerto Rico) participate in LACA activities. The remaining countries do not yet have organized crystallography groups.

The list of the more relevant activities in Latin America related to IYCr 2014 were the Latin-American Summit Meeting (Brazil) and four OpenLabs (Argentina, Uruguay, Colombia–Venezuela and Mexico). In parallel, many educational and crystallographic promotional activities were also organized: the UNESCO Schools Science Teachers Meeting, São Paulo, Brazil; the Agilent OpenLab in La Plata and Buenos Aires, Argentina; the Bruker OpenLab in Montevideo, Uruguay; the Rigaku OpenLab in Bucaramanga, Colombia (collaboration with Venezuela); and the PANanalytical OpenLab in Mexico City, Mexico. Several national meetings of the national Crystallographic Associations took place in 2014 in LACA: the Mexican Crystallographic Association – SMCr, the Asociación Argentina de Cristalografía – AACr, the Red Uruguaya de Cristalografía – RUCr and the Grupos Peruanos de Cristalografía – Peru. Advanced Schools on different crystallographic topics also took place in 2014: the School on Crystallization and Polymorphism (San José, Costa Rica, January 2014); the School on Macromolecular Crystallography (São Carlos, Brazil, April 2014); the Course on Protein Crystallization (Concepción, Chile, May 2014); the Course on Single-Crystal Diffraction for undergraduate students (Merida, Venezuela, June–July 2014); the Course on X-ray Powder Diffraction for the Oil Industry (Merida, Venezuela, October 2014); the Short course on the PDF Technique (Mar del Plata, Argentina, November 2014); and the School on Synchrotron Radiation Techniques (Mar del Plata, Argentina, November 2014). Dissemination and popularization activities, such as the national crystal growing contests and short courses for teachers in Argentina and Uruguay, were among other activities promoting crystallography all over Latin America – lectures, exhibitions, science fairs, art and photographic contests and educational material.

Special mention must be given to the LNLS/CNPEM – Brazilian Summit Meeting 22–24 September 2014, with the participation of 101 scientists from nine Latin-American countries (Brazil, Argentina, Uruguay, Chile, Paraguay, Venezuela, Colombia, Mexico and Peru). The event in Campinas gathered experienced researchers from Latin-American countries, younger scientists (Early Career Research Scientists – ECRS) and renowned world scientists as invited lecturers. The main

objective was to evaluate the advances in the last decades in the field of structural crystallography applied to biological phenomena. One of the main points was the identification of barriers to integration, and the difficulties that hinder the development of competitive scientific research in the Latin-American Region. One of the activities planned for the first day of the event was a press conference with the presence of journalists and other media professionals in which prominent personalities were interviewed. Among them were Ada Yonath (2009 Nobel Prize in Chemistry), Marvin Hackert (President of the IUCr), Glaucius Oliva (President of the Brazilian National Research Council – CNPq), Carlos Henrique de Brito Cruz (Scientific Director of the Research Foundation of the State of São Paulo – FAPESP and Director of the National Laboratory for Biosciences – LNBio), Antonio José Roque da Silva (Director of National Synchrotron Light Laboratory – LNLS), Samar Hasnain (Editor-in-Chief of the IUCr journals).

Some discussion sessions and round tables were organized with the participation of scientists of Latin-American origin who are at present established and working abroad (France, Spain and USA). During the morning of 23 September, Dr Lidia Brito, Regional Director for UNESCO in Latin America, talked about cooperation between UNESCO and the IUCr for the International Year of Crystallography. A letter of intent was written by the participants and read at the closing ceremony of the event. One of the proposals in this letter was the creation of a UNESCO/IUCr Cooperation Fund for the promotion of crystallography in the region. The intention is to request governments, funding agencies, research institutes and enterprises, for contributions towards a fund of USD 100,000, which could be used to support student exchange activities and scientific events, and also to finance the common use of large experimental facilities. The organization of this Summit Meeting was sponsored by the Brazilian funding agencies FAPESP, CNPq and CAPES. An IUCr contribution to finance Early Career Research Scientists is acknowledged. Commercial sponsors were: Molecular Dimensions, Bruker, NanoTemper Technologies, Agilent, GE Healthcare, Rigaku/Dairix, Formulatrix, Astex, TTPLabtech e INCOATEC.

During 2014 the Association was growing its organization to achieve a stable and sustainable situation and continued to be very active in promoting activities involving crystallography in Latin America. The first meeting of the Association: I Reunión de la LACA, took place in São Paulo, Brazil, at Instituto de Física, USP, jointly with the XXII Reunión de la ABCr, 9–11 September 2015. With this important meeting, LACA inaugurated its formal scientific activity as a Regional Association of the International Union of Crystallography.

During 2015, the most relevant activities of the crystallographic groups in Latin-American countries were to a large extent due to the exposure given to research in crystallography during the International Year of Crystallography. Meetings of the National Crystallographic Associations and local crystallography groups, national contests for Primary/Secondary Schools, OpenLabs subsidized by commercial enterprises, and diverse science-related forums were organized by several countries. A major event for the Latin-American Region was the First LACA Regional Meeting, which took place in São Paulo, Brazil, 9–11 September 2015, jointly with the 22nd Meeting of the Brazilian Crystallographic Association (ABCr).

The First LACA General Assembly gathered at the Auditorium of the Physics Institute of the University of São Paulo on 10 September 2015. The IUCr was represented by Professor Santiago García-Granda, Spain. The agenda included key matters related to the formal organization of the association, such as (1) Statutes and By-Laws, (2) creation of a LACA fund, (3) general financial matters and operational budget (Treasurer's accounting of present and future expenses), (4) elections of the new authorities, (5) periodicity of the LACA meetings, countries willing to host the next LACA meeting/possible date, (6) general matters.

The following items were approved unanimously:

It was agreed that all country members that were already active members of the IUCr should automatically be considered LACA members; this applied to the following Latin-American countries (adhering institution): Mexico (Consejo Nacional de Ciencia y Tecnología), Costa Rica [Centro Nacional de Alta Tecnología (CeNAT)], Venezuela (Sociedad Venezolana de Cristalografía), Brazil (ABCr), Argentina (Consejo Nacional de Investigaciones Científicas y Técnicas), Uruguay (Academia Nacional de Ciencias del Uruguay) and Chile (Comisión Nacional de Investigación Científica y Tecnología).

Professor Iris L. Torriani (Brazil) was nominated LACA's Provisional Treasurer.

A period of three years was established to complete the legal status, call for general elections and organize meetings and admissions operations.

Chile's proposal to organize the 2018 III-LACA meeting was accepted.

Mexico's proposal to host the 2016 II-LACA meeting was approved.

More details of scientific, educational and promotional activities related to crystallography in several Latin-American countries during 2015 are reported below.

**Mexico – SMCr.** The last meeting of the Mexican Crystallographic Society was held in the Benemérita Universidad Autónoma de Puebla, Puebla, Mexico, 29 September –1 October 2015. The IV National Diffraction Conference, Acapulco, Guerrero, Mexico, was held 8–11 November 2015. As proposed at the 2015 General Assembly, the II-LACA Regional Meeting will take place in October 2016, in the city of Merida, Yucatán, Mexico.

**Argentina – AACr.** The XI Annual Meeting of the AACr, La Plata, was held 4–6 November 2015. The second edition of the International Crystal Growth Contest in Secondary Schools was held (April to November 2015): 400 schools from across the country participated in this event and 13 prizes and 24 merit awards were granted. The VII AACr Crystallography School, La Plata and Buenos Aires, was held 23 October – 3 November 2015. The IV Workshop of the AACr: Users Meeting of Large Installations, La Plata, was held 7 November 2015. Teachers' Training Courses on Crystallography and Crystal Growth were organized all over the country: 40 courses with a participation of over 1,500 attendees (July to November 2015). The AACr sponsored the participation of Argentinian schools in the international contest: Crystal Growth in Schools. Argentina received the largest number of distinctions: 2 gold medals and 2 bronze medals. Lectures and seminars were presented in several schools as well as Science and Technology Fairs, as part of an outstanding outreach effort on the part of several very active AACr members.

**Brazil – ABCr.** The XXII Annual Meeting of the ABCr, São Paulo, 9–11 September 2015, was held jointly with the First LACA Regional Meeting. The 2015 IUCr High-Pressure Workshop, focused on high-pressure crystallography, was organized as a satellite meeting of the LACA I Congress in São Paulo, 12–15 September 2015, held at the National Center for Research in Energy and Materials – CNPEM, Campinas, Brazil. A one-day ICDD Workshop on Powder Diffraction Techniques and Applications, 8 September 2015, was held at the Physics Institute, UNICAMP, Campinas, SP, Brazil.

The XV edition of the Latin-American Seminar of Analysis by X-ray Techniques (SARX) was hosted at the Imperial Museum (Petrópolis, Rio de Janeiro, Brazil), 18–21 September 2016. The SARX event is an international meeting held in South American countries that assembles the best researchers from around the world to promote the exchange of experiences in research and technology developments by X-ray techniques. Since 1997, SARX has taken place in many countries all over Latin America. SARX-2016 was organized by researchers from Rio de Janeiro State University (UERJ).

**Uruguay – RUCr (Red Uruguaya de Cristalografía).** The hands-on International Macromolecular Crystallography School: From Data Processing to Structure Refinement and Beyond, was held at the Institut Pasteur de Montevideo, Uruguay, 6–16 April 2015. The second National Crystal Growth Contest (<http://www.cncc.fq.edu.uy/>) was organized by Facultad de Química, Universidad de la República and funded by Agencia Nacional de Investigación e Innovacion (PCTI\_2014\_13141). Entrants obtained silver and bronze medal prizes in the International Crystal Growth Competition in 2015. Planned for 2016: Second edition of the IUCr–UNESCO Bruker OpenLab Uruguay 2 – Resolución de Estructuras Cristalinas por Difracción de Rayos X de Monocristal, Montevideo, Uruguay, 23–29 February 2016.

**Peru.** Crystallography groups from Peru organized the II Peruvian Crystallography Congress and Course on Analytical X-ray Diffraction Methods for Polycrystalline Materials at the Universidad Nacional de San Marco, UNSM, Lima, 4–6 August, 2015.

**Costa Rica – UCCr (Unión Costarricense de Cristalografía – Costa-Rican Union of Crystallography).** No crystallographic meetings were reported for 2015, but the 7th Workshop on Green Chemistry and Nanotechnologies in Polymer Chemistry was being organized at the National Laboratory of Nanotechnology in San José, Costa Rica, 21–23 September 2016.

**Venezuela SVC (Sociedad Venezolana de Cristalografía – Venezuelan Crystallographic Society).** Most relevant crystallography groups in Venezuela, acting at the Venezuelan Research Institute (Instituto Venezolano de Investigación Científica – IVIC), the Universities of Los Andes (ULA), Central de Venezuela (UVC) and Simón Bolívar (USV), organized several events celebrating the IYCr2014 in different parts of the country. The 45th anniversary of the Crystallography Laboratory at the University of Los Andes was a special occasion for a major combined crystallographic meeting organized with the National Committee for Crystallography from Colombia. The International X-ray Diffraction Course (Rigaku Open-Lab Colombia) took place in Bucaramanga, Colombia, 27–31 October 2014. The meeting had the participation of instructors

and lecturers from Europe and the USA and young scientists from several neighbouring countries of the region and Central America.

Additional general activities in 2015 worth reporting: participation of the countries' National Committees suggesting members for the IUCr Commissions; representation on the Programme Committee of the Hyderabad Congress; encouragement for the creation of crystallography groups and organization of workshops and OpenLab meetings in countries that at present do not have a formal crystallographic association; during 2015 conversations started to organize events in Bolivia and Paraguay.

In summary, several important resolutions were taken during 2015, including the First LACA Regional Meeting, which will contribute to the formalization of the structure of the Latin-American Regional Associate of the IUCr. The venues and dates of the next meetings and the final discussions of the Statutes and By-Laws were a start for the further growth of the Association. The LACA-II Meeting in Mexico in 2016 will be fundamental in this respect. The activities reported in 2015 by the LACA countries clearly show how the International Year of Crystallography influenced the crystallographic community in Latin America; these will still be important for many years to come.

The LACA Provisional Executive Committee was renewed in October 2016, at the II LACA Meeting in Merida (Mexico), formed by the following members: Diego Germán Lamas, President (Argentina), José Reyes Gasga, Vice-President (Mexico), Graciela Díaz de Delgado, General Secretary (Venezuela), José Roberto Vega Baudrit, Adjoint Secretary (Costa Rica) and Iris Torriani, Treasurer (Brazil). A Deliberative Council was established, formed by the following members: Sebastian Klinke (Argentina), Marcia Fantini (Brasil), Mauricio Fuentealba (Chile), Jesús Ángel Arenas Alatorre (Mexico) and Leopoldo Suescun (Uruguay), with Andrea Araya (Costa Rica) and Alexander Briceño (Venezuela) as alternates.

These authorities remain provisional until the Statutes are registered in Brazil and an election is called following the approved procedures. On the other hand, a Special Education Commission is being organized, which will be in charge of evaluating the proposals for courses and schools that request the support of LACA, and proposing activities for LACA.

The most important LACA activities during 2016 were the 2nd LACA Meeting, Merida, Mexico, 23–27 October 2016, with more than 100 participants from Mexico and LACA countries; three OpenLabs held in Montevideo (23–29 February 2016, with the support of Bruker); and the Third Edition of the IUCr–UNESCO OpenLab Mexico [held at the Advanced Materials Research Center (CIMAV), Chihuahua, 16–18 May 2016] and in La Paz (12–16 September 2016, with the support of Rigaku)]. Another important event was the International School on Fundamental Crystallography – Fifth MaThCryst School in Latin America, Havana, Cuba, 30 October – 4 November 2016.

The following are the activities of national societies 2016–2017.

*Argentina – AACr.* XII Annual Meeting of the AACr, San Luis, 9–11 November 2016. VIII School of the AACr, San Luis, 9–11 November 2016. V Workshop of the AACr: Synchrotron and Neutron Techniques for the Characterization of Materials, San Luis, 8 November 2016. Third Edition of the National Crystal Growing Contest for Secondary Schools (April to November 2016). About 300 schools from across the country participated in this edition; 13 prizes and 21 mentions of honour were granted. Training Courses on Crystallography and Crystal Growth for Teachers were organized all over the country: 42 courses with a participation of over 1,600 attendees (April to July 2016). As in 2014 and 2015, the AACr sponsored the participation of Argentinian Schools in the 2016 IUCr crystal growing competition for schoolchildren and Argentina received the largest number of distinctions: 2 gold medals and 2 bronze medals (as in 2015). As in 2014 and 2015, AACr members organized several dissemination activities, giving lectures and seminars in several primary and secondary schools, Universities as well as at science and technology fairs. Postgraduate courses on X-ray techniques were given in Buenos Aires (two courses), Mendoza and San Luis. One of them was focused on small-angle scattering, while the others included several techniques: diffraction, absorption, low-angle scattering, fluorescence, etc.

*Brazil – ABCr.* The Workshop on Applied Crystallography that is organized every one or two years at the Engineering Department of the Universidade Federal do Espírito Santo, was organized on 13–14 May 2016 in Vitória (ES). At the 68th Annual Meeting of the Brazilian Society for the Progress of Science (SBPC), a short Course on Methods of Molecular Structure Determination was offered by Professors Y.P. Mascarenhas, G. Oliva and M.C.A. Fantini, 4–7 July 2016, at Porto Seguro, BA. A short Course on the Rietveld Method took place at Universidade Federal do ABC, São Paulo, SP, 12–16 September, organized by Professor Fabio F. Ferreira.

Márcia C.A. Fantini represented the Latin-American Crystallographic Association at the First Pan-African Conference on Crystallography in Dschang, Cameroon, 6–11 October 2016.

Professor Yvonne Mascarenhas will receive the IUPAC Prize in ‘recognition of women with outstanding contributions in Chemistry and Chemical Engineering in the world’ in July 2017.

*Costa Rica – UCCr.* Participation in the organization of a European event including conferences and poster sessions entitled 7th Workshop on Green Chemistry and Nanotechnologies in Polymer Chemistry, 4th National Conference on Nanotechnoscience, 4th National Conference on Polymers, and ADAM 2016 Workshop, which included topics related to crystallography in San José, Costa Rica, 21–23 September 2016. A doctoral research internship was held at the University of Cambridge, UK, in the Department of Chemistry of Dr William Jones's research group with the subject *Screening of Cocrystals of Lovastatin and Irbesartan by Means of Mechanical Synthesis*, October to December, 2016. Participation in the VIII National Congress of Crystallography, Merida, Yucatán, Mexico, with the presentation of the poster: *Characterization of the Polymer Biodegradable Bionolle [Poly(butylene succinate)–PBS]*, Merida, Yucatan, Mexico, 23–27 October 2016. A course was given on Polymers and Biopolymers in Medical Devices (that included crystallographic topics) to the Boston Scientific: Heredia, Costa Rica (total 4 months), dictated from 1 February – 30 May 2016. A project entitled High Technology Applied to the Development of Low-Cost Methods to Evaluate Properties that Impact the Bioavailability of Drugs in Original and Generic Medicines Available in the National Market, TEC, UCR, LANOTEC, 2016 was presented and approved. A FEES project called Engineering of Crystals Applied to Natural and Synthetic Bioactive Substances: Polymorphs, Nanocrystals and Cocrystals, coordinated by Andrea Araya, TEC, UNA, UCR, LANOTEC, 2015–2016, ends in 2017.

*Mexico – SMCr.* The VIII National Meeting of Crystallography was held 23–27 October 2016 – a regular meeting of the SMCr, in conjunction with the Second Meeting of LACA. As a joint event, the VI Meeting of Users of Synchrotron Light was also organized [by the TULS Network (Thematic Network of Users of Synchrotron Light)]. Six courses covering topics related to crystallography were also held 22–23 October.

PANalytical Mexico and CIMAV Chihuahua decided to organize the Third Edition of the IUCr–UNESCO OpenLab Mexico, 16–18 May 2016. The programme consisted of a three-day seminar to give participants access to an update about how crystallography has developed in Mexico and about different and new applications related to the X-ray diffraction technique through presentations given by 10 national crystallographers and Dr Scott Speakman, Principal Scientist at PANalytical, all of them having a relevant trajectory in the Academic Research environment. In addition, practical sessions were organized in order to show how to take advantage of the XRD and XRF techniques in the research environment. The event took place at the Advanced Materials Research Center (CIMAV), Chihuahua, and even though the vacancies were limited to 70 people, registrations of about 120 people were received, showing a strong interest in crystallography, which made us extend the vacancies to 100 people.

*Venezuela (SVC) and Colombia Crystallographic Societies.* The exhibit *The Chemistry of the Mineral Kingdom* was presented at Encuentro con la Física, Química, Matemática y Biología, Facultad de Ciencias, Universidad de Los Andes (ULA), 13–15 June 2016, by student members of the Crystallography Laboratory at ULA, Merida, Venezuela, under the direction of Professors J.M. Delgado and G. Díaz de Delgado. This is the third year in a row that the exhibit has been presented and included specimens from the Laboratory’s collection. The event is aimed at encouraging elementary and secondary school students to pursue undergraduate studies in science. The event will take place again in June 2017. During 2016 through May 2017 undergraduate and graduate degree theses including crystallographic work were presented by students from Centro de Química of Instituto Venezolano de Investigaciones Científicas (IVIC) and from Departamento de Química, Universidad de Los Andes (Merida). Venezuelan crystallographers participated in the following national and international events: XX Congreso Venezolano de Catálisis, IVIC, Caracas, Venezuela, November 2016; II Reunión Latinoamericana de Cristalografía (LACA) and VIII Congreso Nacional de la Sociedad Mexicana de Cristalografía (VIII-CNCr) in Merida, Yucatán, Mexico, 22–27 October 2016. Invited talks: Professor G. Díaz de Delgado (ULA-Venezuela), *Characterization of Active Pharmaceutical Ingredients (APIs), New Solid Forms of APIs and of Organic and Metal Derivatives of APIs*; and Professor José Miguel Delgado (ULA-Venezuela), *At One Hundred Years of X-ray Powder Diffraction. A Brief Review of Its Beginnings*.

Professors Miguel Delgado and Graciela Díaz de Delgado (ULA) organized the Workshop on Crystallography Databases, 23 October 2016, at CINVESTAV, Merida, as a Pre-Congress event of the meeting II-LACA. Dr Amy Sarjeant (Cambridge Crystallographic Data Centre, CCDC, USA) and Dr Thomas Blanton (International Centre for Diffraction Data, ICDD, USA) participated as Instructors.

The IUCr-UNESCO OpenLab, co-sponsored by Rigaku Latin America, took place at Universidad Mayor de San Andrés (UMSA), La Paz, Bolivia, 12–16 September 2016. The OpenLab was preceded by a mini-course on 8–9 September. About 100 students and young researchers from different Universities and research Institutes from Bolivia, Chile, El Salvador, Mexico, Nicaragua and Peru attended this unprecedented event. The Instructors were Ing. Mario Blanco Cazas and Ing. Ariana Zeballos (UMSA, Bolivia), Professor Diego Lamas (U. San Martín, Argentina/LACA Vice-President at the time), Professor José Antonio Henao (UIS, Colombia), and Professors José Miguel Delgado and Graciela Díaz de Delgado (ULA, Venezuela), along with Dr Akilesh Tripathy (Rigaku Americas, USA).

Professor José Antonio Henao (Universidad Industrial de Santander, Bucaramanga, Colombia), Professor José Miguel Delgado and Professor Graciela Díaz de Delgado (ULA, Venezuela) were Invited Speakers at the XV Latin-American Seminar of Analysis by X-ray Techniques (SARX 2016), 18–22 September, Petrópolis, RJ/Brazil. A Workshop on the PDF-4 Database was organized by Professor Miguel Delgado and taught by Dr Tom Blanton (ICDD, USA) and by Professor Delgado. Professor José Miguel Delgado visited Universidad Mayor de San Andrés, La Paz, Bolivia, 25–28 January 2016. During this period, he and Dr Akihiko Iwata of Rigaku–Latin America were Instructors at the Workshop de Cristalografía at this University. They participated in meetings with University officials and students and professors of the School of Chemistry of Facultad de Ciencias Puras y Naturales of UMSA to plan the activities for the OPENLab–Bolivia, which took place in September of the same year.

As part of the very fruitful collaboration between Laboratorio de Rayos X at Universidad Industrial de Santander (UIS) in Bucaramanga, Colombia, and Laboratorio de Cristalografía of Universidad de Los Andes (ULA) in Merida, Venezuela, several activities took place in 2016 and in the first semester of 2017. Some are planned for the remainder of 2017 and into 2018. Professors J.M. Delgado and G. Díaz de Delgado (ULA, Venezuela) visited UIS during July–August 2016, February 2017, and April 2017.

A collaborative network in the area of pharmaceuticals and catalysts has been established between the laboratories at UIS–Colombia and ULA–Venezuela. It is hoped that this collaboration will be extended to neighbouring countries such as Ecuador, Peru, and Bolivia, and to other Latin-American countries.

The XVII Congreso Colombiano de Química will take place 25–27 October 2017, at UIS, Bucaramanga, Colombia. Professor José Antonio Henao leads the Organizing Committee. Several Pre-Congress courses are being organized, in particular an X-ray Diffraction Course (22–24 October) where Amy Sarjeant (CCDC, USA), Tom Blanton (ICDD, USA), J.M. Delgado and G. Díaz de Delgado (ULA, Venezuela), John Bonilla (UIS, Colombia), and Hernando Camargo (U. Santo Tomás, UST, Colombia) will be the instructors.

Efforts are being devoted to establishing the Colombian Crystallographic Society. The Congreso Colombiano de Química should provide a venue to reach this goal.

An OpenLab on Powder Diffraction is being planned by J.A. Henao and J.M. Delgado at UIS, Colombia, for 2018. It is worth mentioning that the X-ray Laboratory at UIS, Colombia, has been providing an excellent service to academic institutions and industries within Colombia and in Latin America. This Laboratory is among the best equipped centres in South America.

*Uruguay – RUCr.* A Workshop on Integrative Methods in Structural Biology was held 16–19 February 2016 (<http://pasteur.uy/en/last-news/integrative-methods-in-structural-biology-to-enhance-high-impact-research-in-health-and-disease>); participants: 30 students (Uruguay, UK, Argentina), 13 lecturers (Uruguay, Argentina, France, Spain, Brazil, UK). The IUCr-UNESCO Bruker OpenLab Uruguay 2 was held 23–29 February 2016 (<http://cryssmat.fq.edu.uy/OpenLab/index.html>); participants: 44 students, 11 lecturers. Segundo Encuentro de la Red Uruguaya de Cristalografía (RUCr) was held 30–31 August 2016 (<https://sites.google.com/site/2encuentrorucr/home>); participants: 50 registered (2 invited from Argentina and Brazil).

*Chile (Comisión Nacional de Investigación Científica y Tecnología).* In 2016, three schools or courses were held in different Universities. At the Pontificia Universidad Católica de Chile in Santiago in August of 2016, in conjunction with the University of Notre Dame, A Practical Course in Chemical Crystallography was held. At the Universidad Santa María in Valparaíso, the first and second Schools of Crystallography and X-ray Diffraction were held in March and December 2016, respectively. On the other hand, in the Pontificia Universidad Católica de Valparaíso, the Interschools Contest ‘CristalEscolar’

was held for the third consecutive year, where several institutions carried out experiments and exhibited their crystal growth activities.

During the 2nd LACA Meeting, with the participation of the IUCr President Marvin Hackert, and the IUCr Representative for LACA Santiago Garcia-Granda, an assembly of LACA was held during which the executive authorities were renewed, the Statutes were approved and it was decided to organize a Deliberative Council.

The latest version of the LACA Statutes and By-Laws was approved by the General Assembly in Merida, Yucatán, Mexico, and has now been submitted for registration using the services of a private Law and Accounting firm. Since LACA was founded, the Brazilian Crystallographic Association sponsored the first steps of its registration as a non-profit scientific association. In 2016, using funds from the Brazilian National Research Council (CNPq), an exclusive (.org) domain and host server space was acquired for the LACA web site – with a five-year contract. The same CNPq grant will be used to pay for registration fees.

The LACA Executive Board and Council have now taken office, but one important point to be solved is the way of obtaining a basic yearly contribution from the country members. A flux of continued income will be needed to cover functional expenses for maintenance of the administrative structure. LACA is tax-exempt but every year the registration must be reinstated and there is a cost for the accounting services. This is a task for the present authorities.

During the LACA Assembly it was also decided that the Third Meeting of LACA would be held in Chile in October 2018 and that the organization of the First School of LACA, dedicated to crystallography of small molecules, would be held in Montevideo, Uruguay, in February 2018.

For the year 2017, the participation of Latin-American colleagues is promoted at the Hyderabad Congress, where a workshop will be held to discuss the progress of crystallography in Latin America, and it is hoped that several national meetings will be organized. On the other hand, it is planned to organize a new OpenLab in December 2017 in Costa Rica. Unlike previous OpenLabs, this was promoted by the LACA authorities.

*S. Garcia-Granda, IUCr Representative*

#### A12.5. Worldwide Protein Data Bank (wwPDB)

The Protein Data Bank has been an essential resource for macromolecular crystallographers for more than 40 years, and its policies and development have been strongly influenced by the crystallographic community. Today the PDB is a partnership of four entities, referred to collectively as the Worldwide PDB (wwPDB). The partners comprise the RCSB-PDB in the USA, PDBe in Europe, PDBj in Japan and BMRB (NMR database) in the USA. These centres collaborate intimately and share the load, maintaining a single archive that is accessible to researchers, educators and students throughout the world.

Recognizing the importance of this partnership to the crystallographic community, the wwPDB was formally designated a Scientific Associate of the IUCr in 2015. The IUCr provides a representative – currently Professor Ted Baker – on the wwPDB Advisory Committee. This Committee also has representatives from the NMR and cryo-EM communities, as well as regional representation, and is currently chaired by Dr R. Andrew Byrd.

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

As of April 2017 the archive comprises nearly 130,000 macromolecular structures, of which about 90% have been determined by crystallography. Some 11,000 structures were deposited in the past year, at a rate of increase that places increasing demands on the efficiency of annotation, checking and validation. At the same time much development work is being undertaken, both by the wwPDB partners and in the relevant communities as the range of techniques giving structural data continues to expand.

Some of the major developments that have taken place over the past 3 years are as follows:

A new deposition and annotation tool, called OneDep, has been developed and implemented, and is now in full use across the three partner sites for all new depositions. The new system is more flexible, extensible and efficient, and allows geographic balancing of the workload. These developments have resulted in much shorter processing times, from an average of 4–5 days to a median of ~15 h.

The number of structures being determined by cryo-electron microscopy (cryo-EM) is increasing rapidly as new detectors and more powerful processing protocols are applied. The total number is now almost 1,500, with 400 new structures deposited in the past year. A major effort is under way to develop robust validation tools, informed by the experience from crystallography and adapted for the special properties of EM maps and model building.

To cope with the increase in size of structures being deposited, both from cryo-EM and crystallography, the old ‘card image’ format has been superseded to allow extremely large structures, such as ribosomes, to be presented in a single file. On top of the growth in large cryo-EM structures, crystal structures are also increasing in size; the number with molecular weight >500,000 is growing significantly, as is the number with many chains and more than 100,000 atoms. This underscores the complexity of the data depositions and the demands on the wwPDB to adapt and integrate these data smoothly into the archive.

Validation reports, based on those previously implemented for crystallographic structures, have now been implemented for both NMR and cryo-EM depositions. The relevant Task Forces continue to develop these further, one of their most pressing tasks being to incorporate more robust methods for validation of carbohydrate moieties, ligands and cofactors.

It is pleasing to note that the lead taken by our IUCr journals in requiring that PDB validation reports are provided with paper submissions is now being followed by other journals, including most recently journals from the *Nature* stable. There is a clear and obvious need for referees to be given information that allows them to assess the quality of structural data.

Structure factor amplitudes are now routinely deposited with coordinates, and most journals cooperate well in ensuring that these data are indeed deposited for articles that present crystal structures. The wwPDB partners do not have sufficient resources to act as a repository for complete raw data sets. Processed but unmerged data sets can now be accepted, however.

A Task Force led by Jill Trewella is considering how the data from SAXS studies might be archived, including what data should be deposited and how it should be validated. Similar discussions are taking place on other complementary structural techniques.

The remediation of carbohydrate structures in the archive is continuing, to ensure that they conform to proper conventions of atom labeling and stereochemistry. Glycan chains on proteins are often poorly ordered and many archival entries violate stereochemical rules. Changes can only be made with authors’ consent, however, so remediation is a slow process.

With 1.5 million downloads per day across the three wwPDB sites, it is obvious that the archive is of enormous importance to the whole life sciences community. The IUCr can be proud of the contribution made by the crystallographic community, and I am happy to be able to report that the relationship between the IUCr and the wwPDB is strong, and is much appreciated by the wwPDB.

*E.N. Baker, IUCr Representative*

#### **A12.6. International Centre for Diffraction Data (ICDD)**

The Commission on Powder Diffraction maintains close links with the ICDD and also with the International X-ray Absorption Society (IXAS) (<http://www.i-x-s.org/>).

*P. Whitfield, IUCr Representative*

## A12.7. International Organization for Crystal Growth (IOCG)

The most important event concerning IOCG (<http://www.iocg.org/>) in the triennium was the official meeting of the association, the 18th International Conference on Crystal Growth and Epitaxy ICCGE-18, Nagoya, Japan, 7–12 August 2016. The opening ceremony of the Conference took place in the presence of His Imperial Highness, The Crown Prince of Japan. A lecture was given by the Nobel Laureate Isamu Akasaki.

11 general sessions and 10 topical sessions were organized. The Conference was very successful (about 1,400 participants) and very well organized. In the week before the Conference, the 16th International Summer School on Crystal Growth ISSCG-16 was held at Lake Biwa, Shiga, Japan, with the participation of 120 students. Both the Conference and the School were supported by the IUCr.

Many members and consultants of the Commission on Crystal Growth and Characterization of Materials (CCGCM) were involved in the organization of the conference and the school, but I would like to underline in particular the contribution of Koichi Kakimoto, Chair of ICCGE-18 and member of CCGCM.

Many other members/consultants of CCGCM were directly involved in the organization of both the school and the conference. Here it is important to underline that three symposia of the IOCG Conference have been officially co-organized by representatives of the IUCr, namely Janakiraman Kumar (Defect Formation), François Puel (Industrial Crystallization), and Juan Manuel Garcia Ruiz (Organic and Biological Crystallization).

The IOCG Conference also provides an opportunity to consolidate the officers and Executive Committee members. The new President of IOCG is Koichi Kakimoto (Japan), who is also a member of CCGCM; Co-Vice-Presidents are T.F. Kuech (USA) and E. Vlieg (The Netherlands), both members of CCGCM; the Secretary is H.A. Dabkowska (Canada), and the Treasurer is J. Derby (USA). The members of the Executive Committee are J. M. Garcia-Ruiz (Spain), S. Baldochi (Brazil), J.Y. Wang (People's Republic of China) (all consultants/members of CCGCM), Y. Mori (Japan), S. Krukowski (Poland), A. Voloshin (Russia), M. Heukens (Germany), and J. De Yoreo (USA).

As IUCr Representative, I had the chance to take part in the Executive Committee meeting of IOCG in Nagoya and in Executive Committee discussions via e-mail during the triennium.

The next international meeting and school ICCGE-19 and ISSCG-17 will be held in Keystone, Colorado, USA, in 2019. Tom Kuech, a member of CCGCM, will co-Chair the school. The Chairs of ICCGE-19 accepted our proposal to proceed with the idea to co-organize three symposia in cooperation with IUCr representatives.

Also, the IOCG General Assembly evaluated the proposals for the organization of ICCGE-20 and ISSCG-18 and it was decided that these events in 2022 would be organized in Italy. The Conference will be co-Chaired by myself and the School by Roberto Fornari (Past Chair of CCGCM and Past President of IOCG).

At the end of 2010 the European Network of Crystal Growth (ENCG) was constituted. One of the scopes of ENCG is the organization of a European Conference on Crystal Growth (ECCG). After ECCG4 that was held in Glasgow in 2012, in 2015 the European Conference on Crystal Growth was organized in Bologna, Italy, and co-Chaired by myself together with the First European School on Crystal Growth. Many members/consultants of the CCGCM were involved in the organization of this Conference. Both events were very successful. It was already decided that in 2018 the Sixth European Conference on Crystal Growth together with the Second European School of Crystal Growth would be organized in Varna, Bulgaria. These events are quite important to keep alive the crystal growth tradition in Europe.

Concerning IYCr2014, it must be underlined that in 2014 some national associations started campaigns to promote crystal growth among young students and scholars. They offered visits to crystal growth laboratories and organized crystal growth contests. Initiatives were organized in Spain (<http://www.rtve.es/alacarta/videos/la-aventura-del-saber/aventuracsic/3175138/>), Italy (<https://www.facebook.com/pages/Concorso-Nazionale-Crescita-Cristalli/1589346004681687>) and Germany ([www.dgkk.de/schulen/](http://www.dgkk.de/schulen/)).

In conclusion I wish to emphasize that the IOCG is very active in promoting crystal growth conferences and schools and that the cooperation in this field with the CCGCM is strong.

A. Zappettini, IUCr Representative

### A13. Reports of Representatives on bodies not belonging to the Union

#### A13.1. Interdivisional Committee on Terminology, Nomenclature and Symbols of the International Union of Pure and Applied Chemistry (IUPAC ICTNS)

ICTNS continued its activities on behalf of IUPAC in reviewing and approving Technical Reports and Recommendations submitted to IUPAC for publication in *Pure and Applied Chemistry*, and also for approving, on behalf of IUPAC, publications emanating from international bodies on which IUPAC has representation.

There was only one activity of the ICTNS during the triennium that related to crystallography. A group wrote a technical report concerning the revised definition of the mole; the new definition would change Avogadro's number by less than 1 part in  $10^8$ .

C.P. Brock, IUCr Representative

#### A13.2. International Council for Science (ICSU)

The International Council for Science (ICSU) is a non-governmental organization with a global membership that includes 31 International Scientific Unions, 122 national scientific bodies representing 142 countries, and 22 International Scientific Associates. ICSU was founded in 1931 to promote international scientific activity in the different branches of physical science and its application for the benefit of humanity. It is one of the oldest non-governmental organizations in the world and represents the evolution and expansion of two earlier bodies known as the International Association of Academies (IAA; 1899–1914) and the International Research Council (IRC; 1919–1931).

In 1998, its members agreed that the organization's activities would be better reflected by modifying the name from the International Council of Scientific Unions to the International Council for Science, while retaining the rich history of its existing acronym, ICSU. ICSU's strength and uniqueness lies in its dual membership of National Scientific Members and International Scientific Unions. This wide spectrum of interdisciplinary expertise allows ICSU to address major international scientific issues. The General Assembly of ICSU meets every three years and is responsible for setting the general direction, policies and priorities for the next triennium. The 31st General Assembly of the International Council for Science was held in Auckland, New Zealand, 30 August – 3 September 2014. The next General Assembly will be held in Taipei, 23–24 October 2017.

Traditionally, the IUCr is represented by its Immediate Past President but as Professor Gautam Desiraju has been busy with preparations for IUCr 2017, E.N. (Ted) Baker represented the IUCr at the 31st ICSU GA meeting in 2014 in Auckland.

The Assembly agenda featured a number of excellent guest lectures, including an address by Professor Bruce Alberts, former Editor-in-Chief of *Science* magazine, on the development of problem-solving skills in science that are appropriate to any nation, rich or poor. Posters from delegates were displayed throughout the meeting and were summarized orally in two-minute presentations at intervals through the programme.

Of particular interest to IUCr members at the Auckland meeting was a discussion on Open Access publishing led by Professor John Ball, a mathematician from Oxford University and a member of the ICSU Executive Committee. This session endorsed the principle of open access to the scientific record, while setting out five aspirational goals and recommendations for achieving this end. Cautions were raised against the misuse of metrics and the meeting reinforced that publishers should ensure that research datasets are deposited in *trusted* and *sustainable* repositories – an area in which the IUCr has led the way and remains very active. Subsequently, the IUCr has endorsed the San Francisco Declaration in support of these goals.

The President of ICSU for 2014–2017 is Gordon McBean, a climate-change expert from Canada. He will be followed in 2017 by Professor Dayan Reddy, an internationally recognized mathematician from South Africa, who was elected as President-Elect in Auckland. Heide Hackmann became the new Executive Director for ICSU in March 2015 and works with a staff of

about 18 at its headquarters in Paris. In addition, ICSU has three Regional Offices, serving Africa (Pretoria, South Africa), Asia and the Pacific (Kuala Lumpur, Malaysia), and Latin America and the Caribbean (Mexico City, Mexico).

ICSU's strategic plan 2012–2017 identified key priorities and associated activities that focus on three areas that resonate well with the interests of the IUCr: International Research Collaboration, Science for Policy, and the Universality of Science. In the area of International Research Collaboration, ICSU helps coordinate international research programmes. An example of these interdisciplinary bodies of particular interest to the IUCr are CODATA (Data for Science and Technology) and COSPAR (Space Research). ICSU also has been very active in Climate Research (improved understanding of global and regional climate changes), Disaster Risk (impacts of natural hazards), and Future Earth (sustainability), among others. Under Science for Policy, ICSU works to ensure that science is integrated into policy development. Under the priority of Universality of Science, ICSU seeks to address developing a truly global scientific community with a focus on capacity building, science education and access to data.

ICSU supported a Grants Programme that funded four projects in 2015. The IUCr was the lead applicant of one of the funded awards (with support from the ECA, UNESCO, SAASTA and Indaba) titled *Building Science Capacity in Africa via Crystallography*. The IUCr submitted the proposal on behalf of Andreas Roodt (ECA and Indaba) and Michele Zema (IUCr representative). The award provided EUR 30,000 in support of several conferences for capacity building of crystallography in Africa, with a goal of cementing the African Crystallographic Association. The first of these was the Indaba conference held in South Africa in August 2015, and the most recent the First Pan-African Conference on Crystallography, which took place in Cameroon, 6–10 October 2016.

The 2016–2019 ICSU Grants Programme was revised to support fewer, but larger grants than the one the IUCr helped obtain to support its African initiative in 2015. The IUCr partnered with IUPAP to submit a joint proposal that was one of three funded by ICSU for this period. Congratulations to Michele Zema who led the IUCr efforts and our thanks to IUPAP and the many organizations (UNESCO, TWAS, etc.) and large-scale facilities that supported this joint effort. The acronym LAAMP (Lightsources for Africa, the Americas and the Middle East Project) has been chosen for the initiative. The grant is for EUR 300,000 over three years. In addition to this grant providing support for new initiatives, the scope of the proposal will help support a number of OpenLabs.

ICSU launched Science International as a series of meetings to strengthen the voice of global science in international policy. This was done in cooperation with TWAS, IAP and ISSC. The first such meeting was held in December 2015 in Pretoria, South Africa, with a focus on Big Data and Open Data. A working group was formed to draft an accord on Open Data in a Big Data World, which is now available via the ICSU web site. The IUCr wrote a Response co-authored by B. McMahon, L. Van Meervelt, J.R. Helliwell and M.L. Hackert, which is also available on the IUCr web site. The topic of best practices to sustainably achieve the goals of Open Access continues to be discussed, often with reference to 'FAIR' (Findable/Assessable(Accessible)/Inter-operable/Reusable) data.

As part of an effort led by the United Nations, on 25 September 2015 many countries adopted the 2030 Agenda for Sustainable Development to end poverty, protect the planet, and ensure prosperity for all. This led to the identification of 17 Sustainable Development Goals (SDGs) that include 'no poverty', 'zero hunger', 'good health and well-being', 'gender equality', 'clean water', 'clean energy' among others. ICSU engaged in a study of the 17 SDGs and the 169 underlying targets beneath them and reported that many of the targets rely too much on vague, qualitative language rather than measurable, quantitative targets. Efforts to understand better the interrelatedness of these goals and how to help nations implement steps to achieve them is ongoing.

Many of these global initiatives have a major social science component. This has led to discussions about a possible merger of ICSU with ISSC (International Social Science Council). An Extraordinary General Assembly of ISSC and ICSU was held in

Oslo, Norway, on 24 October 2016 to vote on the principle of the merger of ISSC and ICSU, and on a planning framework for the development of a new, single science organization for both the social and natural sciences. 76% of the ICSU members and 87% of the ISSC members voted in favour of a merger, in principle, of the two organizations, thereby setting the process in motion. Many details remain to be resolved such as dues, identifying any official national representation, the fate of the current working ICSU Commissions, ways to insure equitable representation of both the social and physical sciences, how to include medicine and engineering in the discussion of global concerns, etc. A committee is working on how to address the concerns expressed by many of the International Unions about handling these issues, and the IUCr was fortunate that former General Secretary Sven Lidin agreed to serve as the IUCr delegate at the meeting in Oslo.

I look forward to working with ICSU and representing the IUCr in Taiwan later this fall when ICSU meets to hear reports from its many active committees and on the merger proposal.

*M.L. Hackert, IUCr Representative*

### A13.3. ICSU Committee on Data for Science and Technology (CODATA)

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

The major event for CODATA during 2014 was the biennial conference and General Assembly held in Delhi, India, 2–7 November. Due to time constraints on obtaining a visa, the IUCr was represented at this event by B. McMahon (BM). The 24th International CODATA Conference was organized in partnership with its sister organization the ICSU World Data System (WDS) under the title SciDataCon2014 – International Conference on Data Sharing and Integration for Global Sustainability.

Of especial note for IUCr was that the CODATA Prize 2014, for Outstanding Achievement in the World of Scientific and Technical Data, was awarded to Professor Sydney R. Hall, University of Western Australia, for his leadership in the development of data exchange standards including the Crystallographic Information Framework (CIF). The CODATA web site acknowledged that Professor Hall's work ‘certainly met [the] criteria ... It is particularly fitting that a crystallographer should be so recognized during the International Year of Crystallography’. Professor Hall gave a presentation at the Delhi conference on *The Implementation of STAR/CIF Ontologies*.

BM presented a contribution by J.R. Helliwell on *Sustainability of Life and Molecular Crystallography 3D Data* in the session Open Data Infrastructure and Best Practices. BM also took part in the satellite workshop Data Papers and their Applications.

As always, this conference provided a useful opportunity to survey data management practices across many different disciplines, and to showcase the leadership in data management, evaluation and availability of crystallography and structural science.

Notable decisions taken at the General Assembly in Delhi were as follows:

The Netherlands and Kenya were welcomed as new National Members of CODATA.

The Research Data Alliance (RDA) was welcomed as a new Co-Opted Organization (Memoranda of Understanding were signed in March 2015 between CODATA, WDS and RDA to establish formal collaborations between these bodies).

The next SciDataCon, held in September 2016 in Denver, USA (see <http://www.scidatacon.org/2016/>), was entitled Advancing the Frontiers of Data in Research, and formed part of an International Data Week, organized jointly by CODATA, the Research Data Alliance and the ICSU World Data System. The IUCr organized a Microsymposium on Crystallography and Structural Data Bases (<http://www.scidatacon.org/2016/sessions/>).

In 2015 CODATA played a leading role in the publication of a leadership document entitled *Open Data in a Big Data World: An international Accord* (see <http://www.icsu.org/science-international/accord/open-data-in-a-big-data-world-long> and a shortened version at <http://www.icsu.org/science-international/accord/open-data-in-a-big-data-world-short>). This tackled various issues of open access to data and its ramifications. Of particular relevance to the IUCr were that these documents laid out the responsibilities and duties to be expected of publishers; it explained the approaches taken for data archives to be sustainable and open; it analyzed the approaches taken across the globe. The IUCr has endorsed the Science International

2015 Accord on Open Data in a Big Data World and provided a detailed response to the short form of the Accord in which the position of crystallography is included. Copies of the IUCr position paper are available at the IUCr web site: <http://www.iucr.org/iucr/open-data>. This IUCr position paper was very well received by the CODATA General Assembly and the attendees at Denver. A detailed report on the International Data Week can be found at <http://forums.iucr.org/viewtopic.php?f=21&t=381>.

#### *Other activities*

J.R. Helliwell was a formal contributor, in his role as IUCr Representative to CODATA, to an ICSU draft report on ‘open access to scientific data and literature and the assessment of research by metrics’ that was presented to and approved at the 31st ICSU General Assembly in Auckland, New Zealand, in September 2014. The report is available at <http://www.icsu.org/general-assembly/news/ICSU%20Report%20on%20Open%20Access.pdf>.

The IUCr has also been an active participant in the CODATA–VAMAS Joint Working Group on the Description of Nanomaterials, with participation in a questionnaire on existing practices in different disciplines, and representation by Reinhard Neder and Daniel Chateigner at two Workshops in Paris. The final report, with our approval, has been released by the Chair, John Rumble. Details can be found at <http://www.codata.org/nanomaterials>.

*J.R. Helliwell, IUCr Representative*

*B. McMahon, alternate IUCr Representative*

#### **A13.4. ICSU Committee on Space Research COSPAR)**

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

COSPAR’s highest body is the Council, which meets at the Committee’s biennial Scientific Assembly. COSPAR’s elected President for the period 2014–2018 is Lennard A. Fisk (USA) and the Vice-Presidents are J. Wu (People’s Republic of China) and A. Jayaraman (India). Members of the Bureau are: Ines S. Batista (Brazil), C. Césarsky (France), K.-H. Glassmeier (Germany), M.I. Panasyuk (Russia), S. Sasaki (Japan) and J.-P. St-Maurice (Canada).

In 2014, the International Year of Crystallography (IYCr) provided an opportunity to develop a stronger collaboration between the IUCr and COSPAR. For the IYCr Opening Ceremony on 21 January 2014 in UNESCO Hall in Paris, Professors David Bish and David Blake (USA) were chosen to present talks about recent applications of crystallography in the study of Mars during the session Crystallography for Society and the Future. Aaron Janofsky (COSPAR’s Executive Secretary) and Mariano Mendez (Chair of the Panel on Capacity Building) both attended the IYCr Opening Ceremony in Paris. For the 40th Assembly, Moscow, Russia, 2–10 August 2014, I submitted to the COSPAR Council information about IYCr developments and activities.

Following all these discussions, in April 2016 a very successful Capacity Building Workshop on Crystallography for Space Science (<http://www.inaoep.mx/cospar2016/>) took place in Puebla, Mexico. It was organized and run by Juan M. Garcia-Ruiz, Maria E. Mendoza, Guillermo T. Tagle, Hanna A. Dabkowska and Mariano Mendez. The programme presented the fundamentals of crystallography, minerals in space, reports on crystallographic and crystal-growth experiments performed in space and actual and future investigation of space debris by crystallographic methods, including sample preparation and data collection (also in space). 27 PhD students, post-docs and young staff members, mostly from Latin America, took part in the workshop. For many of them it was their first contact with crystallography. The IUCr helped to cover the costs of bringing some young participants to this meeting and the travel of 3 Visiting Professors teaching the basics of crystallography.

The topic of the workshop *Crystallography for Space Sciences* is very novel as this was the first COSPAR workshop focused on crystallography, which is becoming more important in research on Mars and some comets. There is a proposal to organize a similar workshop in another area of the world soon.

COSPAR acts mainly as a body responsible for organizing biennial Scientific Assemblies. After a great deal of consideration

the 41st Assembly planned for Istanbul, Turkey, 30 July – 7 August 2016, was cancelled owing to the failed coup event of 15 July.

H.A. Dabkowska, IUCr Representative

### A13.5. International Council for Scientific and Technical Information (ICSTI)

ICSTI offers a unique forum for interaction among organizations that create, disseminate, and use scientific and technical information. ICSTI is a Scientific Associate of ICSU, the International Council for Science. ICSTI's mission cuts across scientific and technical disciplines as well as international borders, to give member organizations the benefit of a truly global community.

In July 2015 there was a meeting of ICSTI in Hannover, Germany. At the Annual General Meeting, ICSTI decided that membership fees should go up by 1.5%. For the IUCr this means an increase to EUR 850 (IUCr is a category A member). Category B increases to EUR 1,595. It was also decided that there would be a meeting in Philadelphia in February 2016 (Annual Members Meeting) and the next AGM would be 9–10 September 2016 in Washington, USA. At the meeting there were two workshops.

The first workshop entitled ITOC (Information Trends and Opportunities Committee) was on Open Science and Open Data. The first speaker was Geoffrey Boulton (Edinburgh) who gave an excellent talk entitled *Open Data and the Future of Science*, with examples of this in practice, including possible problems in open data (problems connected with industrial collaborators for instance). Nonetheless, he expressed the view that publicly funded research at least should result in full public access to the data used in the research in future. The IUCr is already well there in any case. This talk was followed by three more: *From Open Access to Open Science* (J. Cotta), *Data Sovereignty VIVO Approach* (L. Heller), and *Legacy of the International Geophysical Year to the World Data System* (M. Diepenbroek). There was a presentation of a number of on-line tools for measuring impact: ReadCube, Overleaf, Altmetric and Figshare.

The second workshop was by the TACC (Technical Activities Coordinating Committee). Martin Fenner from PLOS (Germany) showed that the Public Library of Science requires all accepted papers to include a data availability statement, and to make the data underlying the publication available as supplementary information or in a publicly available repository. Ben Mcleish and Stephen Cawley (UK) gave a joint talk tracking specific investigators using Altmetric. They pointed out that systems like Altmetric should be a boon for Universities required to specify the impact of their research, such as the REF in the UK. Terri Mitton (France) talked about the data available publicly by the OECD. Finally Christian Soltmann described the European Patent System and claims that EPO contributes to innovation (he did not discuss the negative aspects of this, and was questioned about that).

A one-day meeting was held in Denver, USA, on 10 September 2016, which was attended by B. McMahon in place of A.M. Glazer. This comprised: General Assembly Meeting (including Member Initiative Presentations); Information Trends and Opportunities Committee (ITOC) Workshop on Enabling Innovations for Researcher Workflows and Scholarly Communication (Chair: Markus Ekman); Technical Activities Coordinating Committee (TACC) Workshop on Trends in Scientific Software Development, Sharing and Use; WorldWideScience Alliance Annual Meeting; and ICSTI Executive Board Meeting.

In the ITOC Workshop the following talks were presented:

*Innovations in Scholarly Communication: Openness, Efficiency and Reproducibility Drivers* by Jeroen Bosman and Bianca Kramer of Utrecht Library in the Netherlands.

*Wikidata and Wikimedia Commons as a Platform for Collaborative Annotation and Reuse for Scientific Data* by Lambert Heller of the German National Library of Science and Technology (TIB).

*From Principles to Action – The FORCE11 Approach to Innovation in Scholarly Communications* by Cameron Neylon, Professor of Research Communication at the Centre for Culture and Technology at Curtin University, USA.

*An Open Science Framework for Managing and Sharing Research Workflows* by Courtney Soderberg, Center for Open Science, Charlottesville, Virginia, USA.

In the TACC Workshop the following talks were presented:

Jay Billings, Oak Ridge National Laboratory and DOE Office of Scientific and Technical Information, described *The New Department of Energy Software Center*.

Andrea Ross, of the Eclipse Foundation, spoke (rather generally) about the mechanics and advantages of open-source software development in a talk entitled *Eclipse Foundation: A Symphony of R&D Collaboration*.

James Willenbring, Sandia National Laboratories, described *The IDEAS Scientific Software Productivity Project* and how to refactor code to work well on new computing platforms.

Eleonora Presani, Project Manager, Elsevier Research Intelligence, spoke on *Elsevier's SoftwareX journal*. [This provided an interesting comparator to the publication of new programs and software packages in *J. Appl. Cryst.* and we noted that editorial procedures and requirements on authors were broadly similar. The software/code metadata items required by the Elsevier journal may also provide a useful model for enhancing the content of the software directory (formerly 'SinCris') on the IUCr web site.]

Fernando Perez, University of California Berkeley, described the *The Jupyter project*. [The Jupyter project was born out of the IPython Project in 2014 and has evolved to support an open source, interactive data science, scientific computing platform for over 40 programming languages.]

At the ICSTI Executive Board meeting J.R. Helliwell attended in place of A.M. Glazer who was unable to attend. B. MacMahon attended as an Observer. The main items discussed were in the overview report from the ICSTI Executive Secretary Tony Llewellyn. Main items of interest were that the IUPAC and IUPAP delegates were not present but IUCr was heartily thanked for their continued presence. [Our impression was that to have at least one science Union in attendance was important so as to form a touchstone with science, and scientist, viewpoints for the other ICSTI members.]

The ICSTI financial assets were as last year (approximately EUR 100,000). The ICSTI cash flow was in a slight deficit (approximately EUR 3,000).

The plan in recent years of attaching the ICSTI General Assembly and Workshops to a major event was proposed to be continued and was supported as very sensible. Possible events for 2017 included the European Publishers conference in Berlin, Germany, or the next Research Data Alliance Plenary to be held in Barcelona, Spain.

Following the ICSTI meeting in Denver, a memorandum of understanding was signed with RDA (Research Data Alliance) whereby ICSTI becomes an Organizational Affiliate of RDA and RDA becomes an Associate Member of ICSTI.

In April 2017, an ICSTI Executive Committee meeting and workshop took place in Barcelona followed by a meeting of the RDA. The meeting started with a brief discussion of financial problems with income of EUR 96,400 for 2017. Four members have left but three new members joined. The next meeting will be 26 October 2017 in Washington, USA, hosted by the Library of Congress. Possible meetings in 2018 were suggested for Berlin March/April or possibly London or Rome. There were two workshops. The first on ITOC (Information Trends and Opportunities Committee) was based around the problem of reproducibility and verification of scientific results. The second workshop was TACC (Technical Activities Coordinating Committee) dealing mainly with repositories of data and the question of preservation of data. One of the most interesting talks was by Tim Smith (CERN) who spoke about their open research data depository and pointed out that storage of digital data rapidly decays with time (the error rate is high), and so in order to maintain the data over a long time they go through a continuous media verification process of all data held in the repository in order to make early corrections, rather than allow errors to accumulate. This consumes 10% of their drive capacity! Following the two workshops the ICSTI Executive Committee met, mainly to discuss the possibility of refreshing their web site and making it more user friendly and up to date. The problem here, as usual, was the cost of doing this and where the funds would come from.

A.M. Glazer acknowledges with gratitude the close collaboration with the IUCr journals Executive Managing Editor, P.R. Strickland, and with the IUCr's Representatives to CODATA, J.R. Helliwell and B. McMahon.

*A.M. Glazer, IUCr Representative*

#### **A13.6. International Organization for Standards (ISO)**

In 2013 the Liaison between ISO/Technical Committee 12 (TC 12) Quantities and Units and the IUCr was confirmed, and the Chair of the Commission on Crystallographic Nomenclature was appointed Liaison Representative.

There was no activity during the triennium related to crystallography.

*C.P. Brock, IUCr Representative*

### **A14. Budget estimates for period to Twenty-Fifth General Assembly: determination of unit contribution**

#### **A14.1. Budget estimates**

The estimated budget for the General Fund 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 2017 – 31 December 2019.

	CHF	CHF
<b>INCOME</b>		
Subscriptions from Adhering Bodies	486,000	
Yield from investments and banking accounts	120,000	
	606,000	
<b>EXPENDITURE</b>		
Administration	1,445,400	
Subscriptions to ICSU and bodies of ICSU	15,000	
Administrative meetings	306,000	
Scientific meetings	24,000	
	1,790,400	
<b>ESTIMATED PROFIT/(DEFICIT)</b>		(1,184,400)

#### **A14.2. Unit Contribution**

According to Statute 5.10(k), the General Assembly has to determine the Unit Contribution to be paid by the Adhering Bodies for the period to the next General Assembly. The Executive Committee recommends to the General Assembly that the Unit Contribution should remain at its present level of CHF 1,000 (set at the Beijing Congress in 1993) for the years 2018–2020.

## Appendix B. Statutes and By-Laws of the International Union of Crystallography

as Adopted by the Fourth General Assembly in 1957 and Amended by the Fifth General Assembly in 1960, the Sixth General Assembly in 1963, the Seventh General Assembly in 1966, the Eighth General Assembly in 1969, the Ninth General Assembly in 1972, the Tenth General Assembly in 1975, the Eleventh General Assembly in 1978, the Seventeenth General Assembly in 1996, the Eighteenth General Assembly in 1999, by unanimous postal agreement of the Adhering Bodies in 2010 and the Twenty-Second General Assembly in 2011

### Statutes

#### *1. Objects of the Union*

1.1. The objects of the Union are

- (a) to promote international cooperation in crystallography;
- (b) to contribute to the advancement of crystallography in all its aspects, including related topics concerning the non-crystalline states;
- (c) to facilitate international standardization of methods, of units, of nomenclature and of symbols used in crystallography;
- (d) to form a focus for the relations of crystallography to other sciences.

1.2. For these purposes the Union shall have the power

- (a) to adhere to the International Council for Science;
- (b) to organize international meetings and conferences on subjects falling within the purview of the Union;
- (c) to promote international publication of crystallographic research and of crystallographic works;
- (d) to set up Commissions or other bodies for special objects;
- (e) to initiate, promote and coordinate crystallographic research requiring international cooperation;
- (f) to organize Special Projects which shall be financed independently of the regular operations of the Union;
- (g) to participate in Joint Commissions with other Unions or other scientific bodies in matters of interest to the Union;
- (h) to perform all such other legal acts as are essential for or conducive to the objects of the Union including the constitution or organization of separate or independent bodies having an appropriate legal status;
- (i) to receive into association existing regional organizations of crystallographers having substantially the same aims and objects as the Union; these organizations shall be known as Regional Associates of the Union;
- (j) to receive into association existing international scientific organizations whose interests overlap with the aims and activities of the Union; these organizations shall be known as Scientific Associates of the Union.

#### *2. Organization and Legal Domicile*

2.1. Under the name of International Union of Crystallography an Association has been organized and incorporated; it is governed by Articles 60 and following of the Swiss Civil Code and by the present Statutes of Incorporation.

2.2. The duration of the Union is not limited.

2.3. The legal domicile of the Union is in Geneva, Switzerland.

#### *3. Membership*

3.1. The members of the Union are its Adhering Bodies.

3.2. There shall be only one member for each country. Only under extraordinary circumstances the General Assembly may admit a suitably designated additional Adhering Body from a country, provided a corresponding Adhering Body of that country has already been admitted as a National Member of the International Council for Science (ICSU). In this case, each Adhering Body will have separate delegates and will be treated separately in questions of voting and finances.

3.3. The Adhering Body can be a National Academy, National Research Council or similar body, or a scientific society or group of such societies. Each Adhering Body shall form a National Committee for Crystallography to represent it in the Union.

3.4. Any number of Countries may agree to form a group in order to name or establish a single Adhering Body. This Body shall form a joint National or Regional Committee for Crystallography. Wherever the terms Country and National Committee for Crystallography are used in these Statutes or in the By-Laws, they shall be taken to include such groups of Countries and joint National or Regional Committees for Crystallography.

3.5. Membership in the Union shall be fully effective when the nature of the Adhering Body and the membership of the National Committee have been reported to and accepted by the General Assembly. Any replacement of an Adhering Body is subject to the approval of the Executive Committee and acceptance by the General Assembly. Any major change in the nature of an Adhering Body shall be considered valid only after it has been reported to and accepted by the General Assembly.

3.6. Adherence to the Union shall be in one of five Categories I-V with corresponding voting powers and contributions as set out in Statutes 5.5 and 9.4. A Body applying for adherence to the Union shall specify in which Category it wishes to adhere; this choice of Category, or any desired change in the Category, is subject to the approval of the Executive Committee and confirmation by the General Assembly.

3.7. Any extension of a joint adherence formed in accordance with Statute 3.4 is subject to the approval of the Executive Committee and acceptance by the General Assembly.

3.8. Participation in Special Projects [Statute 1.2(f)] shall not be obligatory. The extent of financial participation shall be a matter for special negotiation for each such project, except that the relationship between contribution and voting power within the project shall be that of the Category scheme defined in Statutes 5.5 and 9.4 to determine this relationship in the General Assembly.

3.9. Each National Committee has the right to submit to the Union through the General Secretary questions within the competence of the Union.

3.10. Any Adhering Body may withdraw from the Union if it has given notice of withdrawal at least six months before the end of the current financial year; it is required to fulfil its obligations relating to the time period when it was a member of the Union. Its membership and any further obligations shall then be suspended by the Executive Committee at the expiry of the notice of withdrawal. The withdrawal shall take effect when it has been reported to the General Assembly.

3.11. An Adhering Body which withdraws from the Union in accordance with Statute 3.10, or any Adhering Body whose membership is cancelled in accordance with Statutes 5.12 or 9.6, loses all rights in connexion with the Union.

3.12. If the Countries of a group formed in accordance with Statute 3.4 agree that the group should be dissolved, or if a Country wishes to withdraw from such a group, with or without the agreement of the other Country or Countries of the group, the adherence of the original group shall be suspended by the Executive Committee at the expiry of an appropriate notice, provided that the original group has fulfilled its obligations. The termination of the original adherence shall take effect when the matter has been reported to the General Assembly. Pending this report, the Countries of the group, or any of them, may submit proposals for the continuation of their representation in the Union. In each of such proposals the nature of the Adhering Body, the membership of the National Committee and the desired Category of adherence shall be specified. These proposals are subject to the approval of the Executive Committee, which shall then make *ad interim* arrangements concerning these adherences. These arrangements are subject to acceptance by the General Assembly.

#### 4. Administration

4.1. The work of the Union shall be conducted by

- (a) the General Assembly;
- (b) the Officers of the Union, constituting the Executive Committee;
- (c) the Commissions as defined in Statute 8.1.

The composition and function of these bodies are defined in the following paragraphs, whose application is governed by the By-Laws.

#### 5. General Assembly

5.1. The work of the Union shall be directed by the General Assembly which is composed of delegates appointed by the Adhering Bodies.

5.2. The Executive Committee is responsible to the General Assembly and shall participate in its deliberations. Members of the Executive Committee have no voting power in the General Assembly, except for the casting vote of the Chair [Statute 5.8].

5.3. The General Assembly shall, as a rule, hold an ordinary meeting once every three years. The date and the place of the meeting, unless determined by the previous General Assembly, shall be determined by the Executive Committee. The General Secretary shall communicate the date and the place of the meeting to the National Committees and to the Commissions at least twelve months in advance.

5.4. In special cases, the President of the Union, with the consent of the Executive Committee, may call an extraordinary meeting of the General Assembly. This shall be done at the request of one-fifth of the Adhering Bodies. The routine business of a General Assembly prescribed in Statute 5.10 shall normally be omitted, unless specifically included in the agenda; but an extraordinary General Assembly shall have the same powers, and be subject to the same rules, as an ordinary General Assembly, except where otherwise is stated in the Statutes and By-Laws. The General Secretary shall communicate the date and the place of the extraordinary General Assembly to the National Committees and to the Commissions at least eight months in advance if amendment of the Statutes is contemplated, or at least four months otherwise.

As an alternative, in special cases not requiring an amendment to or a change of the Statutes, the President of the Union with the consent of the Executive Committee may ask for a postal or electronic ballot of the Adhering Bodies. This shall be done at the request of one-fifth of the Adhering Bodies. The voting power of an Adhering Body in a postal or electronic ballot is the same as that at General Assemblies. The General Secretary will communicate the matter for determination to the National Committees and to the Commissions four months before the deadline for the votes to be received by the General Secretary. In order to facilitate a full discussion between the participants in the postal or electronic ballot, the comments and questions of the Adhering Bodies, the responses of the President as well as any amendment to the initial proposal will be circulated among the Adhering Bodies using fast means of communications at the latest one month before the deadline.

5.5. The voting power of an Adhering Body at General Assemblies and in postal or electronic ballots shall be in accordance with its Category of adherence, as follows:

Category	I	II	III	IV	V
Number of votes	1	2	3	4	5

5.6. Each Adhering Body, through its National Committee, shall make known to the General Secretary before the opening of each General Assembly the names of its delegates (and of their alternates, if any), and also the name of the Chair of the national or regional delegation. No Officer of the Union may be a member of any delegation, nor shall any person serve as a member of more than one delegation.

5.7. Normally each of the delegates present at a General Assembly shall have one vote only, but when for special reasons an Adhering Body cannot be fully represented at a General Assembly it may distribute its votes among a number of delegates smaller than the number of votes which that Adhering Body has in accordance with the Category in which it adheres; such a decision has to be made known to the General Secretary before the opening of the General Assembly concerned. Any Adhering Body not represented at a General Assembly may forward its views to the General Secretary by letter, and such views shall be made known to the General Assembly if received before voting takes place.

5.8. Except where otherwise provided in the Statutes and By-Laws, decisions of the General Assembly are taken by a majority of the votes cast. In the event of an equal division of votes the Chair shall take the final decision.

5.9. No question which has not been placed on the agenda of business to be transacted at the General Assembly shall be discussed or put to the vote unless a proposal to that effect be approved by at least two-thirds of the votes there represented.

5.10. The General Assembly shall

- (a) take appropriate action on any matters concerning membership in the Union [Statutes 3.5, 3.6, 3.7, 3.10, 3.12 and 5.12];
- (b) elect the President, the Vice-President, the General Secretary, the Treasurer and the other Officers of the Union [Statutes 6.1 and 6.3];

- (c) consider, and make decisions regarding, the confirmation of the appointments of Editors of publications of the Union [Statute 7.1];
- (d) determine the number of elected members of each Commission set up by the General Assembly [Statutes 5.11(c) and 8.2];
- (e) elect the Chairs and members of the Commissions [Statute 8.2];
- (f) elect representatives of the Union on Joint Commissions with other Unions, and on other scientific bodies [Statutes 1.2(g) and 8.5];
- (g) receive the reports on the activities of the Union and of its Commissions [Statutes 6.8 and 8.4];
- (h) receive the audited accounts for the years elapsed since the previous General Assembly [Statute 9.1];
- (i) on receipt of satisfactory reports or accounts, release the Treasurer, or any other Officer, or the Chair or any member of any Commission or other body, from financial or other liability to the Union;
- (j) determine the budget for general expenditure for the period to the next General Assembly, on the basis of the estimate prepared by the Executive Committee [Statutes 9.2 and 9.3];
- (k) determine the unit contribution for the period to the next General Assembly [Statute 9.5];
- (l) determine the general policy and the timetable for the period to the next General Assembly;
- (m) give preliminary consideration to the activities of the Union for the three-year period following the next General Assembly.

5.11. The General Assembly shall have the power

- (a) to amend these Statutes in accordance with Statute 13.1;
- (b) to formulate and amend By-Laws on any matters not covered by these Statutes;
- (c) to set up any Commission or other body it may deem necessary for the administrative and scientific work of the Union, and to determine the terms of reference of such a body [Statute 1.2(d)];
- (d) to dissolve any Commission or other body set up in accordance with Statute 5.11(c) when its existence is deemed no longer necessary;
- (e) to determine the nature of Special Projects which shall be financed independently of the regular operations of the Union [Statute 1.2(f)];
- (f) to accept Regional Associates, to determine the nature of the association in each case, and to determine any mutual financial commitments;
- (g) to accept Scientific Associates, to determine the nature of the association in each case, and to determine any mutual financial commitments;
- (h) to decide on all other questions falling within the competence of the Union.

*Timetable in preparation for General Assembly*

		Statute	By-Law
12 months	Notice of date and place of ordinary General Assembly to National Committees and Commissions	5.3	-
8 months	Notice of date and place of extraordinary General Assembly to National Committees and Commissions, if amendment of Statutes is contemplated	5.4	-
6 months	Proposals for amendments to Statutes to General Secretary	13.1	-
5 months	Estimated budgets from Commissions to Executive Committee	9.2	-
4 months	Proposals for agenda of General Assembly to General Secretary	-	1.2
4 months	Notice of date and place of extraordinary General Assembly to National Committees and Commissions, if amendment of Statutes is not contemplated	5.4	-
4 months	Proposals for amendments to Statutes to National Committees and Commissions	13.1	-
14 weeks	Reports of Commissions to General Secretary	8.4	-
10 weeks	Report of Executive Committee to National Committees and Commissions	6.8	-
10 weeks	Reports of Commissions to National Committees and	8.4	-

	Commissions		
10 weeks	Budget to National Committees and Commissions	9.3	-
10 weeks	Agenda to National Committees and Commissions	-	1.1

*Timetable during General Assembly*

		Statute	By-Law
‘Before’	Notice by National Committees to General Secretary of names of delegates, alternates and Chairs of delegations, and of distribution of votes if not one per delegate	5.6, 5.7	-
96 hours	Nominations by Executive Committee for Officers of Union	-	8.1
72 hours	Recommendations by Commissions to General Secretary for Chairs and members of Commissions	-	8.3
48 hours	Nominations by Executive Committee for Chairs and members of Commissions	-	8.3
48 hours	Notification of motion to amend or suspend By-Laws	-	9.1
36 hours	Notice to General Secretary of nominations by delegates for Officers of Union	-	8.2
24 hours	Posting of nominations by delegates for Officers of Union	-	8.2
24 hours	Notice to General Secretary of nominations by delegates for Chairs and members of Commissions	-	8.4
12 hours	Posting of nominations by delegates for Chairs and members of Commissions	-	8.4

5.12. The General Assembly may cancel the membership of any Adhering Body of the Union for any serious cause; such a decision may only be taken after the member in question has been previously given an opportunity to furnish an explanation to the Executive Committee for forwarding to the General Assembly. At least three-fourths of the total number of the votes of all Adhering Bodies are required for cancellation.

#### 6. Executive Committee

6.1. The Officers of the Union constituting the Executive Committee are

- (a) the President;
- (b) the Vice-President;
- (c) the General Secretary;
- (d) the Treasurer;
- (e) the immediate Past President;
- (f) six ordinary members.

6.2. The election of Officers of the Union shall be arranged in such a way that there will not be more than two Officers from any one Country and that amongst the six ordinary members there will be at least one Officer from a Country from each of the three geographical regions (i) Europe and Africa, (ii) the Americas and (iii) Asia/Oceania. A person is regarded as belonging to the Country in which he or she is normally resident and where the main part of his or her work is conducted. In cases of doubt the General Assembly shall decide to which Country a person is considered to belong.

If during the period between General Assemblies the number of Officers from a Country is increased above two because of any change of Country of residence, the Officer or Officers who changed their Country of residence may continue to serve until the close of the next General Assembly. If at that time the number of Officers from the Country concerned would remain above two, one or more of the Officers who changed their Country of residence shall be considered to have resigned.

6.3. The offices of General Secretary and Treasurer may be combined and shall then be considered as a single office. Otherwise no person shall hold more than one office simultaneously. The voting power of the Officer holding the combined office of General Secretary and Treasurer shall not be more than that of either the General Secretary or the Treasurer.

6.4. The President holds office as President until the close of the ordinary General Assembly following his or her election, and continues as a member of the Executive Committee until the close of the ordinary General Assembly next but one following that of his or her election. He or she is not then eligible for immediate re-election to the office of President, nor to any other office in the Executive Committee.

The Vice-President holds office until the close of the ordinary General Assembly following his or her election. He or she is not eligible for immediate re-election to the same office.

The General Secretary and the Treasurer hold office until the close of the ordinary General Assembly following that of their election. They are eligible for immediate re-election to the same office, but shall not serve in that office for more than three full consecutive terms.

Three ordinary members are elected at each ordinary General Assembly and hold office until the close of the ordinary General Assembly next but one following that of their election. They are not eligible for immediate re-election to the same office.

In the event of a vacancy, through resignation, death or other cause, any Officer elected by the General Assembly to fill the unexpired term of office shall serve only to the end of the normal term of the Officer he or she replaces; at the end of this service he or she may be nominated for re-election for a full term to the same office.

6.5. The Executive Committee shall carry out the decisions of the General Assembly and give effect to the general policy of the Union as determined by the General Assembly.

6.6. During the periods between General Assemblies the Executive Committee shall have full power to carry on the business of the Union in all matters not specifically assigned by the Statutes, the By-Laws or the General Assembly to individuals or to Commissions or other bodies. If necessary, it may make *ad interim* arrangements in all matters assigned by the Statutes and By-Laws to the General Assembly.

6.7. In the event of an individual, a Commission or another body of the Union failing to act in any matter assigned to him or her or it by the Statutes, By-Laws or the General Assembly, the Executive Committee may, after reasonable notice to the individual or body in question, take action on behalf of the Union.

6.8. The Executive Committee shall report on its activities to the General Assembly. The action taken by the Executive Committee in accordance with Statutes 3.5, 3.6, 3.7, 3.10, 3.12, 6.6, 6.7, 7.1, 7.2, 8.2, 9.6 and 9.9 shall be included in this report. The report to the General Assembly shall be dispatched by the General Secretary to the National Committees and to the Commissions at least ten weeks before the meeting.

## 7. Publications of the Union

7.1. The Editors of the publications of the Union are appointed by the Executive Committee for initial terms extending through not more than six years beyond the ordinary General Assembly following the appointment. Each initial appointment is subject to confirmation by that General Assembly. Reappointments may be made by the Executive Committee for terms of not more than three years, and are subject to confirmation by the ordinary General Assembly following the reappointment.

7.2. Co-editors and Assistant Editors are appointed by the Editors for terms of not more than three years, but they may be reappointed immediately for terms of the same length. The appointments and reappointments are subject to the approval of the Executive Committee.

7.3. Editors and Co-editors are members of the Commissions set up for their respective publications.

## 8. Commissions and Joint Commissions

8.1. The term Commission shall be understood to include all Commissions, Committees, and other bodies of the Union with the exception of National Committees for Crystallography, and the Executive Committee and its subcommittees.

8.2. The Chairs and members of the Commissions are elected at each General Assembly. Subject to the approval of the Executive Committee, Commissions may co-opt further members during the periods between General Assemblies, and may fill vacancies arising from resignation, death or other cause. Members (but not Chairs) may be nationals of or residents in a Country not adhering to the Union.

8.3. The Commissions shall be responsible to the General Assembly. They shall generally have full freedom in arranging their internal structure and work. They may formulate their own Rules of Procedure within the framework of the Statutes and By-Laws of the Union, and within their terms of reference.

8.4. The Chairs shall report on the activities of the Commissions to the General Assembly. These reports shall reach the General Secretary at least fourteen weeks before the General Assembly and shall be dispatched by him or her to the National Committees and the Commissions at least ten weeks before the meeting.

8.5. The representatives of the Union on Joint Commissions and on other scientific bodies [Statute 1.2(g)] are elected at each General Assembly. For each such body one representative shall be designated as the chief representative of the Union. His or her obligations to report are the same as those of the Chairs of the Commissions.

#### *9. Finance*

9.1. The Executive Committee shall be responsible to the General Assembly for all the financial affairs of the Union.

9.2. The Chair of each Commission (or other member approved by the Executive Committee) shall be responsible to the Executive Committee for any expenditure of funds by this Commission. Five months before each General Assembly he or she shall submit to the Executive Committee an estimate of the budget of the Commission for the period between that General Assembly and the one following it. He or she shall submit annually to the Executive Committee a revised budget for the ensuing year and a statement of accounts for the preceding year. These accounts shall be available for audit by the Executive Committee or its appointees.

9.3. The Executive Committee shall prepare an estimate of the budget for the period between the next General Assembly and that following it. This estimate shall be dispatched by the General Secretary to the National Committees and to the Commissions at least ten weeks before the meeting.

9.4. Each Adhering Body shall pay an annual subscription in accordance with its Category of adherence, as follows:

Category	I	II	III	IV	V
Number of unit contributions	1	3	6	10	15

The annual subscriptions are payable during the calendar year to which they apply.

9.5. The unit contribution, stated in terms of a currency to be designated by the Executive Committee, shall be determined by the General Assembly for the period to the next General Assembly.

9.6. Any Adhering Body which is in arrears with its subscription for two years shall be warned and shall be deprived of its voting power. The membership of any Adhering Body which is in arrears for four years shall be automatically suspended and may be cancelled by the General Assembly under Statute 5.12. An Adhering Body whose membership has been suspended shall receive no privileges of the Union and incur no further responsibility for dues; it may be reinstated by action of the Executive Committee.

9.7. The financing and management of publications of the Union shall be kept distinct from general expenditure. Editors and Co-editors shall be responsible to the Executive Committee for any receipts or expenditure of funds by them with respect to their publications.

9.8. The financing and management of Special Projects of the Union shall be kept distinct from the regular operations of the Union.

9.9. No funds may be solicited or accepted on behalf of the Union or any of its Commissions from any international, governmental or other agency or person without the prior approval of the Executive Committee. Any National Committee for Crystallography may however solicit funds within its own Country for the support of its own activities or in its capacity as host for a General Assembly, Congress or other meeting sponsored by the Union. Any funds, in the form of donations, legacies, or grants, accepted by the Executive Committee shall be used so far as is possible in accordance with the wishes of the donors.

#### *10. Liability*

10.1. The Union is liable only to the extent of its assets, and the Adhering Bodies are not individually liable for its corporate debts and liabilities.

10.2. The liabilities of the Adhering Bodies are limited to the payment of their annual subscriptions and to such contributions to the Special Projects of the Union as they may have pledged.

10.3. No Officer of the Union shall be individually liable for the corporate debts and liabilities of the Union. The Union shall indemnify any Officer or former Officer in respect of any claims laid against him or her in respect to his or her authorized actions on behalf of the Union. At its discretion the Executive Committee may extend this indemnity to other persons in respect of their authorized actions on behalf of the Union.

10.4. The Union shall not accept any liability for any personal loss, damage or accident sustained by an individual, not being an employee of the Union, engaged in any activity, including travel, on behalf of the Union.

#### *11. Auditor and Representation of the Union*

11.1. The Auditor of the Union shall be a person or corporation authorized to act as a public accountant. The Auditor shall be appointed by the Executive Committee on the recommendation of the Treasurer and maintained thereafter subject to the approval of the General Assembly.

11.2. With the exception of cheques, all contracts and formal agreements involving the Union shall be signed by two Officers of the Union. The Executive Committee may restrict the power to sign a particular document or type of document to specific persons among the Officers; and it shall determine rules for the signing of cheques.

11.3. The President shall be the official representative of the Union on all other civil and legal occasions and in dealing with other organizations. The President may in this respect delegate his or her powers to another Officer of the Union, or, with approval of the Executive Committee, to any other person.

#### *12. Dissolution of the Union*

12.1. The Union shall not be dissolved except on a motion presented at a General Assembly. If a motion to dissolve is to be presented, the notice for that General Assembly as given under Statute 5.3 or 5.4 shall include a statement of the motion to dissolve and shall refer specifically to this Statute. Such a motion shall be presented to the General Assembly without amendment and at least three-fourths of the votes there represented shall be required for dissolution.

In the event that less than three-fourths of the total number of the votes of all Adhering Bodies are represented at the General Assembly, a postal or electronic ballot may be arranged, and in such a postal or electronic ballot at least three-fourths of the total number of the votes of all Adhering Bodies shall be required for dissolution.

12.2. In the event of dissolution of the Union in accordance with Statute 12.1, the General Assembly shall appoint a special Committee, reporting to the International Council for Science, for the liquidation of the assets of the Union. The available assets will be entirely attributed to one or more institutions in pursuit of a goal of similar public interest to that of this association and that also benefits from tax exemption. In no case can the property be returned to its current or founding members, nor be used for their profit in whole or part in any manner whatsoever.

#### *13. Statutes*

13.1. Amendments to the Statutes require action at a General Assembly. An amendment is adopted at such an Assembly only if (i) at least two-thirds of the votes represented at the General Assembly are affirmative and (ii) if these affirmative votes amount to more than half the total number of the votes of all Adhering Bodies. In the event that the vote on a proposed amendment satisfies condition (i) but not condition (ii), the Executive Committee may refer the proposed amendment to a postal or electronic ballot of the Adhering Bodies. If the proposed amendment then obtains affirmative votes amounting to more than half the total number of the votes of all Adhering Bodies, the amendment is adopted.

Proposals for amendments may be made by the Executive Committee or by any National Committee. Such proposals made by National Committees shall reach the General Secretary at least six months in advance of the General Assembly. The General Secretary shall dispatch these proposals, and those made by the Executive Committee, to the National Committees and to the Commissions at least four months before the meeting.

13.2. The present English text shall be considered the authoritative text in the interpretation of these Statutes. Where disputes arise concerning this interpretation, the matter shall be decided by the General Assembly, or, during the periods between General Assemblies, by a ruling of the President of the Union.

## By-Laws

### 1. General Assembly

1.1. The agenda of business to be transacted at a General Assembly shall be determined by the Executive Committee and shall be dispatched by the General Secretary to the National Committees and to the Commissions at least ten weeks before the meeting.

1.2. Any National Committee and any Commission of the Union may propose business to be transacted at a General Assembly. Such proposals shall reach the General Secretary at least four months before the meeting, and shall be included in the agenda of the General Assembly.

1.3. The General Assembly may determine the date and the place of the next but one ordinary meeting of the General Assembly.

1.4. Chairs of the National Committees and of the Commissions, and representatives of Regional Associates and Scientific Associates may attend the General Assembly and take part in the discussions but shall have no voting power. The President may invite representatives of scientific bodies, or individuals, to attend the General Assembly; such invited guests may take part in the discussions but shall have no voting power. Other interested persons may also attend the General Assembly but they shall not take part in the discussions, unless specifically invited or permitted to do so by the Chair, and they shall have no voting power.

At the discretion of the Chair any or all of the persons attending the General Assembly under this By-Law may be required to withdraw.

1.5. If a delegate to a General Assembly is absent from a session of the Assembly, his or her place may be taken by any of the alternates nominated to the Assembly under Statute 5.6 provided that the Secretary of the Assembly is notified before the beginning of the session of the name of the delegate and of the name of the alternate, either by the delegate or by the Chair of his or her delegation. In general no such substitution may take place during a session of the Assembly, but the Chair of the Assembly may permit substitution to be made under special circumstances.

1.6. The names of the representatives of a Body whose application for adherence to the Union has been received and declared in good order by the Executive Committee under By-Law 2.9(a) shall be made known to the General Secretary as prescribed in Statute 5.6. These representatives shall be seated with the delegates of the Adhering Bodies during the preliminary ceremonies and the initial business of the General Assembly. At the discretion of the Chair or by a vote of the Assembly, the representatives may be required to withdraw during the discussion of and voting on matters concerning adherence to the Union. The delegates of a new member may take their seats among the other delegates as soon as the General Assembly has accepted their Adhering Body as a member of the Union.

1.7. 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, and shall normally precede the reading of the minutes and the discussions of matters arising therefrom.

1.8. Delegates of an Adhering Body may not vote on any matter concerning its membership in the Union.

1.9. In the event of the General Assembly considering a change in a group of Countries according to Statute 3.12, the delegates from the Countries belonging or previously belonging to the group may not vote on any matters concerning the representation in the Union of any of these Countries. After acceptance of the *ad interim* arrangements made by the Executive Committee under Statute 3.12, these delegates have full voting power.

1.10. The delegates of new members may not vote on any matters concerning adherence to the Union, nor on any matters concerning the adoption of the minutes of the previous General Assembly, during the General Assembly at which they themselves are admitted.

1.11. The General Secretary shall post on the official bulletin board of the General Assembly the names of the Chairs and members (and alternates, if any) of the delegations and the numbers of votes represented by them.

1.12. During the General Assembly any delegate (or alternate) and any Officer of the Union is considered to have been notified of any action of the General Assembly, or of the Executive Committee, or of any Commission, if one of the two following procedures is adopted

(a) a notice is placed in the mail box or other location at which the delegate (or alternate) or the Officer is accustomed to receive mail during the course of the General Assembly, or

(b) a notice is handed to the designated Chair of each delegation with the specific request that he or she communicate its contents to his or her delegation, and to the General Secretary with the specific request that he or she communicate its contents to the Executive Committee, provided that in either case a similar notice is posted on the official bulletin board.

1.13. Minutes of the meetings of the General Assembly shall be made. Copies of the draft minutes shall be communicated by the General Secretary to the National Committees, to the Officers of the Union and to the Chairs of its Commissions. After approval at a subsequent General Assembly, two copies of the definitive minutes shall be signed by the Chair and the Secretary of the session at which they are approved, and shall be kept by the President and the General Secretary.

## 2. *Executive Committee*

2.1. The Executive Committee shall meet at each General Assembly. There shall be at least two additional meetings during the period between General Assemblies, unless the Executive Committee by a postal or electronic vote decides otherwise.

2.2. The Executive Committee shall make nominations to the General Assembly for the Officers of the Union, for the Chairs and members of the Commissions, and for representatives on Joint Commissions and on other scientific bodies. Normally these nominations shall be made after a preceding postal or electronic communication with the National Committees. In each case in which an Officer of the Union is nominated for another office, either by the Executive Committee or by delegates to the General Assembly [By-Law 8.2], the Executive Committee shall also include a nomination for the office which would be vacated if the election to the other office occurs. If the election to the other office does not occur and if the Officer's term has not expired, the nomination to the office which would have been vacated shall not be considered.

2.3. In the event of the resignation, death or disability of the President, the Vice-President shall assume the office of President until the close of the next ordinary General Assembly.

In the event of the resignation, death or disability of the Vice-President, the Executive Committee may appoint one of its members to serve as Vice-President until the close of the next ordinary General Assembly.

In the event of such circumstances that the General Secretary or the Treasurer cannot carry out his or her duties, the other shall assume those duties until the Executive Committee has considered the situation. In that event the Executive Committee may, but need not, appoint a new General Secretary or Treasurer to serve until the close of the next ordinary General Assembly.

In the event of the resignation, death or disability of an ordinary member of the Executive Committee, the Executive Committee may co-opt a new member to serve until the close of the next ordinary General Assembly.

The accession of an Officer of the Union to a new office under the conditions of this By-Law shall be accompanied by his or her resignation from the office to which he or she was previously elected, but service under this By-Law shall not affect his or her eligibility for immediate re-election to the new office.

2.4. Any Officer unable to attend a meeting of the Executive Committee may designate a deputy to attend that meeting. Such a deputy shall be named in writing to the President or the General Secretary. He or she shall have no voting power and shall not be counted as part of a quorum.

2.5. The President, on his or her own initiative or at the request of the Executive Committee, may invite any individual to be present at a meeting of the Executive Committee; such an invited guest may take part in the discussions but shall have no voting power.

2.6. At a meeting of the Executive Committee two-thirds (fractional parts neglected) of the Officers specified by Statutes 6.1 and 6.3, excluding any who have resigned or died, shall constitute a quorum; and decisions shall be taken by a simple majority of the Officers present and voting. The Chair of the meeting shall not vote in open ballots; but in the event of an equal division of votes the Chair may take the final decision. In secret ballots required by the Statutes or By-Laws or ordered by the Chair, he or she may vote at his or her discretion. If the Chair does not vote and there is an equal division of votes, he or she may take the final decision. If the Chair has voted in a secret ballot, he or she may not take the final decision, and must leave it to further discussion and ballot.

2.7. During the period between meetings of the Executive Committee, voting may take place by post or electronic means. Adoption of a proposal shall require affirmative votes from two-thirds (fractional parts neglected) of the Officers specified by Statutes 6.1 and 6.3, excluding any who have resigned or died. No decision on any proposal other than calling or cancelling a meeting of the Executive Committee shall be made by postal or electronic vote in the event that at least two Officers express

the wish that the matter concerned should first be given more or further consideration, either by correspondence or at a meeting of the Executive Committee.

2.8. Minutes of the meetings of the Executive Committee shall be made. Two copies of the minutes shall be signed by the Chair and the Secretary of the meeting at which they are approved, and shall be kept by the President and the General Secretary. A summary of the draft minutes of meetings of the Executive Committee shall be despatched by the General Secretary to the National Committees within ten weeks of the conclusion of each meeting.

2.9. In addition to the obligations described in the Statutes and elsewhere in these By-Laws, the Executive Committee shall

- (a) receive and report on applications for adherence to the Union if the nature of the applying Body and the membership of the National Committee have been duly reported to and considered to be in good order by the Executive Committee; pending the next General Assembly the Executive Committee may in the case of such applications provide such services of the Union as it deems proper;
- (b) consider and report on any other questions concerning adherence to the Union;
- (c) present an annual report, including an audited statement of receipts and expenditure, to the National Committees;
- (d) report to the Commercial Registry of Geneva any changes in the registered information concerning the Union;
- (e) have the power to appoint representatives on scientific bodies not belonging to the Union.

### 3. President

3.1. The President of the Union is Chair of the General Assembly and of the Executive Committee. In the absence of the President from a session or meeting, the Vice-President, or if he or she is not present another Officer of the Union designated by the Executive Committee, shall act as Chair.

3.2. The President of the Union is an *ex officio* member, with voting power, of all Commissions of the Union.

### 4. General Secretary

4.1. The General Secretary of the Union is Secretary of the General Assembly and of the Executive Committee. In the absence of the General Secretary from a session or meeting, another Officer of the Union designated by the Executive Committee shall act as Secretary.

4.2. The General Secretary of the Union is an *ex officio* member, with voting power, of all Commissions of the Union.

4.3. The General Secretary is responsible for conducting the ordinary business of the Union, with the exception of the financial administration, and for keeping its records.

4.4. 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.

### 5. Treasurer

5.1. The Treasurer of the Union is responsible for the financial administration of the Union and for keeping its accounts.

5.2. The Treasurer is an *ex officio* member of all Commissions of the Union, with voting power only for those questions which may involve the Union in financial commitments.

### 6. Sub-committees of the Executive Committee

6.1. The Finance Committee is appointed by the Executive Committee to advise on finances, establishment and salaries. The Convener of the Finance Committee should normally be a resident of the same country as the Union Secretariat. If the Convener is not an elected member of the Executive Committee he or she will attend *ex officio* the meetings of the Executive Committee without voting rights.

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.

6.3. The Executive Committee may establish, modify or abolish any other Sub-committees.

## 7. Commissions of the Union

7.1. The Chairs of the Commissions and the chief representatives on Joint Commissions or other bodies shall forward records of all meetings of the Commissions to the President and the General Secretary. They shall report annually on the activities of these bodies to the Executive Committee.

7.2. If funds are provided for the use of a Commission, it may make its own financial arrangements, with the prior approval of the Executive Committee and subject to the provisions of the Statutes and By-Laws. In cases where the Executive Committee has given prior approval, payments toward travelling expenses of Chairs and members of Commissions may be made from the general funds of the Union.

7.3. No person who has served for three consecutive full terms of office on a Commission is eligible for nomination for a fourth consecutive term of service on the same Commission except as Chair. In no case is any person eligible for more than four consecutive full terms of service on the same Commission. These limitations do not apply to Editors [Statute 7.1], Co-editors [Statute 7.2] and *ex officio* members. Any Commission, in its Rules of Procedure, may reduce the length of service specified here.

7.4. In the event of the resignation, death or disability of the Chair of any Commission, the Executive Committee shall appoint a member of that Commission to serve as Chair until the close of the General Assembly following this appointment.

## 8. Nominations and Elections

8.1. All delegates (and alternates) shall be notified of the nominations presented by the Executive Committee under By-Law 2.2 for the Officers of the Union as early as possible and at least ninety-six hours before the scheduled commencement of the session of the General Assembly at which the vote is to be taken.

8.2. After the delegates have been notified of the nominations by the Executive Committee as prescribed in By-Law 8.1, other nominations for Officers of the Union may be made by any six or more delegates. Such nominations shall be made in writing to the General Secretary not less than thirty-six hours before the voting session and shall be accompanied by a written statement that the consent of the nominees has been obtained. These nominations shall be posted by the General Secretary on the official bulletin board not less than twenty-four hours before that session.

8.3. Recommendations from each Commission for the Chair and members of the Commission shall be made in writing to the General Secretary not less than seventy-two hours before the voting session of the General Assembly. These recommendations shall be approved by a majority of the members of the Commission and shall be accompanied by a written statement that the consent of the persons recommended has been obtained. All delegates (and alternates) shall be notified of the nominations presented by the Executive Committee under By-Law 2.2 for the Chair and members of each Commission at least forty-eight hours before the voting session.

8.4. After the delegates have been notified of the nominations by the Executive Committee as prescribed in By-Law 8.3, other nominations for the Chair and members of each Commission may be made by any six or more delegates. Such nominations shall be made in writing to the General Secretary not less than twenty-four hours before the voting session and shall be accompanied by a written statement that the consent of the nominees has been obtained. These nominations shall be posted by the General Secretary on the official bulletin board not less than twelve hours before that session.

8.5. In voting for the President, Vice-President, General Secretary and Treasurer of the Union, each of these offices shall be taken separately and voting shall be by secret ballot. A simple majority of the votes represented by the delegates present at the voting session shall be required for election.

If there is only one candidate for one of these offices, his or her nomination shall be presented to the General Assembly and the candidate concerned shall be considered as elected. If there are two candidates or more, and an election is not achieved after two ballots, the candidate receiving the smallest number of votes in the second ballot shall be removed from the list unless this will lead to a candidate being elected without receiving a simple majority of the votes. If an election is not achieved after a third ballot, this procedure shall be repeated until an election is achieved. Any ballot form showing more than one mark shall be invalid. Any contingency arising during the balloting shall be resolved by a ruling of the Chair of the General Assembly.

8.6. The election of the ordinary members of the Executive Committee shall be by secret ballot, the ballot form showing the nominations presented by the Executive Committee and the nominations made by delegates. Balloting shall be conducted in such a way that the requirements of Statute 6.2 are met. A simple majority of the votes represented by delegates present at the voting session shall be required for election. If there are not more candidates than vacancies, the nominations shall be

presented to the General Assembly and the candidates shall be considered as elected. If there are more candidates than vacancies and all vacancies are not filled by election at the first ballot, a second ballot shall be arranged containing the names of the candidates not elected. If there are vacancies after the second ballot, the balloting procedure shall be repeated until all vacancies are filled; for second and subsequent ballots the name of the candidate receiving the smallest number of votes on the preceding ballot shall be removed from the list unless this will lead to a candidate being elected without receiving a simple majority of the votes. Any ballot form showing more marks than the appropriate number of vacancies shall be invalid. Any contingency arising during the balloting shall be resolved by a ruling of the Chair of the General Assembly.

8.7. In the event that an election must be held to fill the unexpired term of an office vacated by an ordinary member [Statute 6.4], the nominations for this office shall be distinct from the nominations for ordinary members for full terms. A person may be nominated for both categories, but can be elected to only one office [Statute 6.3]. If ballots are required in the elections for both categories, the ballots for the full-term offices shall take place first. A person who has been elected to two consecutive non-full terms is not eligible, on completion of his or her second term, for immediate re-election as an ordinary member of the Executive Committee.

8.8. In voting for the Chairs and members of the Commissions each Commission shall be considered separately. For the election of the Chairs the procedure described in By-Law 8.5 shall be followed. For the election of the members of the Commissions the procedure described in By-Law 8.6 shall be followed except that no more than two ballots shall be held. Any vacancies still remaining may be filled as provided in Statute 8.2.

8.9. The procedure for the nomination and election of representatives of the Union on Joint Commissions and on other scientific bodies is so far as is possible the same as that for the nomination and election of the Chairs and members of the Commissions.

#### *9. By-Laws*

9.1. These By-Laws may be amended or suspended at any General Assembly and at least two-thirds of the votes there represented are required for an amendment or suspension. A motion to amend or suspend, if not already included in the agenda of business of the General Assembly, may be placed there by the procedure of Statute 5.9. No notice is required for a proposal to suspend the time limits prescribed by By-Laws 8.2 and 8.4. Notification of any other motion to amend or suspend the By-Laws must be given by its originators to all delegates (and alternates) and to all Officers of the Union in accordance with the procedure prescribed in By-Law 1.12, at least forty-eight hours before the session of the General Assembly at which the motion is to be considered.

9.2. The present English text shall be considered the authoritative text in the interpretation of these By-Laws. Where disputes arise concerning this interpretation, the matter shall be decided by the General Assembly, or during the periods between General Assemblies, by a ruling of the President of the Union.

## Appendix C. Committees, Commissions and Representatives

### C1. Membership of bodies belonging to the Union

#### Executive Committee

President

S. Lidin, Division of Polymer & Materials Chemistry, Lund University, Box 124, Lund, SE-221 00 Lund, Sweden

Vice-President

H. A. Dabkowska (Canada)

General Secretary and Treasurer

L. Van Meervelt (Department of Chemistry, Katholieke Universiteit Leuven, Celestijnenlaan 200F, BE-3001, Leuven, Belgium)

Immediate Past President

M. L. Hackert (USA)

Ordinary members

W. Depmeier (Germany), G. C. Diaz de Delgado (Venezuela), S. Garcia-Granda (Spain), R. Kuzel (Czech Republic), J. L. Martin (Australia), M. Takata (Japan)

[S. Lidin, H. A. Dabkowska, L. Van Meervelt, M. L. Hackert, W. Depmeier, S. Garcia-Granda and R. Kuzel will hold office until the close of the Twenty-Fifth General Assembly (2020). G. Diaz de Delgado, J. L. Martin and M. Takata will hold office until the close of the Twenty-Sixth Assembly (2023).]

Executive Secretary

A. T. Ashcroft (International Union of Crystallography, 2 Abbey Square, Chester CH1 2HU, UK)

#### Commission on Journals

Chair and Editor-in-Chief of IUCr journals

A. J. Allen (National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899-8523, USA) (*Acta A + B + C + D + E + F; IUCrData; IUCrJ; JAC; JSR*).

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- Ex officio member**
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T. Bekker (Russia)

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J. M. Garcia-Ruiz (Spain, as an Editor of *Journal of Applied Crystallography*)

**Commission on Crystallographic Computing****Chair**

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Chair

K. A. Kantardjieff (College of Science and Mathematics, Craven Hall 6211, California State University San Marcos, 333 South Twin Oaks Valley Road, San Marcos, CA 92096-0001, USA)

Elected members

O. Asojo (USA)

M. Weiss (Germany)

A. Guerri (Italy)

T. Inoue (Japan)

P. Kashkarov (Russia)

J. Moorthy (India)

S. Lopez-Andres (Spain)

D. Lamas (Argentina)

### Commission on Crystallography in Art and Cultural Heritage

Chair

G. Artioli (Dip. Geoscienze, Università di Padova, Via Gradenigo 6, I-35131 Padova, Italy)

Elected members

P. Bezdicka (Czech Republic)

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E. Tereschenko (Russia)

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Chair

Changqing Jin (Institute of Physics, Chinese Academy of Sciences, Zhongguancun South Str 3 number 8, Haidian District, Beijing, 100190, People's Republic of China)

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B. Albert (Germany)

E. Antipov (Russia)

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Chair

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Chair

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Chair

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M. Colmont (France)

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R. Oberti (Italy)

M. Wolcyrz (Poland)

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Chair

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M. T. Fernandez-Diaz (France)

O. Garlea (USA)

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Chair

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Wei Ren (People's Republic of China)  
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Chair

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J. Hernandez-Velasco (Spain)  
C. Alba-Simoniesco (France)  
V. Peterson (Australia)  
Th. Proffen (USA)  
R. Przenioslo (Poland)  
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### **Commission on NMR Crystallography and Related Methods**

Chair

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T. Polenova (USA)  
M. J. Potrzebowski (Poland)  
R. E. Wasylissen (Canada)  
S. Van Doorslaer (Belgium)  
D. Bryce (Canada)  
J. Senker (Germany)

### **Commission on Powder Diffraction**

Chair

D. Billing (School of Chemistry, University of the Witwatersrand, Private Bag 3, PO Wits, 2050, South Africa)

Elected members

A. Altomare (Italy)  
I. Evans (UK)  
B. Kennedy (Australia)

A. Mukherjee (India)  
A. Huq (USA)  
D. Kovacheva (Bulgaria)  
J. Rius (Spain)  
T. Ida (Japan)  
A. Wilkinson (USA)  
Ex officio member  
J. A. Kaduk (USA; as Representative of the International Centre for Diffraction Data)

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Chair  
J.-M. Gillet (Physics, CentraleSupelec, Grande Voie des Vignes, Chatenay-Malabry, 92295, France)  
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P. Dominiak (Poland)  
E. Espinosa (France)  
A. Gukasov (France)  
J. Kozisek (Slovakia)  
C. Matta (Canada)  
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T. Thakur (India)  
Ex officio member  
T. Ishigaki (Japan; as representative from Commission on Neutron Scattering)

**Commission on Small-Angle Scattering**

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E. Gilbert (Australia)  
J. Ilavsky (USA)  
K. Djinovic Carugo (Austria)  
D. McGillivray (New Zealand)  
E. Shtykova (Russia)  
M. Sugiyama (Japan)  
Ex officio member  
J. Westbrook (USA; as Representative of the Worldwide Protein Data Bank)

**Commission on Structural Chemistry**

Chair  
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K. Fromm (Switzerland)  
R. Banerjee (India)  
C. W. Lehmann (Germany)  
L. R. MacGillivray (USA)  
S. M. Peng (Taipei)  
G. Resnati (Italy)  
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**Commission on Synchrotron Radiation and XFEL Radiation**

Chair

P. Grotulska (Canadian Light Source, 44 Innovation Boulevard, Saskatoon, SK S7N 2V3, Canada)

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E. Granado (Brazil)  
T. Hatsui (Japan)  
M. Kozak (Poland)  
Y. Murakami (Japan)  
S. Pascarelli (France)  
S. Ramaswamy (India)  
J. L. Smith (USA)  
T. Tschentscher (Germany)

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Chair

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D. Bhattacharyya (India)  
V. Briois (France)  
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S. M. Heald (USA)  
Y. Inada (Japan)  
C. Lamberti (Italy)  
K. Lawniczak-Jablonska (Poland)  
N. M. Souza-Neto (Brazil)

**C2. Regional Associates****American Crystallographic Association**

Representative

H. A. Dabkowska (Brockhouse Institute for Materials Research, McMaster University, 1280 Main Street, Hamilton, Ontario, L8S 4M1, Canada)

**Asian Crystallographic Association**

Representative

J. L. Martin (Griffith Institute for Drug Discovery, N27, Griffith University, Don Young Road, Nathan, QLD 4111, Australia)

**European Crystallographic Association**

Representative

R. Kuzel (Department of Condensed Matter Physics, Charles University, Faculty of Mathematics and Physics, Ke Karlovu 5, 121 16 Prague 2, Czech Republic)

**Latin-American Crystallographic Association**

Representative

G. C. Diaz de Delgado (Laboratorio de Cristalografía-LNDRX, Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, Mérida, Mérida 5101, Venezuela)

**C3. Scientific Associates****International Centre for Diffraction Data**

Representative

D. Billing (School of Chemistry, University of the Witwatersrand, Private Bag 3, PO Wits, 2050, South Africa; ex officio as Chair of the Commission on Powder Diffraction)

**International Organization for Crystal Growth**

Representative

A. Zappettini (Istituto Materiali Elettronica Magnetismo, Consiglio Nazionale delle Ricerche, Parco Area delle Scienze 37/a, Parma 43010, Italy; ex officio as Chair of the Commission on Crystal Growth and Characterization of Materials)

**Worldwide Protein Data Bank (wwPDB)**

Representative to wwPDB Advisory Board

E. N. Baker (School of Biological Sciences, University of Auckland, Private Bag 92-019, Auckland, New Zealand)

**C4. Representatives on bodies not belonging to the Union****Interdivisional Committee on Terminology, Nomenclature and Symbols of the International Union of Pure and Applied Chemistry**

Representative

C. P. Brock (Department of Chemistry, University of Kentucky, 505 Rose St, Lexington, KY 40506-0055, USA; ex officio as Chair of the Commission on Crystallographic Nomenclature)

**International Science Council (ISC)**

Representative

M. L. Hackert (Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX 78712, USA)

**ICSU Committee on Data for Science and Technology (CODATA)**

Representative

J. R. Helliwell (School of Chemistry, The University of Manchester, Brunswick Street, Manchester M13 9PL, UK)

**ICSU Committee on Space Research (COSPAR)**

Representative

H. A. Dabkowska (Brockhouse Institute for Materials Research, McMaster University, 1280 Main Street, Hamilton, Ontario, L8S 4M1, Canada)

**International Standards Organization (ISO)**

Representative

C. P. Brock (Department of Chemistry, University of Kentucky, 505 Rose St, Lexington, KY 40506-0055, USA; ex officio as Chair of the Commission on Crystallographic Nomenclature )

**Appendix D. Adhering Bodies and National Committees for Crystallography****D1. Adhering Bodies**

Adherence to the Union is in one of five Categories I–V, with corresponding voting powers and contributions as set out in Statutes 3.6, 5.5 and 9.4.

Country	Category	Adhering Body	Secretary of National Committee
Albania and Kosovo	I	Polytechnic University of Tirana - PUT	D. Karaj, Faculty of Mathematical Engineering and Physical Engineering - PUT, 'Muhamet Gjollesha', No.6 , Tirana, Albania
Algeria	I	Algerian Association of Crystallography	D. Mezaoui, Laboratoire Sciences des Matériaux, Université des Sciences et de la Technologie Houari Boumedienne, BP 32 El-Alia, 16111 Bab-Ezzouar Alger, Algeria
Argentina	I	Consejo Nacional de Investigaciones Científicas y Técnicas	A. Serquis, Comision Nacional de Energia Atomica, Centro Atómico Bariloche, Departamento Caracterización de Materiales, Av E. Bustillo km 9,500, (R8402AGP) San Carlos de Bariloche, Río Negro, Argentina
Australia	III	Australian Academy of Science	A. Wright, ISC Liaison Officer, Australian Academy of Science, Ian Potter House, Gordon Street, Acton, ACT 2601, Australia
Austria	I	Österreichische Akademie der Wissenschaften	K. Hradil, X-ray Center, Vienna University of Technology, Getreidemarkt 9, 1060 Vienna, Austria
Bangladesh	I	Bangladesh Crystallographic Association	T. Debnath, Department of Chemistry, University of Dhaka, Dhaka-1000, Bangladesh
Belgium	II	The Royal Academies for Science and the Arts of Belgium	L. Van Meervelt, Biomolecular Architecture, Chemistry Department, K. U. Leuven, Celestijnenlaan 200F, B-3001 Leuven (Heverlee), Belgium
Brazil	I	Brazilian Crystallographic Association	N. M. Souza Neto, Brazilian Synchrotron Light Laboratory, Rua Giuseppe Máximo Scolfaro, 10.000, Polo II de Alta Tecnologia de Campinas, Campinas, São Paulo, Brazil
Bulgaria	I	Bulgarian Crystallographic Association	R. Petrova, Institute of Mineralogy and Crystallography, Acad. G. Bonchev str., Block 107, Bulgaria
Cameroon	I	Cameroon Crystallographic Association	J. Ngoune, Department of Chemistry, Faculty of Science, University of Dschang, PO Box 67 Dschang, Cameroon
Canada	III	National Research Council	M. Fodje, Canadian Lightsource, 44 Innovation Boulevard, Saskatoon, SK, S7N 2V3, Canada

Chile	I	Asociacion Chilena de Cristalografia	A. Galdámez, Department of Chemistry, Faculty of Science, University of Chile, Santiago, Chile
China, People's Republic of	IV	Chinese Association for Science and Technology	Xiao-Dong Su, Life Science College, Peking University, Beijing 100871, People's Republic of China
China, Taipei	II	The Academy of Sciences Located in Taipei	S. M. Peng, Department of Chemistry, National Taiwan University, Taipei
Costa Rica	I	Centro Nacional de Alta Tecnologia (CeNAT)	A. M. Araya Sibaja, Chemistry, University of Costa Rica, San Pedro de Montes de Oca, San José, 2060, Costa Rica
Croatia	I	Croatian Crystallographic Association (under the auspices of the Croatian Academy of Science and Arts)	M. Dakovic, Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, HR-10000, Croatia
Czech and Slovak Republics	II	Regional Committee of Czech and Slovak Crystallographers	I. Kuta Smatanova, Institute of Chemistry and Biochemistry, Faculty of Science, University of South Bohemia, Branišovská 1760, České Budějovice, CZ 37005, Czech Republic
Denmark	I	Royal Danish Academy of Sciences and Letters	A. Ø. Madsen, Department of Chemistry, University of Copenhagen, Universitetsparken 5, Copenhagen, DK-2100, Denmark
Egypt, Arab Republic of	I	Academy of Scientific Research and Technology	A. M. M. Moustafa, Physics Division, Solid State Department, National Research Centre, El-Buhous Street, Dokki, Cairo, Egypt
Finland	I	Suomen Tiedeakatemia (Council of Finnish Academies)	M. Blomberg, Department of Physical Sciences, PO Box 64, University of Helsinki, FIN-00014 Helsinki, Finland
France	IV	Académie des Sciences (Institut de France)	M. Giorgi, Université Aix Marseille, Spectropole, Fédération des Sciences Chimiques de Marseille FR1739, Campus St Jérôme, 52 av. Escadrille Normandie Niemen, 13013 Marseille, France
Germany	IV	Deutsche Gesellschaft für Kristallographie (DGK)	U. Kolb, Johannes Gutenberg-Universität Mainz, Institut für Anorganische Chemie und Analytische Chemie, Duisbergweg 10-14, 55128 Mainz, Germany
Greece	I	Hellenic Crystallographic Association	K. Bethanis, Physics Laboratory, Biotechnology Department, Agricultural University of Athens, 75 Iera Odos, Athens 118 55, Greece
Hungary	I	Magyar Tudományos Akadémia	P. Bombicz, Institute of Chemistry, Chemical Research Center, Hungarian Academy of Sciences, H-1525 Budapest, POB 17, Hungary
India	III	Indian National Science Academy	S. P. Mishra, Assistant Executive Director (International), Indian National Science Academy, Bahadur Shah Zafar Marg, New Delhi 110 002, India
Ireland, Republic of	I	Irish Crystallographic Association	S. E. Lawrence, Department of Chemistry, University College, Cork, Ireland
Israel	I	Israel Academy of Sciences and Humanities	M. Harel, Department of Structural Biology, The Weizmann Institute of Science, Rehovot 76100, Israel
Italy	III	Consiglio Nazionale delle Ricerche	M. Saviano, Istituto di Cristallografia del CNR, via Amendola 122/O, 70126 Bari, Italy
Japan	IV	Science Council of Japan	M. Takata, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Japan

Korea, Republic of	I	Korean Crystallographic Association	M. S. Lah, Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST), Ulsan, Republic of Korea
Mexico	I	Consejo Nacional de Ciencia y Tecnología	G. Gonzalez-Reyes Galindo, National Autonomous University of Mexico, UNAM in Mexico City, Mexico
Morocco	I	Moroccan Crystallographic Association	D. Zakaria, Laboratoire de Physico-Chimie des Matériaux, Université Chouaib Doukkali, Faculté des Sciences, BP 20, 2400 El Jadida, Morocco
Netherlands	II	The Dutch Association for Crystallography (NVK)	M. Lutz, Crystal and Structural Chemistry, Utrecht University, Padualaan 8, Utrecht, 3584 CH, The Netherlands
New Zealand	I	The Royal Society of New Zealand	M. Wickens, The Royal Society of New Zealand, P O Box 598, Wellington, New Zealand
Norway	I	Det Norske Videnskaps-Akademi	B. Fjaerstoft, Institute of Pharmacy, University of Oslo, PO Box 1068, Blindern, 0316 Oslo, Norway
Pakistan	I	Pakistan Academy of Sciences/International Center for Chemical and Biological Sciences	M. I. Choudhary, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan
Poland	I	Polska Akademia Nauk	I. Turowska-Tyrk, Faculty of Chemistry, Wroclaw University of Technology, 27 Wybrzeze Wyspianskiego St., 50-370 Wroclaw, Poland
Portugal	I	Sociedade Portuguesa de Fisica	M. T. L. Duarte, Chemical Engineering Department, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal
Regional Committee – AsCA	I	Regional Committee of Crystallographers from Indonesia, Malaysia, Thailand and Vietnam	Duong Ngoc Huyen, Hanoi University of Science and Technology, No. 1 Daicoviet, Hanoi, Vietnam
Russia	V	Russian Academy of Sciences	N. I. Sorokina and O. A. Alekseeva, Shubnikov Institute of Crystallography, Russian Academy of Sciences, Leninsky pr. 59, Moscow 119333, Russia
Serbia	I	Serbian Ministry for Science and Technology	P. Vulic, Faculty of Mining and Geology, University of Belgrade, Serbia
Singapore	I	Singapore National Institute of Chemistry	J. J. Vittal, Department of Chemistry, National University of Singapore, Singapore 117543
Slovenia	I	Slovenian Chemical Society	A. Meden, Faculty of Chemistry and Chemical Technology, University of Ljubljana, PO Box 537, SI-1001 Ljubljana, Slovenia
South Africa	II	National Research Foundation	L. Ngwenya, South African ICSU Secretariat, National Research Foundation, PO Box 2600, Pretoria 0001, South Africa
Spain	III	Subdirección General de Organismos y Programas Internacionales, Ministerio de Ciencia y Tecnología	E. Gutiérrez Puebla, Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, E-28049 Madrid, Spain
Sweden	II	Kungliga Vetenskapsakademien	A. Sjögren, Svenska Kemistsamfundet, Wallingatan 24, 111 23 Stockholm, Sweden
Switzerland	II	Schweizerische Gesellschaft für Kristallographie	M. Wörle, Head Small Molecule Crystallography Center, Laboratorium für Anorganische Chemie, ETH Zürich, HCI H103, Vladimir-Prelog-Weg 1, CH-8093 Zürich, Switzerland

Tunisia	I	Tunisian Association of Crystallography	W. Cheikhrouhou-Koubaa, Centre de Recherche en Numerique de Sfax, Tunisia
Turkey	I	Ulusal Kristallografi Dernegi	L. T. Yildirim, Department of Engineering Physics, Hacettepe University, 06532 Beytepe, Ankara, Turkey
UK	V	The British Crystallographic Association	A. Stanley, Rigaku Corporation, Oxford, UK
Uruguay	I	Academia Nacional de Ciencias del Uruguay	L. Suescun, Facultad de Quimica, Av. Gral. Flores 1224, Casilla 1157, 11800 Montevideo, Uruguay
USA	V	National Academy of Sciences – National Research Council	K. Bennett, KB Science, Charles Street Station, PO Box 140343, Boston, MA 02114, USA
Venezuela	I	Sociedad Venezolana de Cristalografía	J. M. Delgado, Laboratorio de Cristalografía, Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, La Hechicera, Mérida 5101, Venezuela

## D2. National Committees for Crystallography

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Algeria

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Argentina

D. R. Vega (Chair), S. Klinke, D. Lamas, G. Narde, G. Punte, A. Serquis

Australia

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Austria

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**Switzerland**

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**Venezuela**

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