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international union of crystallography

Acta Crystallographica Section A
**Foundations and Advances**

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# Report of the Executive Committee for 2012

## 1. Meetings

The IUCr sponsored the following meetings held during 2012:

Third African School and Workshop on X-rays in Materials: Some Established Techniques and Practical Applications, Dakar, Senegal, 23–28 January.

Powder Diffraction and Rietveld Refinement School, Durham, UK, 25–29 March.

RapiData 2012, Brookhaven, USA, 22–27 April.

From Genes to Atomic Structures: an Introduction to Synchrotron-Based Structural Biology, Trieste, Italy, 23–27 April.

Third International School on Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials (ISC2012), Granada, Spain, 21–25 May.

Present and Future Methods for Biomolecular Crystallography, Erice, Italy, 31 May – 10 June.

2012 Gordon Research Conference 'Crystal Engineering', Waterville Valley Resort, New Hampshire, USA, 10–15 June.

Electron Crystallography School – New Methods and Applications, Stockholm, Sweden, 17–20 June.

Fourth European Conference on Crystal Growth (ECCG4), Glasgow, UK, 17–20 June.

International Summer School on Crystallography for Health and Biosciences, Como, Italy, 19–23 June.

Sagamore XVII – Great Potentials from Advanced Probes, Hokkaido, Japan, 15–20 July.

Annual Meeting of the American Crystallographic Association, Boston, USA, 28 July – 1 August.

27th European Crystallographic Meeting, Bergen, Norway, 6–11 August.

International Workshop on New Developments of Methods and Software for Protein Crystallography, Xi'An, People's Republic of China, 25–27 August.

International Summer School on Crystal Growth and Photovoltaic Materials, Brasov, Romania, 27 August – 1 September.

XXII Conference on Applied Crystallography, Targanice/Andrychow, Poland, 2–6 September.

Aperiodic 2012, Cairns, Australia, 2–7 September.

Indaba 7, Kruger National Park, South Africa, 2–7 September.

Fifth K. H. Kuo Summer School of Electron Microscopy and Crystallography; International Workshop of Cryo Electron Microscopy and Tomography, Anhui, People's Republic of China, 7–12 September.

Applications of Precession Electron Diffraction, Manchester, UK, 14–15 September.

European Charge Density Meeting (ECDM6), Strbske Pleso, Slovakia, 15–20 September.

Advances in Crystallography at High Pressures, Mito, Japan, 23–27 September.

International Symposium on Radiation Physics (ISRP 12), Rio de Janeiro, Brazil, 7–12 October.

Fundamentals of Modern Methods of Biocrystallography – BioCrys 2012, Oeiras, Portugal, 20–27 October.

Computational Discovery for Novel Crystal Structures and Advanced Materials using the USPEX Code, Lausanne, Switzerland, 21–27 October.

4th School of the Argentinian Crystallographic Association, Santa Fe, Argentina, 5–9 November.

Celebration of 100 Years of X-ray Diffraction (Macromolecular Structure of Biological and Non-Biological Materials) Workshop, Red Sea, Egypt, 18–22 November.

XIII Seminario Latinoamericano de Análisis por Técnicas de Rayos-X, Santa Marta, Colombia, 18–23 November.

International School on Fundamental Crystallography 2012 (ISFC2012), Uberlandia, Brazil, 25 November – 2 December.

AsCA '12/CRYSTAL 28, Adelaide, Australia, 2–5 December.

The Executive Committee met in Boston, USA, in July, and in Adelaide, Australia, in December. The Finance Committee met in Leuven, Belgium, in March and October, to prepare its advice and recommendations on finances, establishment and staff matters.

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

editorial policy, pricing policy and subscription rates, consideration of Report of Journals Review Committee, establishment of Journals Management Board, approval of appointments of Editor-in-Chief, Editors and Co-editors, online-only publishing of journals, launch of *IUCrJ*, archival policy, Special Issues, open access, and other matters concerning the IUCr journals;

review of contract with Wiley-Blackwell for IUCr journals;

International Year of Crystallography (IYCr), Report of IYCr Committee;

approval of audited accounts for the previous year;

General Fund estimates and level of unit contribution;

status of membership subscriptions;

investment policy;

funding and uses of Publications and Journals Development Fund and Research and Education Fund;

sponsorship and financial support for meetings, young scientists' support, Visiting Professorship Scheme;

establishment of Inter-Regional Bursary Fund;

Journal Grants Fund;

cooperation with databases, Working Group on Data Deposition;

progress with Volumes A, A1, B, C, D, E, F and G of *International Tables* and development of associated software, consideration of possible new volumes;

*IUCr Newsletter*;

*World Database of Crystallographers*;

Online Dictionary of Crystallography;

promotional activities;

Ewald Prize Selection Committee;

discussion of arrangements for Montreal and Hyderabad Congresses.

Other items dealt with in this way were:

uses of the Crystallographic Information Framework (CIF), work of the Committee for the Maintenance of the CIF Standard (COMCIFS), provision of checking services to other publishers, chemical information, support of mmCIF project and CIF handling software;

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

Crystallography in Africa;

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

review of activities of Regional Associates;

review of reports of IUCr Representatives on other bodies.

Items concerning the Chester office were:

staffing requirements in the IUCr office in Chester, appointment of IYCr Project Manager, appointment of Business Development Manager;

office premises;

risk analysis;

upgrading of office technology, provision of internet services.

The Executive Committee particularly wishes to thank Professor Gernot Kostorz for his work as Editor-in-Chief through a challenging period in journals publication. The Executive Committee welcomes Professor Samar Hasnain as his successor.

## 2. Publications

Volume 68 of *Acta Crystallographica*, Volume 45 of *Journal of Applied Crystallography* (*JAC*) and Volume 19 of *Journal of Synchrotron Radiation* (*JSR*) were published.

## 3. Adhering Bodies

A list of Adhering Bodies of the Union, with names and addresses of the Secretaries of the National Committees for Crystallography, was published as Appendix D to the Report of the Twenty-Second General Assembly and International Congress of Crystallography [*Acta Cryst.* (2012), A**68**, 607–664].

## 4. Work of the Commissions

### 4.1. Commission on Journals

#### 4.1.1. Overview

| | 2008 | 2009 | 2010 | 2011 | 2012 |
|---|---|---|---|---|---|
| No. of submissions | 5765 | 7129 | 7033 | 7302 | 6628 |
| without *Acta E* | 1919 | 2016 | 1905 | 1831 | 2023 |
| Rejection rate (%) | 24 | 22 | 22 | 22 | 21 |
| No. of published papers | 4795 | 5440 | 5431 | 5650 | 5330 |
| without *Acta E* | 1239 | 1274 | 1318 | 1206 | 1283 |
| No. of open-access papers | 3647 | 4245 | 4232 | 4571 | 4125 |
| without *Acta E* | 89 | 79 | 119 | 127 | 78 |
| No. of pages | 11295 | 12812 | 13156 | 12667 | 13307 |
| without *Acta E* | 7034 | 7704 | 7961 | 7144 | 8136 |
| No. of printed pages | 5847 | 6385 | 6277 | 5470 | 6560 |
| No. of online-only pages | 5448 | 6427 | 6879 | 7197 | 6747 |
| without *Acta E* | 1187 | 1319 | 1684 | 1674 | 1576 |

Towards the end of 2012, the IUCr initiated a major project to extend and expand the scope of its journals to meet the needs and serve the interests of researchers in the crystallographic and wider scientific communities who utilize structural information for addressing their scientific questions. The aim is to make the journals the natural home for many of the high-quality scientific publications that are currently published in journals such as *Nature Structure and Molecular Biology*, *Structure*, *Proceedings of the National Academy of Sciences*, *Journal of the American Chemical Society*, *Angewandte Chemie*, *Chemical Communications etc.*, where structural data underpin these publications. The overall development plan was considered by the IUCr Executive Committee in December 2012. A Journals Management Board was also formed to provide support for implementation of the plan and streamline the management of the journals. A policy of closer interaction with IUCr's Commissions was introduced.

The total number of articles published in IUCr Journals in 2012 was slightly lower than in recent years at 5330. This is primarily due to a decrease in articles published in Section E (397 less than in 2011) following its delisting by the Science Citation Index. The delisting will suppress the impact factors of all journals in the crystallography category of the Science Citation Index, but will have a particularly strong effect on IUCr Journals. A detailed plan is being formulated for Section E to regain coverage by the Science Citation Index in the next few years.

Two IUCr journals were included in the top three ranked crystallography journals, with Section D having an impact factor of 12.6 and *JAC* an impact factor of 5.2. Sections B and C, and *JAC* had cited half-lives of >10 years. *JSR* was ranked sixth in the Instruments and Instrumentation category. A total of 3.2 million downloads of journal articles were made from **Crystallography Journals Online** in 2012. The highest number of downloads (1.5 million) was for Section E.

Very few open-access papers are published in Sections A, B and C, suggesting that a concerted effort to boost open-access publication could pay dividends. For our other journals, the proportion of open-access papers published in recent years has generally been in the 10–20% range, with the highest proportions being in Section D and *JSR*.

A number of Special Issues were produced in 2012. A Special Issue to mark the Laue Centennial was published in Section A. Section C published a virtual Special Issue on Absolute Structure. Proceedings of the CCP4 Study Weekend: Model Building, Refinement and Validation were published in Section D. Papers presented at the International Workshop on Improving Data Quality and Quantity for XAFS Experiments (Q2XAFS2011) were published in *JSR*.

At the end of the year, more than 160 Section Editors and Co-editors worked on IUCr journals. The work of all these dedicated colleagues is highly appreciated. The year marked the retirements of a number of Editors and Co-editors as well as the appointment of a number of Editors and Co-editors reflecting the broadening scope of our journals and emphasizing the 'science-face' of crystallographic research. One hundred years of crystallographic success have made structural data an essential part of all modern science ranging from chemistry to materials science to biological science (and also to medicine through the design of new structure-based drugs). X-ray sources have continued to advance from the humble beginnings of the sealed tubes used by Laue and the Braggs. With the emergence of very powerful and tunable X-ray lasers, structural science and methods are beginning to access non-crystalline systems while beginning to probe their dynamics too. We certainly have some exciting decades ahead in which all of the IUCr journals will continue to play an increasingly important role.

We pay our tribute to Steve Wilkins who passed away suddenly. His legacy as a scientist and one of our committed Co-editors will remain with us in the form of the Bragg Centennial issue of Section A, which is to appear in January 2013.

**S.S. Hasnain**, Editor-in-Chief and Chair

#### 4.1.2. *Acta Crystallographica* Section A

*Acta Crystallographica* Section A *Foundations of Crystallography*, is in general healthy. The number of submissions to the journal is at a

| | 2008 | 2009 | 2010 | 2011 | 2012 |
|---|---|---|---|---|---|
| No. of submissions | 96 | 116 | 100 | 134 | 143 |
| Rejection rate (%) | 33 | 39 | 40 | 40 | 33 |
| No. of published papers | 81 | 56 | 81 | 68 | 83 |
| research papers | 42 | 41 | 66 | 56 | 64 |
| short communications | 6 | 5 | 3 | 5 | 5 |
| lead articles | 0 | 1 | 1 | 0 | 0 |
| feature articles | 24 | 1 | 1 | 0 | 1 |
| editorial | 0 | 0 | 3 | 0 | 0 |
| abstracts | 2059 | 735 | 734 | 2087 | 527 |
| other | 9 | 8 | 7 | 7 | 13 |
| No. of open-access papers | 0 | 0 | 2 | 6 | 3 |
| No. of pages | 702 | 548 | 724 | 565 | 787 |
| Average length (pages) | 10 | 10.3 | 9.8 | 9 | 10.2 |
| Average publication time (months) | 5.3 | 5.0 | 5.7 | 4.7 | 5.1 |
| Impact factor | 2.05 | 49.93 | 54.33 | 2.07 | |
| 5 year impact factor | 2.1 | 30.64 | 24.72 | 30.65 | |
| Cited half life (years) | >10.0 | >10.0 | 6.2 | 3.9 | |

five-year high, along with the number of pages published. The average combined time for review and publication remains steady at around five months. The impact factor dropped in 2012 to 2.07 after two years of exceptionally high values, reflecting the high number of citations of the article on *SHELX* by George Sheldrick, which was published in 2008.

The year started with the first of two Special Issues commemorating 100 years of X-ray diffraction. The January 2012 issue featured four articles and an editorial celebrating the Laue centennial. These articles were simultaneously published in *Zeitschrift für Kristallographie*, with Walter Steurer and Wolfgang Schmahl acting as joint Editors. Towards the end of 2012, the second Special Issue, a collection of articles contributed by speakers at the Bragg Centennial Symposium in Adelaide on 6 December, were published online to coincide with the symposium, and then in print as the first issue of 2013. Steve Wilkins acted as Guest Editor for these articles. Both Special Issues have been very well received.

The November issue included a Feature Article entitled Fifty Years of Aperiodic Crystals, by Ted Janssen.

Walter Steurer stepped down as Editor after the publication of the last issue of the year. He is succeeded in the role by Simon Billinge and John Miao.

Plans for the journal moving forward include expanding its scope to include high-quality, high-impact work in which crystallography and related non-crystalline diffraction-based methods have had a significant role. The subtitle for the journal will be changed to *Foundations and Advances* to reflect this new scope, and a rapid-publication section will be introduced for the highest-quality articles, which will be publicized *via* press releases and well written commentaries to bring them to the attention of a broad audience.

Walter Steurer and the Co-editors for *Acta A* are thanked for all their work in maintaining the high standards that are expected of the journal. Finally, the sad loss of Steve Wilkins early in 2013, only a few weeks after he completed work on the Bragg Special Issue, is noted.

**S. Billinge** and **J. Miao**, Editors of Section A

#### 4.1.3. *Acta Crystallographica* Section B

The February 2013 issue of the journal will be published with its new subtitle *Structural Science, Crystal Engineering and Materials*, indicative of the additional areas from which we are now aiming to attract submissions.

The number of papers published in Section B (79) over the past 12 months has risen somewhat compared with the previous year (57), reversing the monotonic decay seen previously, although this is due to a lower rejection rate (34% *versus* 40%) for a slightly smaller number of submissions (112 *versus* 121). The total number of pages published for 2012 was 685, markedly up from the 2011 total of 581, but the latter was the lowest number since 1985. The average length of an article (9.6 pages) has decreased from the peak of 10.7 pages in 2011, but this is still longer than the average of 8.9 pages in 2007. The impact factor increased to 2.3 having remained around 1.8 for 2009 and 2010.

| | 2008 | 2009 | 2010 | 2011 | 2012 |
|---|---|---|---|---|---|
| No. of submissions | 134 | 138 | 96 | 121 | 112 |
| Rejection rate (%) | 35 | 34 | 40 | 40 | 34 |
| No. of published papers | 91 | 90 | 73 | 57 | 79 |
| research papers | 81 | 76 | 71 | 52 | 67 |
| short communications | 5 | 4 | 0 | 1 | 4 |
| feature articles | 0 | 3 | 1 | 1 | 1 |
| other | 5 | 7 | 1 | 3 | 7 |
| No. of open-access papers | 1 | 2 | 3 | 5 | 0 |
| No. of pages | 791 | 790 | 706 | 581 | 685 |
| Average length (pages) | 9.3 | 9.6 | 9.8 | 10.7 | 9.6 |
| Average publication time (months) | 5.0 | 4.9 | 5.2 | 4.6 | 4.7 |
| Impact factor | 2.34 | 1.80 | 1.83 | 2.29 | |
| 5 year impact factor | 2.33 | 2.03 | 2.03 | 2.00 | |
| Cited half life (years) | >10.0 | >10.0 | >10.0 | >10.0 | |

Following on from the meetings of the Commission on Journals in Madrid in 2011, under the Editorship of Sander van Smaalen the journal has just begun to publish the first of a series of Feature Articles and Lead Articles on topics of high current interest. The status of Lead/Feature Articles and planned Special Issues is given below.

Lead/Feature Articles

| Title | Author | Date |
|---|---|---|
| The charge-flipping algorithm in crystallography | L. Palatinus | February 2013 |
| The generalized invariom database | B. Dittrich | April 2013 |
| Crystal structure prediction | S. L. Price | August 2013 |
| MOFs at high pressure | S. Moggach | Invited |

Special Issues

| Title | Guest Editor(s) | Date |
|---|---|---|
| Crystal engineering | A. Bond | August 2013 |
| Non-ambient crystallography | A. Katrusiak and D. Billing | December 2013 |
| Crystal structure prediction | G. M. Day and C. H. Görbitz | 2014 |

I am enthusiastic about the potential for Special Issues to attract new authors and readers, although they need to be planned and organized carefully to avoid longer publication times for the standard papers that we hope to attract.

On a very positive note the Director of the Cambridge Crystallographic Data Centre, Dr Colin Groom, has confirmed that they plan to submit both a 'must-cite' CSD paper and a series of follow-on ones to IUCr journals, starting in 2014.

I am happy to welcome Andrew Bond, University of Southern Denmark, to the *Acta B* Editorial Board. I would also like to thank retiring members Sander van Smaalen, former Section Editor, and J. Manuel Perez-Mato for all their past contributions to the journal.

I welcome the recent appointment of a second Section Editor, Marc de Boissieu, and look forward to shaping a brighter future for the journal building on its reputation and strength. Future appointments of Co-editors will emphasize our commitment to publishing high-quality results from the research areas they represent.

There are close and ongoing discussions with Tony Linden as Editor of Section C, in order to ensure that the development of the two journals proceeds efficiently, with maximum collaboration and management of possible overlaps.

**A. J. Blake**, Editor of Section B

#### 4.1.4. *Acta Crystallographica* Section C

| | 2008 | 2009 | 2010 | 2011 | 2012 |
|---|---|---|---|---|---|
| No. of submissions | 751 | 687 | 592 | 479 | 504 |
| Rejection rate (%) | 60 | 52 | 53 | 50 | 49 |
| No. of published papers | 332 | 331 | 284 | 239 | 232 |
| research papers | 328 | 328 | 280 | 234 | 229 |
| editorial | 1 | 1 | 0 | 2 | 2 |
| other | 3 | 2 | 4 | 3 | 1 |
| No. of open-access papers | 2 | 1 | 1 | 0 | 0 |
| No. of pages | 1197 | 1258 | 1134 | 993 | 984 |
| Average length (pages) | 3.6 | 3.8 | 4.0 | 4.2 | 4.2 |
| Average publication time (months) | 1.8 | 1.9 | 1.9 | 2.0 | 2.0 |
| Impact factor | 0.56 | 0.78 | 0.75 | 0.52 | |
| 5 year impact factor | 0.57 | 0.7 | 0.63 | 0.44 | |
| Cited half life (years) | >10.0 | >10.0 | >10.0 | >10.0 | |

2012 was a modest year for *Acta Crystallographica* Section C. Of concern was the low number of papers submitted during the early part of the year, although things picked up slightly towards the end of the year. At one point we were close to the minimum printable size for an issue. Although the total number of submissions for 2012 ended slightly above that for 2011, the total number of published papers decreased slightly. The impact factor for 2011 also dropped to 0.52, whereas it had been hovering near 0.75 in the preceding two years. Clearly, the downward trend for Section C cannot continue and the matter was the subject of discussions during the review of the IUCr journals and at a meeting in Chester in July 2012. A special report on the situation with Section C, along with some proposals for improving the journal, were submitted to the IUCr Executive Committee in April 2012. This document formed the basis for discussions in late 2012 and in January 2013 on future directions for the journal.

In late 2012, the chairs of the IUCr Commissions that are relevant to the activities of Section C were contacted to seek their thoughts on how Section C might better serve their communities and how we might encourage more authors to submit papers to the journal. The feedback was very useful, as were comments and suggestions solicited from the Section C editorial and co-editorial team. Consequently we plan to implement a significant broadening of the scope of Section C during 2013. There will be a sea change to the style and scope of Section C papers with a view to making the journal attractive to the broader scientific community, significantly increasing its size and more than doubling its impact factor within the next 2–3 years. The title of the journal will be changed to *Acta Crystallographica* Section C *Structural Chemistry*. Initial activities will include the publication of five Special Issues during late 2013/early 2014, a first for Section C. This initiative is already underway. The Notes for Authors for 2013 will be simplified to make them more author-friendly and the journal will accept submission of the text sections of a paper as a Word document, thereby overcoming a point of resistance by some authors to submitting papers entirely in CIF format.

The average publication time for Section C papers has been rising slowly, which is undesirable for a journal that promotes itself as a rapid publication journal. In some cases we have been significantly slower than some of our main competitors. This is mainly due to bottlenecks in the review process resulting from the difficulties some Co-editors have in finding a reviewer who actually responds to a request. It is planned to establish a review board during 2013, along the lines of the review board set up previously for Section F, which will hopefully alleviate some of these difficulties.

The virtual issue dedicated to the subject of absolute structure was released in December 2012 and includes papers relating to this topic published in Section C between January 2011 and November 2012. The issue is available at http://journals.iucr.org/special_issues/2012/absolutestructure/ and received favourable comment. The next virtual issue is planned for December 2013 and will be on the topic of metal organic frameworks. Another virtual issue mentioned in my last report as being organized on the topic of unexpected structures has been abandoned as the Guest Editor, despite his own enthusiasm, did not find much interest from prospective authors.

One Co-editor retired during the year: John Gallagher. I am very grateful for his support and enthusiasm for the journal. John remains active as a Section E Co-editor. I also warmly thank all current Section C Co-editors, the Chester Editorial Office staff and the Editor-in-Chief for their continued support and dedication, especially at this time of change.

**A. Linden**, Editor of Section C

#### 4.1.5. *Acta Crystallographica* Section D

| | 2008 | 2009 | 2010 | 2011 | 2012 |
|---|---|---|---|---|---|
| No. of submissions | 191 | 205 | 201 | 239 | 340 |
| Rejection rate (%) | 19 | 19 | 22 | 26 | 29 |
| No. of published papers | 152 | 160 | 167 | 131 | 193 |
| research papers | 135 | 136 | 148 | 119 | 173 |
| short communications | 13 | 16 | 11 | 5 | 8 |
| feature articles | 0 | 0 | 0 | 0 | 0 |
| editorial | 1 | 1 | 4 | 0 | 2 |
| other | 3 | 7 | 4 | 7 | 10 |
| No. of open-access papers | 33 | 43 | 37 | 27 | 39 |
| No. of pages | 1294 | 1349 | 1354 | 1077 | 1700 |
| Average length (pages) | 9.1 | 9.1 | 8.7 | 8.8 | 9.4 |
| Average publication time (months) | 4.4 | 4.5 | 5.1 | 4.0 | 5.1 |
| Impact factor | 2.94 | 2.26 | 6.33 | 12.62 | |
| 5 year impact factor | 1.83 | 2.01 | 4.10 | 7.04 | |
| Cited half life (years) | 9.7 | 9.4 | 9.0 | 6.9 | |

*Acta Crystallographica* Section D is currently in very good shape. The impact factor rose to 12.6 this year, and has clearly played a part in attracting many more submissions to the journal. Submissions increased by nearly 40%, to 340, and the number of papers published rose by a similar amount, to 239. Given the volatility of impact factors and the influence a few very highly cited papers can have on them, we do not expect this figure to be sustained. Nevertheless, it has raised the profile of the journal, and by attracting many more excellent structural papers has increased its core strength.

Papers on crystallographic methods remain central to the journal and are responsible for a large proportion of its citations. The annual CCP4 Special Issue, for which Roberto Steiner, Bernhard Rupp and Charles Ballard were Guest Editors, focused in 2012 on Model Building, Refinement and Validation. These are all topics of very high interest in the wider structural biology community. Paradoxically, an article published in *Science* during 2012 on the use of weak data in refinement has further heightened interest in crystallographic methods; while we might have wished it had appeared in *Acta D*, it is likely to be positive for our journal because of the light it shone on fundamental issues of crystallography.

It is our clear impression that the structural papers published in 2012 have been of distinctly higher quality than in previous years. Both Co-editors and authors have taken on board the requirement for significant biological or chemical impact as a key requirement for publication. Application of this criterion has led to an increased rejection rate (29%) but will help to ensure a continuing high profile for the journal. The procedures and criteria for transfers between *Acta D* and *Acta F* are by now well understood and are working well.

A related issue for the journal, currently under active discussion, is the extent to which it should broaden its focus. Several IUCr Commissions have been approached as part of an in-depth consul-

tation. Structural papers increasingly combine crystallography with biochemical and biophysical analyses, and a recent article in the journal on publication standards for biological SAXS data has attracted great interest. It may be desirable to widen the range of expertise covered by our Co-editors to deal with a broadened scope for the journal.

At present two countries, the USA and the UK, account for almost 40% of submissions. Both countries are well represented among our Co-editors (5 and 4, respectively). Submissions from Asia are increasing, however, notably from the People's Republic of China, India and Korea, and further Co-editor appointments from these countries are desirable for the future. We are extremely grateful to all current Section D Co-editors, most of whom have had to carry a higher load in 2012, and to Louise Jones and the Chester Editorial Office staff for their dedicated support and continuing concern for the quality of the journal.

**E. N. Baker** and **Z. Dauter**, Editors of Section D

**4.1.6. *Acta Crystallographica* Section E**

| | 2008 | 2009 | 2010 | 2011 | 2012 |
|---|---|---|---|---|---|
| No. of submissions | 3846 | 5113 | 5128 | 5471 | 4605 |
| Rejection rate (%) | 16 | 18 | 18 | 19 | 17 |
| No. of published papers | 3556 | 4166 | 4113 | 4444 | 4047 |
| research papers | 3533 | 4151 | 4091 | 4434 | 4039 |
| editorial | 1 | 1 | 1 | 0 | 0 |
| other | 22 | 14 | 21 | 10 | 8 |
| No. of open-access papers | 3558 | 4166 | 4113 | 4444 | 4047 |
| No. of pages | 4261 | 5108 | 5195 | 5523 | 5171 |
| Average length (pages) | 1.2 | 1.2 | 1.3 | 1.2 | 1.3 |
| Average publication time (months) | 0.8 | 0.7 | 0.7 | 0.7 | 0.7 |
| Impact factor | 0.37 | 0.41 | 0.41 | 0.35 | |
| 5 year impact factor | 0.37 | 0.38 | 0.34 | 0.28 | |
| Cited half life (years) | 2.4 | 2.7 | 3.1 | 3.3 | |

2012 was a relatively good year for *Acta Crystallographica* Section E, despite the fall in submissions following our deselection from the Web of Science. The main reason for the removal was a high self-citation rate.

Papers have been submitted from 81 countries; the six top contributors are People's Republic of China (31.6%), India (10.7%), Malaysia (7.3%), South Africa (4.2%), the USA (4.1%) and Germany (4.1%). However, submissions from People's Republic of China are down by *ca* 7% and those for Malaysia by *ca* 2%, whereas the submissions from India and Germany have risen by *ca* 1%. Contributions from other countries are relatively stable.

There were a total of 4605 articles submitted, compared to 5471 in 2011, and 5171 pages published. The proportion of organic (71%) papers increased, while the proportion of metal-organic papers (27%) decreased and the proportion of inorganic papers remained the same (2%).

Publication times remained low with an average submission-to-publication time of 0.7 months.

At the summer 2012 meeting of the Section Editors various propositions were put forward to counter the effects of the deselection from the Web of Science. These discussions are ongoing.

Developments continue to be made to the submission system and to the online content. There is an improved 3D page, which now shows a chemical view of structures and improved ellipsoid representations. The proofs sent to the authors now include the Supplementary Material as well as the short-format paper.

This year has been free of fraudulent structure submissions and we continue to maintain a vigilant watch for potentially fraudulent structures. The validation procedures continue to be improved and reduced-cell checking combined with checks for similar structure factors are a routine part of the review process.

A number of Co-editors retired during the year, and it is our pleasure to record here our sincere appreciation of their sustained outstanding efforts and their support of the journal. The retirees are: David Watson, Catharine Esterhuysen and Andreas Fischer.

Four new Co-editors were appointed during the year and we are pleased to welcome aboard Petra Bombicz, Ann Chippindale, Viktor Khrustalev and Tim Prior.

We are extremely grateful to all current Section E Co-editors and the Chester Editorial Office staff for their dedicated support and contributions to the ongoing daily operations of the journal.

**W. T. A. Harrison**, **H. Stoeckli-Evans**, **E. R. T. Tiekink** and **M. Weil**, Editors of Section E

**4.1.7. *Acta Crystallographica* Section F**

| | 2008 | 2009 | 2010 | 2011 | 2012 |
|---|---|---|---|---|---|
| No. of submissions | 349 | 422 | 421 | 401 | 375 |
| Rejection rate (%) | 10 | 9 | 9 | 8 | 9 |
| No. of published papers | 302 | 333 | 377 | 385 | 362 |
| research papers | 293 | 328 | 362 | 365 | 351 |
| editorial | 5 | 2 | 4 | 3 | 3 |
| other | 4 | 3 | 11 | 17 | 8 |
| No. of open-access papers | 8 | 11 | 41 | 41 | 15 |
| No. of pages | 1187 | 1319 | 1684 | 1674 | 1576 |
| Average length (pages) | 4.0 | 4.0 | 4.5 | 4.4 | 4.4 |
| Average publication time (months) | 2.6 | 2.8 | 3.6 | 3.9 | 3.2 |
| Impact factor | 0.61 | 0.55 | 0.56 | 0.51 | |
| 5 year impact factor | – | – | 0.48 | 0.46 | |
| Cited half life (years) | 2.3 | 2.7 | 2.7 | 3.2 | |

In 2012, its eighth year of publication, Section F has seen a small (about 5%) reduction in the number of papers published compared with the previous year. Nonetheless, with 351 original science articles in 1576 pages, it remains an important journal for the macromolecular crystallography (MX) community.

In both 2010 and 2011, *Acta F* published 99 structure and laboratory communications; totals that reflect an approximate doubling over previous years, and that represent 27 and 26% of the papers published, respectively. In both of those years, an entire issue was devoted to the product of a single structural genomics (SG) group. As an example, the September 2011 issue was entirely the output of the Seattle Structural Genomics Center for Infectious Disease (SSGCID). With one overview article, eight laboratory communications and 21 structure communications, the SSGCID Special Issue was thus the single most important contributor to the high percentage of structure and laboratory communications. In 2012, no such Special Issue was assembled, but *Acta F* nevertheless published 88 structure and laboratory communications, which amounts to 25% of all papers published in that year. This shows that the increase first caused by the SG Special Issues could be maintained and that *Acta F* has moved into a position where it is attracting more structure and laboratory communications. We do hope that this trend will continue in the coming years.

A very positive development is that we managed to reverse the drift upwards of the average time from the submission of a paper to its publication. After a maximum of 3.9 months in 2011, the average publication time was down to 3.2 months. It was still higher than 2008 and 2009 but lower than in the two previous years. We should not forget that rapid publication has been the mandate of our journal since its inception. This reversal is therefore a significant move in the

right direction. We need to continue our efforts to investigate the factors lengthening publication time in order to develop measures to bring publication times down further.

An important development in this respect is the new version of the publication tool *publBio*. It is now possible to produce crystallization and structural communications that meet all the journal's formatting and data requirements using this tool with or without an existing PDB entry. This should facilitate the writing and submission of such manuscripts, and should also make refereeing and editing of such papers much easier. After the positive feedback from participants at IUCr luncheons at the DGK 2012 conference in Munich, Germany, and the ACA 2012 meeting in Boston, USA, we are currently considering when to make the use of *publBio* mandatory for crystallization communications.

2012 also featured another first: the publication of an article that identified a previously published structure as likely to be based on fabricated data. This article has proved to be another shock to the crystallographic community worldwide as evidenced by its high number of downloads (more than 4000). While it is unlikely that a policy of critiquing the publications of potential authors is a winning strategy for our journal in the long term, ignoring or masking serious errors is most definitely harmful to the field as a whole and our authors clearly recognize this. We will therefore, while exercising the greatest caution, continue to publish such articles in the future and have two such publications already in the pipeline for 2013.

Despite the fact that we publish a steady 25% of structure and laboratory communications, our impact factor for 2012 remains stalled at about 0.5. The reason for this is not clear and we will continue to search for causes. We still strive to reach an impact factor of one within the next three years.

**H. M. Einspahr** and **M. Weiss**, Editors of Section F

#### 4.1.8. *Journal of Applied Crystallography*

| | 2008 | 2009 | 2010 | 2011 | 2012 |
|---|---|---|---|---|---|
| No. of submissions | 258 | 282 | 309 | 266 | 321 |
| Rejection rate (%) | 39 | 34 | 32 | 34 | 30 |
| No. of published papers | 161 | 172 | 222 | 180 | 180 |
| research papers | 117 | 126 | 165 | 131 | 127 |
| short communications | 9 | 9 | 11 | 8 | 6 |
| lead articles | 1 | 0 | 0 | 0 | 0 |
| editorial | 0 | 0 | 2 | 0 | 0 |
| other | 34 | 37 | 44 | 41 | 47 |
| No. of open-access papers | 10 | 11 | 10 | 6 | 6 |
| No. of pages | 1197 | 1212 | 1543 | 1306 | 1338 |
| Average length (pages) | 8.5 | 7.9 | 8.0 | 8.1 | 8.4 |
| Average publication time (months) | 5.8 | 5.4 | 5.7 | 5.1 | 5.4 |
| Impact factor | 3.21 | 3..02 | 3.79 | 5.15 | |
| 5 year impact factor | 4.87 | 3.82 | 4.19 | 5.66 | |
| Cited half life (years) | >10.0 | >10.0 | >10.0 | >10.0 | |

The journal has had a successful year, with an increase in the number of submissions and pages published. The impact factor has increased to 5.15.

*JAC* continues to publish high-quality articles covering an exceptionally broad range of fields. It is perceived that the main challenges for the future are to ensure that we maintain both the scope and the quality of the journal's scientific content. To this end we aim to appoint several new Co-editors in the coming year, in order to replace retiring Co-editors and to fill gaps in expertise, both in areas that currently feature well in the journal and in emerging areas.

Work began in 2012 on the journal's first virtual Special Issue. This issue on X-ray diffraction microscopy, which was finalized in March 2013, collects together a series of specially commissioned articles originally published in the journal between August 2012 and April 2013 and highlights new methods and instrumentation. Two further Special Issues, focusing on highlights of the 11th Biennial Conference on High Resolution X-ray Diffraction and Imaging (XTOP2012) and the International Small-Angle Scattering Conference (SAS2012), are currently in production.

The number of authors choosing to make their articles open access remains low. The Editorial Office is therefore considering ways in which the benefits of open access can be more actively promoted to both authors and funding agencies in order to reverse this trend.

**A. Kaysser-Pyzalla**, Editor of *JAC*

#### 4.1.9. *Journal of Synchrotron Radiation*

| | 2008 | 2009 | 2010 | 2011 | 2012 |
|---|---|---|---|---|---|
| No. of submissions | 140 | 166 | 186 | 191 | 228 |
| Rejection rate (%) | 31 | 21 | 27 | 28 | 22 |
| No. of published papers | 120 | 132 | 114 | 146 | 154 |
| research papers | 73 | 109 | 96 | 123 | 124 |
| short communications | 37 | 8 | 5 | 8 | 6 |
| feature articles | 0 | 0 | 2 | 0 | 0 |
| editorial | 0 | 0 | 0 | 2 | 1 |
| other | 10 | 15 | 11 | 13 | 23 |
| No. of open-access papers | 35 | 11 | 25 | 42 | 15 |
| No. of pages | 666 | 883 | 816 | 948 | 1066 |
| Average length (pages) | 5.8 | 7.5 | 7.7 | 7.0 | 7.3 |
| Average publication time (months) | 6.4 | 5.3 | 5.2 | 5.4 | 4.9 |
| Impact factor | 2.33 | 1.99 | 2.34 | 2.73 | |
| 5 year impact factor | 2.63 | 2.83 | 3.11 | 2.57 | |
| Cited half life (years) | 6.2 | 6.1 | 6.4 | 6.6 | |

2012 was a good year for the *JSR*, with a modest increase in the impact factor to 2.73 and a record number of submissions and accepted papers. Among other important events, the journal added two Main Editors: J. Friso van der Veen, Head of Research, Department of Synchrotron Radiation and Nanotechnology, Paul Scherrer Institut, and Professor of Experimental Physics, ETH-Zürich, Switzerland; and Ilme Schlichting, Director, Department of Molecular Mechanisms, Max Planck Institute, Heidelberg, Germany. Both are well known scientists with impressive credentials. Ilme Schlichting adds expertise and name recognition in free-electron laser-based research and strengthens the efforts of *JSR* to attract free-electron laser-based submissions. To further encourage papers from newly commissioned or soon-to-be commissioned free-electron laser facilities, Ilme Schlichting is organizing a Special Issue on free-electron lasers and the message 'including free-electron lasers' now appears on the front cover of *JSR*. Friso van der Veen is also considering a Special Issue on ultimate synchrotron sources. Samar Hasnain has relinquished his role as the current-events editor owing to his new duties as Editor-in-Chief of IUCr journals and currently Gene Ice is serving as the current-events editor.

The journal actively recruited beamline papers so that the broad user community has access to peer-reviewed documentation of the instrumentation deployed for their science.

**G. Ice**, **I. Schlichting** and **J. F. van der Veen**, Editors of *JSR*

### 4.2. Commission on *International Tables*

*International Tables for Crystallography* is currently composed of eight volumes (A–G and A1) plus the Brief Teaching Edition of

Volume A. A new edition of Volume F (*Crystallography of Biological Macromolecules*) was published in January 2012. New editions of Volumes A and D are nearing completion. Creation of a ninth volume (Volume H, *Powder Diffraction*) is proceeding well. Coordinated revisions of Volumes B and C are being planned (see below), and a revision of Volume G is being considered.

New volumes covering XAFS/XRF and magnetic structures are being discussed; it is expected that Editors for the two volumes will be appointed during 2013. A related development is the 2013 publication of the pdf format e-book *Magnetic Group Tables: 1-, 2- and 3-Dimensional Magnetic Subperiodic Groups and Magnetic Space Groups* by D. B. Litvin, which is now available to download from the IUCr web site at http://www.iucr.org/publ/978-0-9553602-2-0. This e-book, in which more than 12K page images are compressed into *ca* 100 MB of file space, was approved by the Commission on Magnetic Structures.

Sales of the print editions are showing some decline, but sales of access to the online volumes remain strong. This development was expected. Expanded content available in the online version only was already a feature in Volume A, and was already being planned for Volumes C and H.

Reports for the individual volumes follow.

**4.2.1. Volume A (*Space-Group Symmetry*; Editor M. Aroyo) (including the Brief Teaching Edition and the Symmetry Database server)**. Although work on the preparation of the 6th edition continued through 2012, there has been some delay relative to previous publication plans. Currently, most of the table and text material for the three parts of the new Volume A are at an advanced stage of preparation. Publication is expected in 2014.

Part 1 (Introduction to Space-Group Symmetry). Preliminary versions of most of the chapters are available. Some of the texts have already been peer-reviewed while others need further improvement before sending them to referees. The typesetting process is estimated to start during the second half of 2013.

Part 2 (Tables of Plane and Space Groups). The newly designed tables are ready with the exception of those for the cubic groups. For these groups novel general-position diagrams in orthogonal and slightly tilted projections are being generated. The guides to the use of the tables are at a rather advanced stage and the typesetting of the material of Part 2 could start during the second half of 2013.

Part 3 (Advanced Topics in Space-Group Theory). The material for all six chapters has been successfully peer-reviewed and practically all the texts (with the exception of the new sections of the point-group chapter) are ready for typesetting.

*Symmetry Database server of the online edition of International Tables*. The work on the enhancement of the Symmetry Database of the Online Edition of *International Tables for Crystallography* continued through 2012 within the framework of a new project between the IUCr and the software company eFaber (Bilbao) under the supervision of M. I. Aroyo. The main activities have been focused on the development of databases and computer tools for the analysis of symmetry relations between space groups including group–subgroup relations of any index. The programs for the calculation of chains of maximal subgroups for any group–subgroup pair of space groups are being tested. A preliminary version of a set of new graphic tools for interactive visualization of group–subgroup relations has been developed.

*Brief Teaching Edition*. The first part of the *Brief Teaching Edition* will be an adapted version of the Introductory part of the 6th Edition of Volume A, and will present a practical guide to the use of the crystallographic symmetry data. Owing to the delay of the preparation of the material of Part 1 of Volume A, the initial versions of the texts for the Introductory part of the *Brief Teaching Edition* are expected for the second half of 2013. The material for Part 2 (selection of space-group tables and the corresponding guides) is expected to be ready for the second half of 2013.

**4.2.2. Volume A1 (*Symmetry Relations Between Space Groups*; Editor U. Müller)**. The second edition of Volume A1 was published in 2010. It has not been changed since. It consists of three parts.

Part 1 deals with group-theoretical aspects of space groups, group–subgroup relations and the underlying mathematical background. There is a chapter giving instructions on how to relate crystal structures by group–subgroup relations and how to construct trees of group–subgroup relations for crystal structures that can be derived from a high-symmetrical structure type (aristotype). A chapter deals with the publicly accessible Bilbao Crystallographic Server with descriptions of those databases and computer programs that are related to the subjects of this volume.

Part 2 contains the complete listings of the maximal subgroups for each plane group and space group, including their general positions or their generators, their conjugacy relations and the transformations to the conventional settings. In addition, the minimal supergroups are listed.

Part 3 lists the relations between the Wyckoff positions for every maximal subgroup of every space group including the cell transformations and coordinate transformations.

In both Parts 2 and 3, the infinitely many maximal isomorphic subgroups are included in a parametrized form.

**4.2.3. Volume B (*Reciprocal Space*; Editor G. Chapuis) and Volume C (*Mathematical, Physical and Chemical Tables*; Editor T. R. Welberry)**. The Editors of Volumes B and C met for discussions in September 2012 during the Aperiodic 2012 meeting in Cairns, Australia.

The contents of the current volumes were reviewed with the aim of identifying whether:

(i) there were any parts of the current volumes that were now redundant;

(ii) current material was generally up to date and only required light revision;

(iii) current material was substantially lacking in latest developments and required substantial revision;

(iv) there were serious omissions of new developments in crystallography for which new articles should be sought;

(v) the distribution of material between the two volumes was appropriate.

It was also decided to seek expert opinion, for areas outside the range of expertise of the volume Editors, on whether the current content was appropriate and up to date.

*Some particular issues.* It has been suggested that for Volume C, the subtitle *Mathematical, Physical and Chemical Tables* is no longer justified. Currently, Volume C contains a hotch potch (*i.e.* a variety of miscellaneous things) with no clearly defined focus. Since Volume B focuses on 'reciprocal space', Volume C should perhaps focus on 'direct space'.

Opinion has also been expressed that the tables should be reduced to the absolutely necessary in the printed book; the rest should be available online only.

The current volumes contain a significant amount of material pertaining to powder diffraction; it is anticipated that this will largely be covered in the new Volume H *Powder Diffraction* and there appears little purpose in duplication. On the other hand, there are areas of overlap where, for example, particular methodologies used in powder diffraction have a role to play in single-crystal areas. For example, the methods of total scattering and pair distribution func-

tion analysis, which have developed in the powder diffraction area, have clear parallels and are becoming increasingly important in single-crystal diffuse-scattering analysis. A decision needs to be made whether the powder diffraction material is removed completely from Volumes B and C, greatly abbreviated with many cross-references with Volume H, or retained but with a focus more on the single-crystal connections.

Another field falling in this category is the use of pole figures and preferred-orientation analysis, which has overlap with the methods of X-ray diffraction microscopy and coherent diffraction imaging highlighted recently in the Special Issue of *Journal of Applied Crystallography*.

There are currently two articles about aperiodic crystals, one in B4.6 and one in C9.8, neither of which is ideally placed. This material should be combined and perhaps extended into one coherent whole.

*Possible topics for new articles (and ones requiring substantial upgrade)*:

(1) XFELS, X-ray free-electron lasers, including serial femtosecond crystallography.

(2) New developments in synchrotron radiation.

(3) New developments in X-ray detectors – CCDs, pixel detectors *etc*. Also, latest developments for neutron and electron detection.

(4) Atom probe microscopy.

(5) New iterative numerical techniques developed for solving the phase problem by using dual-space refinement. These include the methods for phasing Fraunhofer diffraction patterns from single molecule or nanoparticles. For example, see J. Miao *et al.* [(1999) *Nature*, **400**, 342]. Related is the 'charge flipping' algorithm of G. Oszlányi and A. Süto [(2008) *Acta Cryst*. A**64**, 123–134]. Connected to this is the *VLD* algorithm of Giacovazzo.

(6) Diffuse scattering and disorder. There has been a great deal of development in the last ten years both experimentally and in analysis, including use of genetic and evolutionary algorithms, simulated annealing and 3D PDF methods. (Note the connections with powder diffraction.)

(7) The bond-valence sum technique should be introduced as it is now widely used in a number of areas.

(8) Molecular modelling and visualization. A survey has shown that many of the most highly cited papers in the IUCr journals fall into this category and a major article on the latest developments would be valuable.

(9) The time-of-flight neutron section requires extensive revision. This is particularly pertinent with the advent of new and powerful sources: SNS in Oak Ridge, USA, and the European facility to be built in Lund, Sweden.

(10) 'Combined analysis' – a method that includes the refinement of structure, texture, residual stresses, phase, particle size, shape and microstrains *etc.* and including MQTA (Magnetic Quantitative Texture Analysis).

(11) Data mining – how to make use of the large structural databases.

(12) Methods for structure prediction.

(13) Methods for high-pressure crystallography and other non-ambient-conditions crystallography, crystallography in electric/magnetic fields.

This list of topics is not all-inclusive and other possible topics are still being sought.

**4.2.4. Volume D (*Physical Properties of Crystals*; Editor A. Authier)**. A second edition is being prepared actively:

(1) A new chapter on the tensorial properties of local X-ray susceptibility by Vladimir Dmitrienko and Elena Ovchinnikova has been commissioned. The manuscript is expected in the very near future.

(2) Chapters 1.1 (Introduction to the properties of tensors), 1.2 (Representations of crystallographic groups), 1.3 (Elastic properties) and 1.10 (Tensors in quasiperiodic structures) have been updated.

(3) Chapter 1.5 (Magnetic properties) has been updated; in particular, section 1.5.8.3 (Ferromagnetic and antiferromagnetic ferroelectrics) has been substantially revised by a new author and has received a new title, 'Multiferroics'.

(4) Chapters 3.3 (Twinning of crystals) and 3.4 (Domain structures) are being revised substantially.

(5) A proposal for an additional section in Chapter 3.1 (Structural phase transitions) has been submitted and has been sent to reviewers for comments.

**4.2.5. Volume E (*Subperiodic Groups*; Editors V. Kopský and D. B. Litvin)**. There were no new developments during 2012.

**4.2.6. Volume F (*Crystallography of Biological Macromolecules*; Editors E. Arnold, D. M. Himmel and M. G. Rossmann)**. The second edition of Volume F was published in January 2012.

The second edition dropped five articles that appeared in the first volume, updated 26 articles, and added 19 new articles, covering a range of topics in macromolecular crystallography and allied fields such as electron microscopy. The new articles include such topics as standard definitions for macromolecular crystallographic statistical indicators, expression of membrane proteins, protein engineering, radiation damage, detection of merohedral twinning, determining structures in the presence of merohedral twinning, low resolution *ab initio* phasing, robotic crystal loading, whole-cell X-ray diffraction imaging and halogen interactions in biological crystal structures. The second edition also presents articles on software in current use by macromolecular crystallographers and structural biologists, including software for electron microscopy. The aim of the second edition is to maintain an up-to-date reference for structural biology, to provide standards for the quality indicator metrics of X-ray structure refinement as well as atomic model validation, and to bring to the crystallographer an overview of methods for low- and high-resolution structure determination used in both crystallography and electron microscopy.

The volume is now also available online. As of March 2013, a total of 200 copies of the second edition of Volume F have been sold.

**4.2.7. Volume G (*Definition and Exchange of Crystallographic Data*; Editors S. R. Hall and B. McMahon)**. During 2012 S. R. Hall published with co-workers three papers in the *Journal of Chemical Information and Modeling* that specify the next-generation STAR File syntax (forming the basis for CIF syntax developments) and a methods-based dictionary definition language [Spadaccini, N. & Hall, S. R. (2012) 'Extensions to the STAR file syntax', *J. Chem. Inf. Model*. **52**, 1901–1906; Spadaccini, N. & Hall, S. R. (2012) 'DDLm: a new dictionary definition language', *J. Chem. Inf. Model*. **52**, 1907–1916; Spadaccini, N., Castleden, I. R., Du Boulay, D. & Hall, S. R. (2012) 'dREL: a relational expression language for dictionary methods', *J. Chem. Inf. Model*. **52**, 1917–1925]. New chapters in Volume G will be commissioned to describe this work and its implications for new dictionaries. A timetable for a new edition will be drawn up following a specialist workshop on building DDLm dictionaries and tools for CIF, to be held in August 2013.

**4.2.8. Volume H (*Powder Diffraction*; Editors C. J. Gilmore, J. A. Kaduk and H. Schenk)**. Volume H is a new volume devoted to powder diffraction. This is a subject of great industrial and academic importance that hitherto has only been discussed in *International Tables* in a fragmented way.

The volume consists of three sections:

(1) Instrumentation and Methods.
(2) Defects, Texture, Microstructure and Fibres.
(3) Applications.

This volume will comprise 63 chapters from over 80 authors and co-authors, totalling 690 pages.

Work is proceeding well: to date 36 chapters have been received, with many more expected within the next month.

The Editors met with IUCr staff in Chester in December 2012 to review manuscripts and progress; they will meet again in June 2013 for a major review of all aspects of this volume.

As always with a project of this size and complexity there are delays in the schedule. The Editors and Chester staff are hopeful, however, for a publication date that will coincide with the 2014 Montreal Congress during IYCr.

Further information about the volumes can be found at the home page of the Commission, http://www.iucr.org/resources/commissions/international-tables.

**C. P. Brock**, Chair

### 4.3. Commission on Aperiodic Crystals

2012 was a very active year for the Commission (CAC), following the award ceremony of the Nobel Prize in Chemistry to our colleague Dan Shechtman in December of the previous year. This Prize, awarded almost 30 years after the discovery of quasicrystals, served to invigorate the whole community, and helped to introduce the notion of aperiodic crystals to the greater scientific community as well as to the general public. The Prize inspired the organization of special meetings and sessions throughout the year, as well as the publication of Special Issues of journals, dedicated to quasicrystals. One of these Special Issues was published by the *Israel Journal of Chemistry*, edited by Patricia Thiel; another was published by *Chemical Society Reviews*, edited by Walter Steurer. Both contain a highly recommended collection of articles by leading members of our community.

As always, in 2012 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 central activity for the Commission in 2012 was its triennial flagship meeting Aperiodic 2012, Cairns, Australia, 2–7 September 2012. The meeting was organized by Ray Withers and Siegbert Schmid, with CAC acting as its Scientific Programme Committee. This was the seventh in a series of such meetings, inititated by CAC in 1994, bringing together all the different disciplines involved in aperiodic crystals. More than 110 delegates attended the conference, coming from 23 different countries. Dan Shechtman delivered a special celebratory Nobel lecture on the 30th anniversary year of his pioneering electron-diffraction characterization of the first quasicrystal on 8 April 1982. An introductory tutorial talk by Ted Janssen highlighted the fact that we also celebrated half a century of work on aperiodic crystals, which could be considered as dating back to the pioneering work of Pim de Wolff around 1962 (published in 1964). Presentations at the conference included 2 additional introductory tutorials, 11 invited talks, 46 contributed talks and 43 poster presentations. The Commission wishes to express its utmost gratitude to Ray Withers and Siegbert Schmid for their excellent work. The next meeting, Aperiodic 2015, will be held in Prague, Czech Republic, organized by Michal Dusek and Lukas Palatinus.

In addition to the above, a festive international conference on quasicrystals was held in Taipei, 7–9 May 2012 (Quasicrystals @TaipeiTech), celebrating the 30th anniversary of the discovery of quasicrystals, alongside the award of the 2011 Nobel Prize in Chemistry. ECM27 (the 27th European Crystallographic Meeting), which was held in Bergen, Norway, 6–11 August 2012, included a number of Microsymposia related to aperiodic crystals as well as a special Microsymposium dedicated to a review of state-of-the-art research in quasicrystals. A number of symposia were dedicated to quasicrystals at the Fall Meeting of the Materials Research Society, Boston, USA, 25–30 November 2012, including a Plenary Lecture on quasicrystals given by Dan Shechtman. Finally the series of *ad hoc* Workshops on *JANA2006* continued strongly in 2012 with a number of workshops organized by Michal Dusek in Prague, as well as additional workshops held during international events, such as the 3rd Turkish Crystallographic Meeting, the 3rd Shanghai Workshop on X-ray Crystallography, and the International School on Fundamental Crystallography held in Uberlandia, Brazil.

The most important upcoming meeting for the Commission is ICQ12, the 12th International Conference on Quasicrystals (http://icq12.fis.agh.edu.pl), to be held in Krakow, Poland, 1–6 September 2013, and organized by Janusz Wolny. ICQ12 will be a satellite of ECM28, Warwick, UK, 25–29 August 2013, which will also include two Microsymposia related to aperiodic crystals, a Keynote Lecture by Lukas Palatinus, as well as a Plenary Lecture on quasicrystals by Dan Shechtman. In addition, CAC will hold the 2nd International School on Aperiodic Crystals in Bayreuth, Germany, 7–12 April 2013, to be organized by Marc de Boissieu, Andreas Schönleber and Sander van Smaalen (http://old.crystal.uni-bayreuth.de/aperiodic_crys-school_2013/).

In 2012 CAC continued its process of coordinating and integrating its web site on the IUCr servers (http://www.iucr.org/iucr/commissions/cac.html) with the highly popular and active web site dedicated to all aspects of the crystallography of aperiodic crystals (http://www-xray.fzu.cz/sgip/aphome.html). The latter is maintained by Michal Dusek, for the special interest group on aperiodic crystals of the European Crystallographic Association. We hope to complete the integration of the web sites in 2013 as part of our preparations for the International Year of Crystallography in 2014.

**R. Lifshitz**, Chair

### 4.4. Commission on Biological Macromolecules

Commission (CBM) members have held frequent discussions over the internet, and the Chair has written more than ten letters to support meetings concerning macromolecular crystallography.

The Chair and Commission consultant Manfred Weiss visited Hergada, Red Sea, Egypt, in November 2012, representing the IUCr by attending the ESCA (Egyptian Society of Crystallography and Its Applications) meeting to support local crystallography in Egypt.

The Chair also organized a meeting on behalf of the Chinese Crystallographic Society (CCrS): with the help of the IUCr an International Workshop on New Developments of Methods and Software for Protein Crystallography, Xi'An, People's Republic of China, 24–27 August 2012, was held.

The CBM also played active roles duing the December 2012 Adelaide AsCA meeting and Bragg Centennial celebration meeting, and some discussions on various issues were held there.

The CBM also held extensive discussions over a proposal to change *Acta D* and *Acta F*'s journal directions; the overwhelming

view among the CBM members was that the present status of the journals' status should be maintained as *Acta D* is really doing very well. The issue should be how to keep *Acta D* as it is and not to change it in an unknown direction.

The CBM has also had extensive discussions on the preparation for the Montreal Congress and its nominations for membership of the International Programme Committee. There were many good proposals and suggestions for the Keynote Lectures and for Microsymposia speakers and Chairs; for example, a proposal for a half-day symposium in honour of Professor David Eisenberg was discussed and agreed upon by all CBM members.

In 2011, CBM member Tom Terwilliger (USA) was appointed as a member of the Diffraction Data Deposition Working Group (DDDWG), and will work as liaison between CBM and the databases in an effort to promote communication between the IUCr and the globally critical resources such as the Protein Databank that store and provide convenient access to biological structural data. Tom Terwilliger proposed that the CBM focuses on next-generation deposition expectations for the PDB and provided a high-level vision of key concepts for this discussion. The CBM members enthusiastically supported Tom's ideas and chose this as one of the top focuses for the Commission's future work. The CBM has appointed Tom as the leader of this effort within the CBM. Tom Terwilliger carried out a great deal work on DDDWG-related activities during 2012–2013, and CBM members have held frequent discussions concerning DDD issues. In particular, the CBM has participated in workshops in Bergen, Norway, and Boston, USA, to obtain community input on deposition of diffraction data, contributed to an online set of articles on visions for archiving and using raw diffraction data, and set in progress the commissioning of a set of articles for *Acta D* on archiving and using raw diffraction data.

Some of the meetings that have been supported by the Commission are:

Celebration of 100 years of X-ray Diffraction (Macromolecular Structure of Biological and Non-Biological Materials) Workshop, Hergada, Red Sea, Egypt, 18–22 November 2012.

Biomolecular Forms and Functions: A Celebration of 50 Years of the Ramachandran Map, Bangalore, India, 8–11 January 2013.

Macromolecular Crystallography School 2013: From Data Processing to Structure Refinement and Beyond, Montevideo, Uruguay, 8–16 April 2013.

RapiData 2013, Brookhaven, USA, 21–26 April 2013. This is one of the most important recurring schools for macromolecular crystallography and has been held every year since 1999.

International Conference on Structural Genomics 2013 – Structural Life Science, Hokkaido, Japan, 29 July – 1 August 2013. This meeting belongs to a series of conferences, and is the seventh biennial International Structural Genomics (ICSG) meeting and is organized by the International Structural Genomics Organization (ISGO); it is designed to serve as a forum to discuss the most recent developments in structural genomics and their impact on research in biology, medicine and disease.

Synchrotron Radiation Techniques and Nanotechnology: a Synergic Approach to Life Sciences and Medicine, Cape Town, South Africa, 11–22 November 2013.

**Xiao-Dong Su**, Chair

#### 4.5. Commission on Charge, Spin and Momentum Densities

The most important event in 2012 was the Sagamore XVII conference held in Hokkaido, Japan, in July 2012. The conference was organized by M. Takata (SPring-8), Y. Sakurai (SPring-8) and Yu Wang (NTU), with the support of the Commission. The role of advanced probes for next-generation science on charge, spin and momentum density was especially discussed during the conference, hosted by the RIKEN SPring-8 Center at the RIKEN Harima Institute and co-hosted by the national neutron and synchrotron institutes in Japan and in Taiwan (NSRRC). About 100 participants, about half from Japan, attended the conference.

The conference started with a session dedicated to the century's pioneers in the field of charge, spin and momentum densities on the occasion of the centennial of Laue's discovery of X-ray diffraction by crystals in 1912, the Braggs' demonstration of crystal structure determination by X-rays in 1913 and also the birth of crystallography in Japan by Terada's demonstration of X-ray diffraction [T. Terada (1913). *Nature*, **91**, 135] and Nishikawa's report on X-ray patterns of fibrous, lamellar and granular substances [S. Nishikawa & S. Ono (1913). *Proc. Tokyo Math-Phys. Soc.* **II**-7, 131].

A special evening session was held in honour of Professor R. Bader, who developed the quantum theory of atoms in molecules – a real breakthrough in the domain of electron-density analysis, which permitted the development of a fruitful dialog between crystallographers and theoreticians for studying chemical interactions.

Besides the sessions on new trends in charge, spin and momentum density science, an important part of the programme was devoted to the study of dynamics in novel materials, including high-$T_c$ superconductors, multiferroics and chiral magnets by inelastic X-ray and neutron scattering. A fascinating session showed the potential of the new XFEL sources.

The proposal of Professor C. Gatti (Milan, Italy) to organize the next Sagamore Conference near Lake Como in Italy was accepted in the closed Commission meeting.

At the European Crystallographic Meeting ECM27 in Bergen, Norway, in August 2012, the field of charge density was represented by one Keynote Lecture (KN14) given by M. Spackman on Charge Density and Crystal Engineering, and two Microsymposia, proposed by special-interest group SIG2, entitled New Perspectives for Charge Density Analysis: Materials Properties from Inorganic to Macromolecules (MS18) and The Importance of Low Temperature in Charge Density Studies: History and Future (MS19).

The 6th European Charge Density Meeting (ECDM6) took place in High Tatras, Slovakia, in September 2012 and gathered about 80 participants mainly from Europe. The meeting was organized by S. Biskupic and J. Kozisek from Bratislava University.

This Commission and the Commission on Electron Crystallography decided to support a joint IUCr project, proposed by P. Nakashima (Monash University, Australia), who will be leader of the project, on electron distribution in the metallic bond by QCBED techniques and X-ray diffraction.

At the request of the IUCr Executive Committee, a round-robin test on charge-density studies on a molecular compound using synchrotron radiation was undertaken this year in collaboration with the Commission on Synchrotron Radiation. The chosen compound is a molecule-based compound, manganese formate dihydrate, $Mn(HCOO)_2(H_2O)_2$, for which several data collections on different synchrotron-radiation beamlines (APS, DESY) and conventional X-ray sources are already available from B. Iversen (Aarhus University, Denmark), who agreed to share his data for the project.

**B. Gillon**, Chair

### 4.6. Commission on Crystal Growth and Characterization of Materials

In 2012 the members of the Commission collaborated actively but mostly *via* the internet. However, in June, at the European Conference on Crystal Growth in Glasgow, some of us had the opportunity to meet in person and exchange opinions. The main points discussed were: (1) the future of crystal growth around the world, (2) the organization of the Montreal Congress and (3) the organization of activities related to the International Year of Crystallography.

During 2012, Hanna Dabkowska decided to step down as a member; she continues to be strongly related to the work of the Commission as a member of the IUCr Executive Committee. Hanna suggested Ewa Talik as her replacement on the Commission. The whole Commission agreed with this choice and the Executive Committee approved her appointment. So, we wish to take the opportunity to thank Hanna for all her incomparable work for the Commission and welcome Ewa to our group.

At the end of August 2012, we were informed about the passing away of Arkady Glikin, who was a great scientist, a consultant of this Commission and a friend to most of us. Again, we wish to express our condolences to his family. Taking into account the relevance of the Russian crystal-growth community as well as the need of a consultant close to the mineralogy community, I invited Tatiana Bekker to serve as a consultant for our Commission. So, welcome also Tatiana to our group.

In August 2013 there will be the IOCG Conference in Warsaw, Poland. Our Commission is involved at different levels in the organization of this important event, and more details are given in my report as IUCr Representative to the IOCG. Here it is important to underline that with the particular aim of celebrating the International Year of Crystallography, three symposia of the IOCG Conference will be officially co-organized by representatives of IUCr, namely Thierry Duffar (Defect Formation/Elimination), Abel Moreno (Biological and Biogenic Crystallization) and Kullaiah Byrappa (Industrial Crystallization).

Moreover, for celebrating the International Year of Crystallography in 2014 we are discussing the organization of a web site to show people a collection of artificially grown crystals.

In 2012 the IUCr supported the following schools/meetings that were important for the crystal-growth community:

International Summer School on Crystal Growth and Photovoltaic Materials, Brasov, Romania, 27 August – 1 September 2012.

3rd International School on Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials (ISC2012), Granada, Spain, 21–25 May 2012.

Fourth European Conference on Crystal Growth (ECCG4), Glasgow, UK, 17–20 June 2012.

In 2012 the Commission received an increasing number of requests for letters of support for several local and international crystal-growth meetings in 2013.

As in previous years, many Commission members and consultants (H. A. Dabkowska, T. Duffar, J. M. Garcia-Ruiz, K. Kakimoto, E. Vlieg, J. Wang and myself) were involved in the work of the International Organization of Crystal Growth.

Finally, I would like to express my great honour and pleasure to continue chairing this Commission. I hope I am giving my own contribution to all the work carried out until now by the Commission to bring more understanding of the role of crystals and their influence on many aspects of life and technology.

**A. Zappettini**, Chair

### 4.7. Commission on Crystallographic Computing

There were two changes in the membership of the Commission in 2012. The Chair R. W. Grosse-Kunstleve resigned in June 2012. He was replaced by vote of the Commission and IUCr Executive Committee approval by R. B. Von Dreele; P. Mercier was appointed to take his place as a new Commission member. The full roster of members and consultants is posted on the Commission web site (http://www.iucr.org/iucr/commissions/crystallographic-computing).

Planning for the 2014 Computing School has continued and the tentative title Crystallographic Computing Life after Fortran? has been proposed. It will be at Carleton University, Ottawa, Canada. P. Mercier (National Research Council) has volunteered to be the local organizer.

The Commission has received an offer of support for a poster prize from OlexSys to be awarded to the best poster focused on crystallographic software.

**R. B. Von Dreele**, Chair

### 4.8. Commission on Crystallographic Nomenclature

*Discussion forum for the Commission on Crystallographic Nomenclature*. A forum has been created for discussion of nomenclature issues by members of the Commission, with Michael Glazer as moderator (Crystallographic Nomenclature), but there has been unfortunately very little response by Commission members, despite repeated reminders.

*Proposal for the addition of Seitz notation for symmetry operations to the symmetry operations subtables of International Tables for Crystallography Volume A*. Two proposals have been submitted for inclusion of Seitz symbols in the *International Tables*, one by D. B. Litvin and V. Kopsky, the other by A. M. Glazer, differing in the symbols used. The Commission has decided that the Seitz symbols should not be included in the printed version of the *Tables*, but may be included in the online version. Discussion on whether one or both types of symbols should be included in the online version of Volume A are ongoing in close cooperation with the Editor, Mois Aroyo. Mike Glazer is to present a complete proposal with examples of the 'rotational' part of the symbols in the cubic and hexagonal cases.

Otherwise few matters related to nomenclature have arisen in the course of the past year.

**A. Authier**, Chair

### 4.9. Commission on Crystallographic Teaching

The Commission has continued its efforts to reach out to the crystallographic community, the scientific community and the community at large by using social media. The Commission Facebook page (http://www.facebook.com/IuCrCommissionOnCrystallographicTeaching) has 87 'likes'. Our Twitter feed (@IUCrTeach) has 13 followers. In the next several months, the Commission will increase activity on both social media outlets to disseminate better exciting findings and important information as we approach the International Year of Crystallography and the Montreal 2014 Congress. We also plan to review our web pages on the IUCr web site, reorganize content as appropriate and update information.

The Chair represents the Commission (CCT) on the International Programme Committee (IPC) for the Montreal Congress. The IPC met in May to develop the programme for Montreal, and the CCT is sponsoring two half-day Microsymposia (MS) entitled Crystal-

lography Education and Training in the 21st Century: New Pedagogies, New Paradigms. These MS will provide a platform for speakers on a wide variety of topics, from technology, to K-16 education and outreach, to community engagement, to post-baccalaureate innovations. We hope that these sessions will also provide a venue for individuals and groups to showcase their ongoing efforts during the IYCr. The CCT has also agreed to co-sponsor the Microsymposium entitled Beginner's Guide to Validation of Crystallographic Results, sponsored by the Commission on Crystallographic Computing.

In the coming months, the CCT will further explore effective strategies for education and outreach during the International Year of Crystallography in 2014. A suggested format for talks aimed at the general public is the 'speed round' format. Here, during a 90 minute period, a moderator will introduce eight crystallographers/diffraction scientists, each of whom will have five minutes to talk about a topic of their choice, which is followed by five minutes of questions. This format is used regularly during national science festivals in the USA, and this type of event will be highly entertaining, engaging and illuminating.

In the past year, the Commission has reviewed and written supporting letters for workshops and summer schools focused on areas relevant to the discipline. These include:

I Latin-American Meeting on Crystallography and IX Annual Meeting of the Argentinean Crystallographic Association, Cordoba, Argentina, 29 October – 1 November 2013.

V School of the Argentinean Crystallographic Association, Cordoba, Argentina, 4–8 November 2013.

X-ray Powder Diffraction: Fundamentals and Applications, Santa Fe, Argentina, 5–9 November 2012.

School of Crystallization and Crystallography for Latin America ECRISLA2013, Florianópolis, Brazil, 14–25 October 2013.

III International Conference on Crystallogenesis and Mineralogy, Novosibirsk, Russia, 27 September – 1 October 2013.

5th Moroccan School of Crystallography – EMC5, Oujda, Morocco 23–27 October 2013.

School of Crystallization and Polymorphism, San Jose, Costa Rica, 27–31 January 2014.

Because a few of the proposals reviewed were poorly written, vague in details and/or did not justify the funds requested, the CCT plans to develop more formalized rubrics for evaluating such proposals in the future, along with criteria and guidelines to be presented to those individuals or groups making proposals to the IUCr for support. Guidelines will enable proposers to make the best possible case in their request. Rubrics will enable the CCT to determine more easily whether the proposals meet the mission and goals of the IUCr, to better compare and contrast the proposals, and to provide more useful feedback to the Executive Committee.

**K. A. Kantardjieff**, Chair

### 4.10. Commission on Crystallography in Art and Cultural Heritage

In 2012, the Commission was involved in the organization of the following two major events:

(1) The meetings X-ray Techniques in Investigations of the Objects of Cultural Heritage, and Celebrating the 100th Anniversary of Crystal X-ray Diffraction were held in Kraków, Poland, 17–19 May 2012, with 80 participants and more than 110 authors of lectures and posters. More information can be found at the Commission web site at http://www.chemia.uj.edu.pl/konferencje/downloads/abstracts_WEB.pdf.

(2) The Metropolitan Museum of Art of New York, the Conservation Center at the Institute of Fine Arts of New York University, the Winterthur Museum, Cornell University, and Brookhaven National Laboratory organized the Fifth International Conference on Synchrotron Radiation in Art and Archaeology (SR2A 2012), in New York City, USA, 5–8 June 2012. The conference consisted of three full days of oral presentations and poster sessions at The Metropolitan Museum of Art. A welcome reception was held at The Institute of Fine Arts, New York University. More information may be found at http://www.bnl.gov/sr2a/. There were 125 participants.

**E. Doorhyhée**, Chair

### 4.11. *ad interim* Commission on Crystallography of Materials

This Commission was established *ad interim* at the July 2012 meeting of the Executive Committee, with the following Terms of Reference:

(1) To organize Keynote Lectures, symposia and workshops (also in collaboration with other Commissions) on the hottest topics at the crossroads between crystallography and materials science, and raise the presence of materials scientists at crystallographic meetings.

(2) To strengthen the links and interactions among crystallographers and materials scientists, solid-state physicists and chemists.

(3) To organize workshops to increase crystallographic proficiency of materials scientists and physicists, and to train a new generation of crystallographers working in various fields of materials science.

(4) To promote scientific collaboration and mobility of scientists across these disciplines.

(5) To spearhead the recognition of crystallography as an interdisciplinary science (not just as a technique or as a tool).

(6) To encourage the publication of materials science research in the journals of the Union.

(7) Finally, the Commission will act in accordance with the general statement of principles regarding Commissions of the IUCr.

The Chair was appointed as Commission representative on the International Programme Committee for the Montreal Congress. The Commission proposed Microsymposia and one Keynote Lecture.

The Commission was indirectly involved in two highly successful international workshops on crystal structure prediction, which were organized by the Chair. One took place in Lausanne, Switzerland, 22–26 October 2012, and the other was held in Stony Brook, USA, 10–15 December 2012.

**A. Oganov**, Chair

### 4.12. Commission on Electron Crystallography

We stand at a crossroads in electron crystallography. The Commission seeks opportunities to take a leadership role in schools for 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.

*In Asia*. The International Workshop of 3D Molecular Imaging by Cryo-Electron Microscopy was organized with support from the Commission in the University of Science and Technology of China, Anhui, 7–12 September 2012. This workshop offered hands-on training of cryo-electron microscopy, tomography and 3D reconstruction, and attracted more than 200 participants from North America, Europe and Asian countries. The 6th ATOM workshop was organized 8–12 April 2012 in Taipei; this workshop focused on

understanding atomic structure using diffraction and imaging, especially aberration-corrected electron microscopy techniques.

*In Europe*. In order to promote electron crystallography as a science for structure determination, members of the Commission formed a special interest group (SIG) and organized several national or international schools. These included: (1) Applications of Precession Electron Diffraction, Manchester, UK, 14–15 September 2012, which was mainly concerned with the theory and application of precession electron diffraction to a wide range of crystallographic research areas and first-hand experience of using the technique. (2) Crystallography in Croatia, 25 January 2012, in which the Croatian crystallographers reported their scientific activity during more than 20 years and electron crystallography used in investigations in physics, chemistry, geology and mineralogy. (3) Electron Crystallography School, RWTH in Aachen, Germany, 23–24 April 2012. (4) Electron Crystallography School – New Methods and Applications, 16–20 June 2012, and The International Symposium on X-ray and Electron Crystallography – from Materials Sciences to Biology, 20–22 June 2012, both held in Stockholm, Sweden. A new EU fp7 Network called ESTEEM 2 was organized and includes activity in electron diffraction, and workshops on electron diffraction are planned within this framework. In addition, one poster prize for a young researcher in electron crystallography was awarded at the 27th European Crystallography Meeting (ECM27), Bergen, Norway, 6–11 August 2012, and two poster prizes for young researchers in electron crystallography were awarded at the European Microscopy Congress, Manchester, UK, 16–21 September 2012.

*In the USA*. The Workshop on Ultrafast Electron Sources for Diffraction and Microscopy Applications was held at the University of California, Los Angeles, 12–14 December 2012, with the aims to inform the broad scientific communities – accelerator, electron scattering and ultrafast science – about the latest developments in ultrafast electron sources, and to identify critical technologies and high-impact scientific opportunities. The Arizona State University 2012 Winter School on High-Resolution Electron Microscopy was organized from 4–7 January 2012; this aims to introduce the theory and practice of high-resolution electron microscopy to scientists currently using transmission electron microscopes for materials science studies.

The Commission recognizes the increased use of tools such as precession electron diffraction and cryo-EM, and aims to involve more biologists in the Commission, an area where there is currently under-representation. A biennial workshop on Electron Crystallography of Membrane Proteins was held in Basel, Switzerland, 19–24 August 2012; the workshop dealt with methods to determine biological membrane protein 3D structures from electron crystallography data of 2D membrane protein crystals.

The Commission also seeks to take a leadership role in reviewing the current contents of the *International Tables for Crystallography* for content relevant to electron crystallography. J. C. H. Spence has co-authored a new section for the sixth edition of Volume A with the title Methods of Space-Group Determination. J. M. Zuo has co-authored the electron powder diffraction part for the new volume H.

**Lian-Mao Peng**, Chair and **U. Kolb**, Vice-Chair

### 4.13. Commission on High Pressure

*2012 Commission Workshop*. The Commission organized its 2012 annual workshop, entitled Advanced Crystallography at High Pressures, in Mito, Japan. The meeting was held in conjunction with the International Symposium of the Quantum Beam Science Directorate (QuBS), Japan Atomic Energy Agency (JAEA), 23–27 September 2012. The Local Organizing Committee was chaired by Commission member Yoshinori Katayama (QuBS, JAEA), and Toyotaka Osakabe (QuBS, JAEA) acted as conference secretary. The workshop was well attended (95 participants from 14 countries). The topics of this workshop covered the whole range of activities of the Commission, and ten scientific sessions were held: (1) crystal structures, phase transitions and dynamic phenomena; (2) amorphous, liquid, non-crystalline and nanocrystalline phases; (3) magnetic and electronic phenomena at high pressure; (4) organic and biological systems; (5) water, ice and other molecular systems; (6) materials science; (7) chemistry; (8) geosciences and planetary sciences; (9) theory and computation; and (10) techniques for high-pressure studies. Each session was organized by two Chairs, of whom at least one was selected from the Commission members and consultants. The programme comprised 1 Keynote Lecture, 2 introductions, 25 invited talks, 11 contributed talks and 44 posters. A tour to the Japan Proton Accelerator Research Complex, J-PARC, was organized after the scientific sessions, and a newly built high-pressure neutron beamline, PLANET, at the Materials and Life Science Experimental Facility, MLF, was shown to the participants. The proceedings will be published as a special section in the journal *High Pressure Research*. The meeting was financially supported by JAEA, the project 'Earth Science Based on the High Pressure and Temperature Neutron Experiments (Grant-in-Aid for Scientific Research on Innovative Areas from MEXT)', the Japan Society of High Pressure Science and Technology, the IUCr and the ICDD. The meeting web site can be found at http://nsrc.jaea.go.jp/iucrhp2012/. A closed Commission meeting was held at the Mito Workshop during which current business was discussed. The main topic of discussion was the plans for the 2013 Commission workshop.

*Participation in the discussions on crystallographic data standards and deposition*. The Commission was represented by F. Fabbiani and K. Dziubek in the discussions on crystallographic data standards and deposition, which took place during the 27th Meeting of the European Crystallographic Association in Bergen, Norway, in August 2012.

*Preparations for the 2013 Commission Workshop*. The 2013 Commission workshop on Advances in Static and Dynamic High-Pressure Crystallography will take place at DESY, Hamburg, Germany, 8–11 September 2013. The Local Organizing Committee is headed by Hanns-Peter Liermann (DESY). This conference will cover the whole range of activities of the Commission.

The tentative list of scientific sessions reads:

(1) Crystallographic controls on rheology and elasticity (Chairs: Simon Redfern and Nori Nishiyama).

(2) Polymorphism and crystal chemistry (Chairs: Kamil Dziubek and Przemyslaw Dera).

(3) Computational approaches (Chairs: Nangini Garg and Rajeev Ahuja).

(4) Amorphous, liquid, non-crystalline and crypto-crystalline solids (Chairs: Andrew Goodwin and Vadim Brazhkin).

(5) Materials science (Chairs: Wilson Crichton and Vladimir Turkevich).

(6) Chemistry (Chairs: Vladimir Solozhenko and Alexandr Talyzin).

(7) Studies of organic and biological systems (Chairs: Andrzej Katrusiak and Elena Boldyreva).

(8) New frontiers in extreme conditions (Chairs: H.-P. Liermann and Ingo Loa).

(9) Rising stars (Chairs: Yoshinori Katayama and Francesca Fabbiani).

(10) Electronic and magnetic phenomena (Chairs: B. Winkler and K. Kamenev).

*Preparations for a 2016 Erice School on High Pressure Crystallography*. Commission member Francesca Fabbiani and former Commission member John Parise are organizing a training event for students and young researchers – an Erice School on High-Pressure Crystallography, which will take place in May/June 2016 and has been endorsed by the Commission. This will be the third school dedicated to the field of high-pressure crystallography and follows in the footsteps of the successful editions of 2003 and 2009. The school is expected to run over a course of eight days, with approximately 35 lectures in addition to demonstrations and workshops. Funding for the school is being sought from a variety of sources, including NATO, as well as other national and international organizations and industry.

*Preparations for the Montreal Congress*. The Commission is represented on the International Programme Committee by its Chair. The Commission submitted a proposal comprising two Keynote speakers and 8 Microsymposia (one co-sponsored with the Commission on Synchrotron Radiation, and one with the Commission on Crystal Growth and Characterization of Materials).

**P. Dera**, Chair

#### 4.14. Commission on Inorganic and Mineral Structures

Members and consultants of the Commission (CIMS) discussed various issues *via* e-mail. Other forms of communication were in person at occasional 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 maintain their links. A. Beatty is the representative of CSC in CIMS while P. Mercier represents CIMS in CSC.

P. Mercier continues to act as liaison officer of CIMS with the *IUCr Newsletter*. He is also the representative of CIMS on the IUCr's Working Group of Database Users.

Strong links exist between CIMS and Special Interest Group 5 of the European Crystallographic Association (ECA-SIG5, http://sig5.ecanews.org/). At present, the secretary of SIG5 is O. Siidra, the Chair is S. Krivovichev and F. Hatert is Vice-Chair.

There are very good relationships between CIMS and the European Mineralogical Union (EMU, http://eurominunion.org/); R. Oberti (EMU Past President since 2013) is a member of CIMS.

CIMS was involved in the following meetings held in 2012:

The third SMARTER Crystallography Workshop, Versailles, France, 10–13 September 2012 (http://www.smarter3.uvsq.fr). J. Rocha was one of the organizers (member of the Board Committee). Almost 100 people attended and 34 lectures were delivered.

An Italian two-day symposium celebrating The Centennial of X-ray Diffraction (1912–2012), Rome, 8–9 May 2012 was co-organized by the Accademia Nazionale dei Lincei, the Accademia delle Scienze di Torino and AIC. R. Oberti and G. Ferraris were members of the Organizing Committee. This symposium obtained the patronage of the ECA. More than 100 persons attended the lectures (delivered by outstanding scientists, among whom were two Nobel laureates and one recipient of the Ewald Prize), which focused on the history of crystallography and its revolutionary impact on many scientific disciplines. The lectures have been published in *Rendiconti Lincei* (2013), **24** (Suppl. No. 1); G. Ferraris acted as Co-editor.

Preparation of the 2013 Goldschmidt Conference to be held in Florence, Italy, 25–30 August 2013. R. Oberti is Co-Chair of the theme The Cutting Edge in Mineralogy and Mineral Physics, and a member of the Organizing Committee.

CIMS has also been much involved in the preparation for the Montreal Congress, suggesting Microsymposia, Workshops and Keynote Lectures.

CIMS supported the application for financial funding by IUCr of the following meetings to be held in 2013:

III International Conference Crystallogenesis and Mineralogy, Novosibirsk, Russia, 27 September – 1 October 2013.

EMU School on Minerals at Nanoscale, Granada, Spain, 3–6 June 2013.

CIMS also gave ('moral') support to the following meetings to be held in 2013:

Short course entitled Uranium: Cradle to Grave, Winnipeg, Canada, May 2013, organized under the auspices of the Mineralogical Association of Canada.

GEOLIFE – Geomaterials for the Environment, Technology and Human Activities, included in the theme The Cutting Edge in Mineralogy and Mineral Physics of the 2013 Goldschmidt Conference, Florence, Italy, 25–30 August 2013.

2012 Gordon Research Conference on Crystal Engineering, Waterville Valley Resort, New Hampshire, USA, 10–15 June 2013.

*Personal achievements*. M. Nespolo is CIMS representative on the Advisory Committee of the 2014 Meeting of the International Mineralogical Association where CIMS is in charge of the Mineralogical Crystallography sessions.

O. Yakubovich became an officer of the European Crystallographic Association (ECA) Executive Committee for the period 2012–2015.

**J. Rocha**, Chair

#### 4.15. Commission on Magnetic Structures

The Commission on Magnetic Structures (CMS) was established by the General Assembly in 2011 at the Madrid Congress. In May 2012, Branton Campbell was appointed as Commission Chair after Laurent Chapon left to take on a new assignment at the ILL. In December, Harold Stokes (BYU, USA) and Mois Aroyo (UPV/EHU, Spain) were appointed as new consultants to the Commission.

The scope of our Commission's efforts encompasses a broad range of magnetic structure types, including commensurate magnetic structures, modulated and otherwise aperiodic magnetic structures, low-dimensional magnetic structures, disordered magnetic structures *etc*. Our formal objectives are listed at http://www.iucr.org/iucr/commissions/magnetic-structures.

In 2012, the Commission reviewed and approved the extensive Magnetic Group Tables (almost twelve thousand pages of tabulated data and graphics) prepared by Daniel Litvin for online publication by the IUCr. The tables include magnetic point groups in 1, 2 and 3 dimensions, magnetic space groups in 1, 2 and 3 dimensions, magnetic Frieze groups, magnetic rod groups and magnetic layer groups. The data presented for each group include graphical and tabulated information following the format of the *International Tables for Crystallography* Volume A, and also include standard sets of coset representatives, maximal subgroups of index $\leq 4$, and a comparison of Belov–Neronov–Smirnova and Opechowski–Guccione symbols. The tables are accompanied by a 100-page book, which contains examples that guide the user in the interpretation and use of each type of table. This monumental work took many years to complete, and is of great value to all who work with magnetic symmetry and/or

magnetic structures. We thank Professor Litvin for the rare passion that led him to undertake such a project.

The Commission conducted a review of the coordinate systems used to describe magnetic structures, and of the refinement packages that implement each one. The report is available on the Commission wiki at http://cmswiki.byu.edu/wiki/Magnetic_Coordinates.

Commission member Wieslawa Sikora (Poland) has been appointed to serve on the International Programme Committee for the Montreal Congress.

A three-day satellite meeting on Magnetic Symmetry and Structure, to be associated with the Montreal Congress, is under consideration. This meeting would be co-sponsored by the Commission on Magnetic Structures, the Commission on Mathematical and Theoretical Crystallography and the Commission on Neutron Scattering.

A schedule of meetings of interest to members of the Commission was set up on the Commission web site at http://www.iucr.org/resources/commissions/magnetic-structures/meetings.

Considerable correspondence was focused on the proper description of a magnetic structure. We have considered three primary description types: the supercell description, the wave 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. Having standards for the various descriptions and their interconversions would make the communication of magnetic structures much more reliable.

Commission members gave featured presentations, developed workshop components, and organized or hosted workshops and Microsymposia at a variety of meetings in 2012. These were not specifically organized under the auspices of the Commission, but substantially furthered its objectives of promoting magnetic neutron scattering and magnetic structure determination:

Magnetic Neutron Diffraction Course, Ural Federal University, Russia, March–June (Alexander Pirogov);

JANA half-day workshop at the colloquium of the Czech and Slovak Crystallographic Association in Klatovy, Czech Republic, 12 June 2012 (Michal Dusek and Vaclav Petricek);

Tutorial on Magnetic Structure Determination, Korea University of Technology and Education (Alexander Pirogov);

9th International Workshop on Polarized Neutrons in Condensed Matter Investigations, Paris, France, 2–5 July 2012 (Laurent Chapon);

14th *ad hoc* JANA 2006 workshop on Magnetic Structures, Prague, Czech Republic, 15–16 October 2012 (organized and hosted by Michel Dusek and Vaclav Petricek);

ORNL Workshop on Magnetic Structure Determination, Oak Ridge National Laboratory, USA, 17–20 October 2012 (Juan Rodriguez-Carvajal);

13th European Powder Diffraction Conference, Grenoble, France, 28–31 October 2012 (Juan Rodriguez-Carvajal and Laurent Chapon).

**B. Campbell**, Chair

### 4.16. Commission on Mathematical and Theoretical Crystallography

*Scientific activity in 2012*. During 2012 the Commission (MaThCryst) organized two main activities and actively participated in a third:

School on Fundamental Crystallography, Mahdia, Tunisia, 9–13 April 2012, in cooperation with the IUCr Commission on Crystallographic Teaching (CCT). This school was originally planned in April 2011 but owing to the events commonly known as the 'Arab Spring' it was postponed by one year. The school was attended by 37 participants from four French-speaking countries (http://www.crystallography.fr/mathcryst/mahdia2012.php). Lectures were partly delivered in French to reduce the difficulties related to the language barrier. A selection of photographs is available at the *ad hoc* section of the IUCr web site (http://www.iucr.org/gallery/2012/mathcryst,-mahdia).

Third School on Fundamental Crystallography in Latin America, Uberlandia, Brazil, 25 November – 3 December 2012. After the schools held in Havana, Cuba (2007) and Montevideo, Uruguay (2010), the series of schools in Latin America continues with a biennial frequency (the fourth and fifth being planned in Argentina in 2014 and in Ecuador in 2016). The school was attended by 50 participants from five countries (http://www.crystallography.fr/mathcryst/uberlandia2012.php). A selection of photographs is available at the IUCr web site (http://www.iucr.org/gallery/2012/mathcryst,-uberlandia).

MaThCryst was also involved, although not directly in the organization, in a further activity: the Special Session on Modeling Crystalline and Quasi-Crystalline Materials at the American Mathematical Society Section Meeting in Tampa, Florida, USA, 10–11 March 2012 (http://www.ams.org/meetings/sectional/2188_program_ss5.html#title). Massimo Nespolo, Commission Chair, and Marjorie Senechal, former Commission consultant, were invited speakers. A selection of photographs is available at the IUCr web site (http://www.iucr.org/gallery/2012/mathcryst,-tampa).

*Scientific Activities in 2013 and later*. Planned activities include, at present:

2013 SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, USA, 9–12 June 2013, with three Minisymposia on Mathematical Crystallography (see http://www.crystallography.fr/mathcryst/siam2013.php).

A School on Topological Methods in Crystal Chemistry and Materials Science, Lausanne, Switzerland, 3–9 September 2013 (http://www.crystallography.fr/mathcryst/lausanne2013.php).

A School on Fundamental Crystallography, Gjulechitza, Bulgaria, 30 September – 5 October 2013 (see http://www.crystallography.fr/mathcryst/bulgaria2013.php).

The fourth School on Fundamental Crystallography in Latin America, La Plata, Argentina, 27 April – 9 May 2014 (see http://www.crystallography.fr/mathcryst/laplata2014.php).

A satellite meeting on Magnetic Symmetry and Structure during the Montreal Congress, co-organized with the Commission on Magnetic Structures and the Commission on Neutron Scattering.

The second School on Fundamental Crystallography in South Africa, organized as a satellite meeting of the 21st Meeting of the International Mineralogical Union, Bloemfontein, South Africa, 25–29 August 2014 (see http://www.crystallography.fr/mathcryst/SouthAfrica2014.php).

*Other activities*. The following activities, already mentioned in previous reports, have not seen further development.

Commission consultant Dhananjai Pandey proposed a workshop in India: perhaps this could be held within the framework of IYCr 2014.

Commission member Stephen Hyde proposed a workshop on the manifold description of modulated structures and the use of differential geometry to describe crystal structures; perhaps this, too, could be held within the framework of IYCr 2014.

A School on Graph Theory in Crystallography and Crystal Chemistry is envisaged soon after the publication of the book with the same title, planned for late 2013 or early 2014.

The planned School on Geometric Algebra in Crystallography is still pending because of the delayed publication of the book with the same title.

*News from commission members*. Commission member Heidrun Sowa is MaThCryst representative on the Diffraction Data Deposition Working Group of the IUCr.

Commission member Sybille Gemming resigned because of lack of time to dedicate to the Commission. The place is vacant and will not be filled until the Montreal Congress.

**M. Nespolo**, Chair

### 4.17. Commission on Neutron Scattering

The Commission (CNS) has continued to promote access to neutron facilities for crystallographers worldwide through a number of different initiatives. Several members of the Commission are involved in organizing and teaching in regional neutron schools, which remain the best way of training the next generation of neutron users and raising awareness about the use of different neutron techniques.

The 6th American Conference on Neutron Scattering (ACNS) was held in June 2012 in Washington, USA. This was a very successful event, attracting over 380 participants from a broad range of scientific disciplines that make use of neutron-scattering studies. Ahead of the conference, a tutorial session on time-of-flight powder diffraction was chaired by Thomas Proffen. At the annual meeting of the American Crystallographic Association in July 2012, Thomas Proffen also organized a session on Local Structure/Partially Ordered Systems as well as a workshop on Modeling and Refinement of Nanoparticle Structures from Diffraction Data. He was also speaker at the 9th Canadian Powder Diffraction Workshop held in May at the University of Saskatchewan, Canada, which was organized by Ian Swainson.

In October 2012, as a satellite event of the EPDIC conference in Grenoble, France, a colloquium was organized at the Institut Laue–Langevin in honour of Alan Hewat. Alan was a very active member of our Commission and remains a reference for the powder diffraction community.

Throughout 2012, the Commission was actively involved in a variety of activities related to the 100th anniversary of X-ray crystallography and the International Year of Crystallography. The celebration of the centenary of the Laue/Bragg discoveries started with a 'Laue day' organized by Wolfgang Schmahl during the 20th annual meeting of the German Crystallographic Society (DGK) held in Munich, Germany, 12 March 2012. A second 'Laue day', attended by more than 160 participants, was organized on 13 November at the Institute Laue–Langevin by Maria Teresa Fernandez-Diaz and Maria-Helene Lemee-Cailleau. The CNS is also participating in a joint Committee involving several European and French Institutions from Grenoble [Institut Laue–Langevin (ILL), European Synchrotron Radiation Facility, CNRS, CEA, Université J. Fourier, Grenoble-INP, SiMAP, Institut Néel, INAC, GIANT, Grenoble Education Authority, La Casemate science museum, French Association of Crystallography]; this Committee is coordinating a number of events for the International Year of Crystallography in 2014.

We have re-established contacts with the publication *Neutron News* in order to revitalize communications between the more expert neutron-scattering community that is the target audience of *Neutron News* and the wider community of neutron users within the IUCr.

The Commission is also closely involved in the development of crystallographic instrumentation at various facilities. It is important to note the continued high levels of investment in new upgrade projects at existing facilities, such as the Millennium Programme at the ILL (France), where the new cold neutron Laue diffractometer LADI-III on a new guide is now two times brighter than before and has delivered results for the smallest sample ever measured for biocrystallography. Similarly, at ISIS (UK) construction is now well under way of four new Second Target Station instruments.

Following a recovery shutdown to repair the damage caused by the earthquake of 11 March 2011, the number of experimental proposals received in 2012 by the Materials and Life Science Experimental Facility (MLF) at J-PARC in Japan actually exceeded pre-earthquake levels. Several dedicated diffraction instruments have been commissioned and made available to users. Moreover, in November 2012 an intensity of about 65 trillion neutrons per pulse was achieved, allowing the MLF to be crowned the world's highest-intensity pulsed neutron source.

Finally, in collaboration with Sax Mason (a former member of the Commission), we are currently initiating a project to measure the same single-crystal sample of one or more compounds on various single-crystal neutron diffractometers around the world in order to perform a comprehensive study of these materials from data collection to reduction and structure analysis. The aim of this study will be to provide insight into the strengths and application specifics of each of the instruments used.

**M. T. Fernandez-Diaz**, Chair

### 4.18. Commission on Powder Diffraction

Unfortunately, 2012 was notable for a large amount of work by various Commission (CPD) members for not much gain. The workshop being organized on structure validation was moved from the ECM to EPDIC for organizational reasons. In the end, however, the workshop was cancelled owing to a perplexingly low level of interest from the European powder-diffraction community in an event being held in Europe. This, despite some late but sustained efforts to promote the meeting (which had already secured some excellent invited speakers), perhaps showed that an educational school format as opposed to a workshop may have been more appropriate given the lack of abstracts from the people who did register. The planned formal CPD meeting at EPDIC did not happen owing to the low turnout. Informal discussions were held instead during the course of the conference.

Work on Volume H of *International Tables for Crystallography* continued in the background with chapters trickling in over the year. A number have been sent out for corrections after review. It has been accepted that the original timescale for the volume was too ambitious given the time constraints on authors these days. Jim Kaduk updated the members present at EPDIC on the progress behind the scenes.

CPD planning for the IYCr largely revolves around a workshop being organized in South Africa for January 2014. It is hoped that it will attract people from around Africa and aims to support the mining industry that is so important to the region. It is hoped that a desktop XRD instrument can be borrowed from a vendor so that some hands-on practical sessions may be held as well as the more conventional presentations.

The CPD has been supporting the organization of the meeting Accuracy in Powder Diffraction IV being held at NIST in April 2013. This meeting was also notable in being the only powder meeting in North America in at least six years to apply for IUCr sponsorship. Hopefully, the tendency toward severe geographical imbalances in sponsorship requests to the CPD will rectify itself in future years. This imbalance is evident in the applications approved and meetings held during 2012 – four from South America, one from Europe and one from Australia. One significant application from Europe was received too late to be considered by the Sub-committee on the Union

Calendar, so some efforts in informing the wider community about the application deadline for IUCr support might be in order.

**P. Whitfield**, Chair

### 4.19. Commission on Small-Angle Scattering

*Commission meetings and communication*. Commission (CSAS) members communicated by e-mail or during personal meetings at national and international conferences. In 2012, most communications were accomplished by e-mail, but several members and consultants were able to meet in person at the 15th triennial International Small-Angle Scattering Conference (SAS 2012), Sydney, Australia, 18–23 November 2012. Virtually all CSAS members and consultants contribute to the various activity categories on an ongoing basis. What follows is a summary of highlights for calendar year 2012.

*Commission activities*. The most significant CSAS activity in 2012 was our involvement in the SAS 2012 Conference held in November in Sydney, Australia. J. Trewhella and D. McGillivray were Co-Chairs of the Scientific Programme Committee, which also included Y. Amemiya and D. Svergun. U.-S. Jeng, R. Serimaa, N. Yagi, J.-S. Pedersen, D. Svergun and I. Torriani were on the International Advisory Panel.

In April 2012, the Commission and the SAS 2012 Organizing Committee, *via* the SAS list-server and SAS 2012 Conference web site, called for nominations for the Guinier Prize, a USD 5000 prize, sponsored by the IUCr, for lifetime achievement in small-angle scattering. Members of the Commission, with others from the conference Organizing Committee, then formed a panel of judges to select the recipient. Finally, on 22 November at SAS 2012, Commission Chair, A. Allen, was delighted to present the 2012 Guinier Prize to Professor Otto Glatter of the University of Graz, Austria, *for his dedicated development, application, propagation and dissemination of small-angle X-ray, light and neutron scattering methods over more than 40 years; for his pioneering work on the development of the indirect Fourier transform method and its application to solve practical problems in real materials across many fields, especially in polymer science, soft matter and nanoparticle systems, and its extension to concentrated systems; and for his universally recognized service in building up the international small-angle-scattering community through teaching and training, software development and publication, development of instrumentation, and the writing of a widely used teaching text.*

In a similar way, also, in April 2012, the Commission and the SAS 2012 Organizing Committee called for bids to host SAS 2018, *i.e.* two conferences ahead of SAS 2012. (During SAS 2009 in Oxford, UK, the site of SAS 2015 was chosen to be Berlin, Germany.) An evaluation committee was convened composed of CSAS members and members of the Organizing Committees of past and present SAS conferences, chaired by the SAS 2012 Conference Chair, E. Gilbert. After a bid presentation session at SAS 2012, SAS 2018 was awarded to Argonne National Laboratory, USA, to host the conference at Grand Traverse Resort and Spa, Traverse City, Michigan.

An Open Meeting of CSAS was held during SAS 2012 to inform the international SAS community of the activities of the Commission. Issues discussed included future SAS Conference venue selection, Guinier Prize selection, development of common SAS data formats (also see canSAS, below), publication standards for bioSAS (see below), planning for the Montreal Congress, proposed development of the CSAS web pages, future membership of the Commission and IUCr celebration of the International Year of Crystallography (IYCr) in 2014. CSAS consultant D. McGillivray also explained the ongoing development of the 'SAS Portal' web pages (http://smallangle.org) – an independent effort to provide useful SAS information, linked to the canSAS work (see below). A. Allen and D. McGillivray also explained plans to develop the IUCr CSAS web pages in 2013 (now underway) and to provide better links to both the canSAS and SAS portal sites, as well as the bioSAS web sites (see below).

The Commission is proposing that, starting with SAS 2015, the Guinier Prize Award should be decided sufficiently in advance of the conference for the Guinier Prize recipient to be invited to deliver a Prize Lecture as part of the Award Ceremony. The Commission has also initiated discussions with both the SAS 2015 and the SAS 2018 Organizers for the triennial SAS conferences, as well as being showcases for SAS science, also to include task-force workshops that focus on addressing SAS issues to improve and enhance SAS practice, integrity and impact. Such workshop groups might be invited to report both at the triennial SAS Conferences and at the IUCr Congresses when appropriate.

Also at the SAS 2012 conference, CSAS member P. Jemian chaired an Open Meeting of the canSAS group, updating on the progress of the group and reporting on a workshop held in Uppsala, Sweden, earlier in the year. For some years, this group of SAXS and SANS beamline scientists, users and software developers (currently including P. Jemian and D. McGillivray from CSAS) has been working to reduce impediments for researchers using multiple instruments at different facilities. This includes exploring the scope for common data formats for SAXS and SANS, and comparing instruments against an agreed measurement standard. [Release v1.1 of the canSAS standard for storing 1-D SAS data and metadata in XML files has been released in March 2013.] This allows better portability of SAXS and SANS data between instruments and experiments, and will help in establishing guidelines for 'recommended' and 'required' information to be incorporated into the metadata (resolution, wavelength, geometry *etc.*) accompanying the actual SAS data. A third aspect to the canSAS work is in simplifying access to information about SAS, in the newly developed web portal as mentioned above. The canSAS group are intending to issue a report on their work in 2013.

Earlier in the year, following discussion among CSAS members, on behalf of the Commission, CSAS Chair A. Allen contributed an SAS-oriented discussion posting to the IUCr Working Group on Diffraction Data Deposition (DDWG) Forum site.

*Educational activities*. CSAS members and consultants organized the following courses to improve awareness of SAS-related methods in 2012:

R. Serimaa – course on X-ray Scattering Methods for Structural Studies of Lignocellulosic Material, National Graduate School of Biomass Refining, University of Helsinki, Department of Physics, Helsinki, Finland (for PhD students with no background in X-ray physics or physics).

V. Volkov – lecture course Supra-Atomic Structures in Nanomaterials, developed as an extension of a course on theory and practice of SAS in investigation of non-crystalline systems, Institute of Nuclear Physics and Physics Department, Moscow State University (MSU), Russia (for undergraduate and postgraduate students); lecture course on SAS Methods, Physics Department, MSU; training course on Study of Structure of Polydisperse and Monodisperse Systems, Institute of Crystallography, Moscow, Russia, with staff from EMBL, Hamburg, Germany (for students and young scientists from Ukraine, Kazakhstan and Byelorussia). Meanwhile, two students at MSU defended diploma research on investigation of nanomaterials and protein molecules by SAS methods, while two others started

SAS-related diploma research in 2012. Two postgraduate students started SAS-related PhD research at the Institute of Crystallography and at the Physics Department of MSU.

D. Svergun – educational lectures in 2012 at events in several different countries.

J. S. Pedersen – undergraduate and graduate lectures in SAS techniques, Aarhus University, Denmark, in courses Biophysical Chemistry 2 (including hands-on application of SAS to protein samples), Protein Biophysics, and Physical Chemistry of Soft Matter; also continued to support new SAXS users at Aarhus University, and from Universities/Research Institutes in Denmark, Scandinavia and the rest of Europe.

N. Yagi – Chair, Local Organizing Committee, conducted SAXS beamline practicals for the 12th SPring-8 summer school, July 2012, and for the 6th AOFSRR (Asia/Oceania Forum for Synchrotron Radiation Research) Cheiron school, SPring-8, September/October 2012.

P. Jemian presented lectures at 'Beyond Rg 2012', a short course in small-angle X-ray scattering given at the Advanced Photon Source. Also assisted in courses on *Irena*, *Indra* and *Nika* software packages in *IgorPro* for SAS analysis given at the Advanced Photon Source, ANL and at the Australian Synchrotron.

*Community-building activities*. CSAS members and consultants served on various SAS-related Committees and panels and editorial boards in 2012 (excluding SAS 2012):

R. Serimaa – board member, Finnish Synchrotron Radiation Users' Organization, 2009–2012.

D. Svergun – main organizer, EMBO Global Exchange Lecture Course on Structural and Biophysical Methods for Biological Macromolecules in Solution, Hyderabad, India (650 applicants, of which 50 were selected). A team of 14 lecturers and tutors gave comprehensive coverage for synergistic use of methods applicable to study biological macromolecules in solution. This was the first event of this kind in India, and clearly a successful SAS-oriented outreach. (SAS Commission member, J. Trewhella was also involved.)

G. Kostorz – co-organizer and speaker at TMS (Theory of Modelling and Simulation) symposium on scattering methods in materials science (Orlando, Florida) – a continuation of efforts to familiarize materials scientists with scattering methods; lectures in Japan and USA; continued service as Co-editor for *Journal of Applied Crystallography*.

A. Allen – SANS beam-time allocation committee at NIST Center for Neutron Research; continues to serve as Co-editor for *Journal of Applied Crystallography*.

P. Jemian – chair, SAXS proposal review panel at the Advanced Photon Source, Argonne National Laboratory.

*Consultant activities*. Several CSAS members and consultants served on SAS-related proposal and design evaluation committees:

D. Babonneau – Peer Review Committee 3 Matter & Material Properties: Structure, Organization, Characterization, Elaboration for beam-time allocation at SOLEIL synchrotron, France.

V. Volkov and the Institute of Crystallography (Moscow) – continued to consult in 2012 for about six scientific and engineering institutes in Russia, and the nanoscale features of some 250 samples of different kinds were investigated by SAS on a collaborative basis.

N. Yagi – advisor for design of proposed LIX (High-Brightness X-ray Scattering for Life Sciences) beamline at NSLS-II, Brookhaven, NY, USA; also adviser for Advanced Soft Material Beamline, SPring-8 (a dedicated SAXS beamline for industry-oriented polymer and soft materials science).

*Organizational activities*. Chaired by J. Trewhella and also including D. Svergun, the world-wide Protein Data Bank (wwPDB) Small-Angle Scattering Task Force (SAStf) met in July 2012 to consider whether deposition of SAS-based models would be of value to the structural biology community, and, if so, what kinds of accompanying data and validation would be required. This Task Force is made up of experts in crystallography, NMR spectroscopy, electron microscopy, and molecular modeling (http://www.wwpdb.org/workshop/sasTaskForce.html). A meeting report describing their recommendations is in review for publication in the journal *Structure*.

With SAS being increasingly used by structural biologists to develop 3D models, this work can be of significant value in advancing understanding of biomolecular structure and function. While SAS is a long-established technique for structural characterization, the capacity easily to generate 3D models from SAS data is a relatively recent development. It was therefore timely for experts in the community to work to establish agreed guidelines for publication that will aid in reviewing and evaluating modelling results. Draft publication guidelines for structural modelling of SAS data from biomolecules in solution were developed by CSAS and have been adopted by the IUCr journals (http://journals.iucr.org/d/issues/2012/02/00/me0456/index.html). A paper describing the basis for the guidelines was published in *Acta D* in 2012 (Jacques *et al.*) and is freely available for download at http://journals.iucr.org/d/issues/2012/06/00/be5200/index.html. While some of these guidelines may apply to a broader class of SAS experiments, they were developed explicitly to inform those performing or evaluating the results of 3D biomolecular structural modelling. Members of CSAS and the Commission on Journals, the wwPDB and the SAStf led a discussion of the draft guidelines and the SAStf recommendations at the SAS 2012 meeting in Sydney, Australia (November 2012), and there was general support for the guidelines but a request for a mechanism for community input. To that end, a web site has been established with the SAS2012 presentation material and the capacity to accept submissions (http://sas.wwpdb.org/), which has been announced through sa_scat, the discussion list-server of CSAS (http://mailman.iucr.org/mailman/listinfo/sa_scat). It is hoped that journal Editors may wish to consider using the guidelines as an aid in the review process; noting that these were developed not to impede publication of SAS results, but to ensure that sufficient detail is provided for adequate review and confidence in the results presented, and for others usefully to test and develop models with further experiments. Communication of the guidelines to relevant journals should follow in 2013.

SAS Commission members and consultants served on several programme or organization committees for SAS-related conferences and workshops in 2012 (excluding SAS 2012):

D. Babonneau – Scientific Committee for Symposium on Carbon- or Nitrogen-Containing Nanostructured Thin Films, EMRS Spring 2012 Meeting.

D. Svergun – co-organizer, EMBL Advanced Course on Hybrid Structural Biology Approaches, and co-organizer, EMBO Practical Course on Protein Expression, Purification Characterization and Crystallization, both courses in Hamburg, Germany, also co-organizer, EMBO Practical Course on Solution Scattering from Biological Macromolecules (devoted to SAXS and SANS analysis of biomacromolecular solutions with over 200 applicants, out of which 26 were selected). (SAS Commission member, J. Trewhella was also involved.)

U-Ser Jeng – organizer, session on Protein/Lipids Non-Crystalline Structures with X-ray Scattering, Annual Meeting of the Biophysical Society of Taiwan, Institute of Biomedical Sciences, Academia Sinica, Taiwan, May 2012 (about 350 attendees with 10 overseas and 20 domestic invited speakers).

J. S. Pedersen – Organizing Committee, 11th European Summer School on Scattering Methods Applied to Soft Condensed Matter, Bombannes, Gironde, France, June 2012.

*Technical activities*. Several CSAS members and consultants presented Invited, Plenary or Keynote SAS-related talks around the world, or took part in other technical activities not included above:

D. Babonneau – invited talk, GISAS 2012 (satellite of SAS 2012): GISAXS Studies of Ion-Beam Nanostructured Hard Materials.

A. Allen – developing NIST standard reference material (SRM) for SAXS intensity calibration, based on glassy carbon (in collaboration with others at NIST and at the Advanced Photon Source, Argonne National Laboratory), now intended for issue by end of 2013; also continued contributions to late drafts of an ISO TC24/SC4 (particle-size committee) SAXS particle size (best practice) standard.

P. Jemian – implemented the goals of the canSAS 1D standard in XML and supporting code packages and documentation. Working on coordinating the goals of the canSAS standard for multidimensional SAS data within the scope of the organizers and also within the scope of the NeXus standard. Continued as member of the NeXus International Advisory Committee that oversees the development of the NeXus data standard for storing data and metadata from X-ray, neutron, electron and muon science experiments.

**A. J. Allen**, Chair

### 4.20. Commission on Structural Chemistry

Most of the interactions among the members and consultants of the Commission (CSC) has taken place through e-mail exchange and, in some cases, timely discussions have been spontaneously carried out when some of the members met in regional ECA, AsCA or ACA meetings. A. Beatty has maintained her activities as link from the CSC with the Commission on Inorganic and Mineral Structures (CIMS), while P. Mercier will act as link from CIMS. J. L. Flippen-Anderson links to the *IUCr Newsletter*.

*Commission activities*. Three major activities have occupied the efforts of the Commission during 2012: discussion and evaluation for Commission support of different proposals submitted to the Subcommittee on the Union Calendar; designation of Commission representatives for the International Programme Committee of the Montreal Congress; and participation of some members of the Commission in the Working Group on Diffraction Data Deposition. Additionally, some Commission members participated in the organization of or as Programme Committee members of workshops or meetings held in 2012.

During the year four proposals reached the Commission asking for formal support for an application for financial assistance from the IUCr. The Erice International School submitted a proposal for an interesting school to be focused on The Future of Dynamic Structural Science, directed by Judith A. K. Howard (UK), Paul R. Raithby (UK), Hazel A. Sparkes (UK), and Andrei V. Churakov (Russia), with a large number of well known specialists in the field. A second event, related to the previous one, unanimously supported by the Commission, was the Workshop on Dynamic Structural Photocrystallography for Chemistry and Material Science, led by Professor Philip Coppens; this is a subject that is clearly at the cutting edge of chemical crystallography.

A third application positively evaluated by our Commission was that of the MISSCA2013 meeting. This international meeting was planned as an open international meeting scheduled to bring together more than 200 people from the Spanish, Italian and Swiss Crystallographic Associations. The topics to be covered included Microsymposia of clear interest for the Commission: Covalent and Supramolecular Functional Materials; Crystallography at Non-Ambient Conditions; and Crystallography of Materials with Novel Electronic Properties.

In July 2012, Jim Britten, Chair of the International Programme Committee for the Montreal Congress, contacted the Commission asking for potential candidates for representing the scientific interests of our Commission. Four first-priority names (together with another four as alternatives) were suggested to allow for compensation of gender and geographic distribution within the IPC. Eventually two candidates were selected for the Committee: Susan Bourne (South Africa) and Paul R. Raithby (UK). These two colleagues will have to design excellent topics and powerful arguments to compensate for the presence of three members in the previous IPC for the Madrid Congress.

The Commission has also being active in the discussions and meetings of the IUCr Working Group on Diffraction Data Deposition (WGDDD). Some of the Commission members have been active in the IUCr forum associated with this initiative, and some have also participated in a couple of meetings of this working group. Patrick Mercier was in attendance at the WGDDD meeting held in Boston, USA (accompanying the ACA meeting), while Fernando J. Lahoz was present at the one-day symposium that took place in Bergen, Norway, on the day the ECA meeting started.

Two events that took place in 2012, supported by the Commission and involving some members/consultants of the Commission, also merit mention. In September, Indaba 7 was held in Kruger National Park, South Africa. More than 100 participants attended this interesting workshop, carried out under the direct supervision of Len Barbour (Organization Chair) and Peter Comba (Programme Chair), dealing with a list of topics clearly fitting the scope of CSC (polymorphs, host–guest compounds, co-crystals, crystal engineering, symmetry, computational modelling, structure determination *etc*.)

Another relevant activity supported by the Commission was the 2012 Gordon Research Conference on Crystal Engineering, held in New Hampshire, USA, in the spring. The local organizers, R. D. Rogers, Michael J. Zawarotko and Christer Aakeröy, brought together more than 150 participants (more than 80 young crystallographers) with most of the relevant authors in the area: S. Gao, F. Grepioni, L. Addadi, J. Berstein, G. R. Desiraju, B. Jones and many others.

**F. J. Lahoz**, Chair

### 4.21. Commission on Synchrotron Radiation

*Introduction*. The purpose 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 (X-FELs) and Energy Recovery Linacs (ERLs).

The progress of synchrotron-radiation user facilities and science continued at a rapid pace during 2012. Several new high-brightness storage-ring facilities are in their final stages of construction, led by the NSLS II at Brookhaven National Laboratory (USA) and the Taiwan Photon Source in Hsinchu, Taiwan. The original three third-generation hard-X-ray facilities, ESRF, APS and SPring-8, are either undertaking or planning significant upgrade programmes.

Impressive scientific output is being reported by the two operating hard-X-ray XFEL projects, LCLS in the USA and SACLA in Japan. It is becoming increasingly apparent that major immediate impacts will be made in structural biology, with the development of nanocrystallography to the point that the first unknown structures are being solved, the introduction of additional novel techniques such as the SLAC development of two colour laser pulses, and with work continuing towards the goal of single-molecule imaging.

*Membership*. The Commission membership was stable during 2012. Two consultants were added in 2011 to represent the SACLA (Japan) and European X-ray Free Electron Laser facilities. The search for a suitable consultant from LCLS (USA) is ongoing.

*SRI 2012, Lyon, France*. The conferences on Synchrotron Radiation Instrumentation are the peak international meetings, staged triennially, bringing together synchrotron facility staff and users from around the world to report on instrumentation and scientific developments. The SRI meetings are always hosted by a major synchrotron user facility, or facilities, and the 2012 conference was jointly hosted by the ESRF and SOLEIL.

SRI 2012 was attended by six members or consultants of the Commission, and a lunchtime meeting was arranged during the conference to discuss issues relevant to the Commission. The major topic of discussion was the recurring problem of recognition and career advancement of beamline scientists at synchrotron facilities; more detail is given below.

*Supported Meetings, Schools and Workshops*. The Commission provided letters of support and endorsement for the following meetings:

International Workshop on Resonant Elastic X-ray Scattering, Diamond Light Source and Oxford, 15–19 July 2013;

the RapiData 2013 course to be held at Brookhaven National Laboratory, USA, 21–26 April 2013;

International Workshop on Dynamic Structural Photocrystallography in Chemistry and Materials Science, Buffalo, USA, 16–20 June 2013;

the International Conference on Structural Genomics, Hokkaido, Japan, 29 July – 1 August 2013;

the 11th International Conference on Biology and Synchrotron Radiation (BSR), Hamburg, Germany, 8–11 September 2013;

Innovation in Polymer Science and Technology 2013 (IPST 2013), Yogyakarta, Indonesia, 7–10 October 2013.

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

*Recognition and Career Development for Synchrotron Beamline Scientists*. The Commission Chair attended the International Advisory Committee (IAC) meeting at the SRI 2012 conference; the IAC is composed of the directors of all major synchrotron user facilities. The Chair and Professor Sine Larsen addressed the meeting about the role of beamline staff scientists and how best their work could be acknowledged and credited by the community. This is a longstanding issue in fields of core interest to the Commission and the Union as a whole, such as protein crystallography, small-molecule crystallography, powder diffraction and XAFS, and has been a long-standing area of concern for the Commission. As these techniques have matured it has become less and less common to give proper acknowledgement to the scientists who have developed and operate the methods/instruments. This can significantly impact career advancement, especially for scientists contemplating a transfer to a university/academic career, and general job satisfaction. The presentation was successful in triggering a lengthy discussion and some subsequent follow-up communication, but the issue is a complex one and no clear solutions were forthcoming.

The Chair also took the opportunity to promote the short-format beamline publication facility available in the *Journal of Synchrotron Radiation*.

*Collaboration with other Commissions*. The Commission together with the Commission on Charge, Spin and Momentum Densities has undertaken a round-robin test for determining high-resolution electron density on a small molecular compound using different synchrotron sources. A molecule-based compound, Mn formate, has been chosen as the sample for the round robin.

*Other Activities*. The Commission will promote and be actively involved in various additional activities related to the 100th year of X-ray crystallography and the International Year of Crystallography. The joint AsCA 2012–CRYSTAL28 conference, and the associated Bragg Symposium, was held in December 2012 in Adelaide, Australia, and was attended by several Commission members. In addition, Commission consultant Soichi Wakatsuki was a member of the International Science Advisory Committee.

The next International Conference on Structural Genomics (ICSG) will be held in Tsukuba, Japan, in 2013 with Soichi Wakatsuki chairing the Organizing Committee. The conference was endorsed for IUCr support by the Commission on the basis that it will include a greater component of crystallography than have recent editions of the conference, and because it will include a special session on the 100th year of X-ray crystallography.

Colin Nave and Soichi Wakatsuki were two of the organizers of the Seventh International Workshop on X-ray Radiation Damage to Biological Crystalline Samples, Diamond Light Source, UK, 14–16 March 2012 (see http://www.diamond.ac.uk/Home/Events/2012/RD7---2012.html for details).

Colin Nave represented the Commission at the IUCr Diffraction Data Deposition Working Group (DDDWG). He carried out a survey of data archiving at synchrotron sources carrying out macromolecular crystallography and submitted a report to the DDDWG.

The sixth Asia–Oceania Forum for Synchrotron Radiation Research (AOFSRR) conference was held in Bangkok, Thailand, in July 2012, after the 2011 event was cancelled owing to the Thailand floods. Commission members Richard Garrett and Shih-Lin Chang were members of the Organizing Committee. The AOFSRR is continuing its efforts to promote the use of synchrotron radiation in the Asia–Oceania region, in particular in the ASEAN (Association of South-East Asian Nations) countries, and the conference was attended by representatives of a number of ASEAN countries. In recent years Malaysia and Vietnam have been admitted as associate members of the AOFSRR; discussions are underway with Indonesia, and Professor Prayoon Songsiriritthigul of the Thailand synchrotron facility has been appointed as a special advisor to the AOFSRR President on ASEAN matters.

**R. F. Garrett**, Chair

### 4.22. Commission on XAFS

2012 involved consolidation of the achievements of the Commission (CXAFS) with the IUCr Congress, the Q2XAFS meeting and the development of Dictionary Definitions. The Q2XAFS meeting, the International Workshop on Improving Data Quality and Quantity for XAFS Experiments, co-chaired by I. Ascone (CXAFS) and H. Oyanagi [International X-ray Absorption Society (IXAS)], December 2011, was a huge success. The new third-generation synchrotron-radiation sources have enabled high-quality and high-

throughput XAFS measurements and new types of experiments. These require new standards and criteria for XAFS spectroscopy, and this was the driving force behind the Q2XAFS workshop. The aim of the workshop was to establish new standards and criteria for XAFS experiments and analyses as well as to establish a new data format, and a database for data deposition. It was attended by 71 people, including 25 from outside Japan (USA, UK, France, Italy, Germany, Canada, Australia, Korea, People's Republic of China and Thailand). The workshop was held with five oral sessions and one poster session.

Developments of the field and papers on major future initiatives have been published in the *Journal of Synchrotron Radiation* [(2012), **19**(6), 849–1066], with Guest Editor I. Ascone (CXAFS). Many of these papers will lead to significant advances for the field and community over the next few years.

The Commission supported and had visibility at the International X-ray Absorption Spectroscopy conference in Beijing, People's Republic of China, 22–28 July 2012. C. T. Chantler was the CXAFS observer at the IXAS Executive Council Meeting, a great statement of the effective relations between the two organizations and a comment on our capacity to work together to further the field. Commission members and consultants (C. T. Chantler, B. Hedman) were on the International Advisory Committee and the International Programme Committee (P. Glatzel). Commission member P. Glatzel was elected Vice-President of IXAS. A well attended Commission meeting was held at this conference. As a particular highlight, the IXAS agreed on the importance of continuing the Q2XAFS meetings to develop and define standards and reporting of structures. Another highlight was the progress on the data deposition format investigation, reported by several speakers; and a particular highlight was the announcement that the winning conference bid for the 2018 (or 2017) IXAS meeting was that of Poland, led by K. Jablonska, one of our new Commission members.

The 12th International Symposium on Radiation Physics, ISRP12, Rio de Janeiro, Brazil, 7–12 October 2012, also held a joint IUCr/CXAFS and ISRP session. A meeting was held at ISRP in Brazil, where the Commission was also able to secure funding support from the IUCr for the symposium. From the front page of the web site for the conference: 'The ISRP12 shall include a Joint Session with the International Commission on XAFS (CXAFS) from the International Union of Crystallography which links up to both XAFS and development and applications together with the fundamental physics and chemistry underlying XAFS and XANES. It will deal also with contributions from Crystallography, Data Deposition, and other areas of interest to the radiation Physics Community and IUCr'. The joint session had the following programme: XAFS and Developments for the Future. Speakers included Y. Joly on theory, J. Hester on data formats and C. T. Chantler on accuracy and opportunities. The Scientific Programme Committee included a member of the Commission (C. T. Chantler) and senior members of the IUCr. The Commission is currently preparing joint symposia and workshop proposals for the Montreal Congress, and work towards securing solid funding from the IUCr for the next Q2XAFS meeting proposed for Poland.

**C. T. Chantler**, Chair

## 5. Sub-committee on the Union Calendar

The Sub-committee receives and considers requests for IUCr sponsorship and nominal financial support, and makes recommendations to the Executive Committee. Acting on the recommendations made by the Sub-committee, during 2012 the Executive Committee approved sponsorship of various schools and meetings, mostly with financial support. Those held in 2012 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 2013, but approved in 2012, are listed below.

Biomolecular Forms and Functions: A Celebration of 50 Years of the Ramachandran Map, Bangalore, India, 8–11 January 2013.

XIV Intensive Teaching School in X-ray Structure Analysis, Durham, UK, 6–14 April 2013.

Macromolecular Crystallography School 2013: From Data Processing to Structure Refinement and Beyond, Montevideo, Uruguay, 8–16 April 2013.

RapiData 2013, Brookhaven, USA, 21–26 April 2013.

Accuracy in Powder Diffraction IV, Gaithersburg, USA, 22–25 April 2013.

The Future of Dynamic Structural Science, Erice, Italy, 30 May – 8 June 2013.

Gordon Research Conference on Electron Distribution and Chemical Bonding, Les Diablerets, Switzerland, 2–7 June 2013.

EMU School on Minerals at Nanoscale, Granada, Spain, 3–6 June 2013.

Zürich School of Crystallography – Bring Your Own Crystals, Zürich, Switzerland, 8–22 June 2013.

Dynamic Structural Photocrystallography in Chemistry and Materials Science, Buffalo, USA, 16–20 June 2013.

XX Conference of Serbian Crystallographic Society, Belgrade, Serbia, June 2013.

Resonant Elastic X-ray Scattering (REXS 13), Oxford, UK, 15–19 July 2013.

Annual Meeting of the American Crystallographic Association, Hawaii, USA, 20–24 July 2013.

International Conference on Structural Genomics 2013 – Structural Life Science, Hokkaido, Japan, 29 July – 1 August 2013.

15th International Summer School on Crystal Growth, Gdansk, Poland, 4–10 August 2013.

17th International Conference on Crystal Growth and Epitaxy (ICCGE-17), Warsaw, Poland, 11–16 August 2013.

International School on Fundamental Crystallography: Introduction to *International Tables for Crystallography* Volumes A and A1, Gjulechitza, Bulgaria, 30 September – 5 October 2013.

8th International Workshop on Bulk Nitride Superconductors 2013 (IWBNS-VIII), Kloster Seeon, Bavaria, Germany, 30 September – 5 October 2013.

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

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

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

European Crystallographic Association), the applicants for sponsorship must seek approval of the Chair of the Regional Associate Organizing Committee.

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

Explicit support from the relevant IUCr Commission(s) is required for any international meeting (except for the meetings of Regional Associates).

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

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

## 6. Committee for the Maintenance of the Crystallographic Information File Standard (COMCIFS)

COMCIFS is charged with maintaining and developing the Crystallographic Information Framework (CIF). CIF covers syntax and dictionary language standards as well as a number of dictionaries written according to these standards, and COMCIFS also develops policies on relevant data-handling issues as necessary.

*Core standards*. Work on the next-generation CIF2 syntax and DDL3 dictionary language has shifted from development of the standards to implementation. This year three important papers were published describing (i) an enhanced STAR syntax, (ii) a new DDLm dictionary language and (iii) the dREL methods language, which allows the relationships between data items to be expressed algorithmically such that unknown values can be automatically derived from known values of other items. Given that COMCIFS' CIF2 and DDL3 development efforts were based on previous drafts of this material, the final forms of the standards adopted by COMCIFS are likely to be close to those outlined in these papers.

The IUCr Executive Committee agreed to fund development of a browser-based Javascript package that is able to read arbitrary DDLm dictionaries including derivation of unknown data item values using dREL methods. In accordance with a resolution at the Madrid Congress, this package will be initially tested at the IUCr offices in order to verify both the software and the practicality of the standards on which it is based. This software is on schedule for public release in mid-2013.

*Dictionaries*. The twinning dictionary is unfortunately still not in final form, with a draft version at an advanced stage. A materials properties dictionary has been independently developed and its relationship to IUCr-sponsored dictionaries is being clarified as part of the namespace policy described below.

*Policies*. Another initiative arising out of the Madrid Congress was development of a namespace mechanism for CIF dictionaries. By the end of 2012 a consensus appeared to have been reached on a way to allow other scientific disciplines to use CIF technologies while shielding IUCr users from potentially ambiguous data names. An allied policy has been developed to handle COMCIFS' relationship with dictionaries produced by third parties. While such dictionary work is very welcome, some simple guidelines are needed to ensure that data definitions are consistent, unambiguous and accessible both now and in the future.

The increasing use of formal data-transfer frameworks in science is creating pressure for CIF to interoperate with ontologies produced by neighbouring disciplines. NeXus is an important data framework increasingly used for data archiving at large-scale facilities. Promising progress has been made toward establishing a cooperative relationship between the NeXus effort and CIF. In September 2012 H. J. Bernstein joined the NeXus International Advisory Committee (NIAC) as a COMCIFS representative and discussions are underway for a meeting between NIAC and COMCIFS in summer 2013. In collaboration with BNL and DLS, Professor Bernstein is working on a preliminary proof-of-concept implementation of integrated software for CBF/imgCIF, NeXus and HDF5, with an integrated ontology.

A list of requirements for a standard CIF API was also produced early in the year. At present, it is not clear whether adoption of an existing CIF programming library or creation of a completely new library is the most effective way to meet these requirements.

Looking forward, the Executive Committee approved two Diffraction Data Deposition Working Group recommendations in late 2012. The second recommendation charges IUCr Commissions with defining metadata relevant to their fields. COMCIFS, with its experience in data handling and metadata, is well placed to provide IUCr Commissions with help in meeting this objective.

*Membership*. Ralf Grosse-Kunstleve resigned from COMCIFS voting membership midway through the year as part of his move to new employment outside crystallography. His thoughtful contributions to discussions will be missed.

**J. Hester**, Chair

## 7. *IUCr Newsletter*

All issues of Volume 20 were 24 pages in length. As in previous years, the content covered topics such as activities of the IUCr, its Regional Associates and Commissions, Letters to the Editor, news concerning crystallographers and crystallography in general, awards, election results, resources, meeting reports, book reviews, future meeting announcements, and a general meeting calendar.

Each issue carried a President's column written by Gautam Desiraju. Editorial responsibilities were shared by Bill Duax and Judy Flippen-Anderson. Patti Potter was responsible for layout and all phases of production and distribution.

Each issue devoted at least two pages to brief summaries of selected articles recently published in IUCr journals. Issues 1 and 2 contained reports on the Madrid Congress. Issues 3 and 4 contained

reports on annual meetings of two of the three Regional Associates (ECM and ACA).

Additional meeting and workshop reports were published covering activities in Argentina, Australia, Canada, Croatia, Cuba, Germany, Hungary, India, Italy, Slovenia, the UK and the USA. Future meeting announcements included the Montreal Congress as well as meetings in Austria, India, Italy and the USA.

Distribution was carried out electronically for all four issues. Messages were sent to approximately 11 200 people for the electronic version. Print copies went to 558 libraries and individuals, and copies were sent to several meetings, including the annual meetings of the Regional Associates.

**W. L. Duax** and **J. L. Flippen-Anderson**, Editors, **P. Coley**, Production Manager

## 8. IUCr/Oxford University Press (OUP) Book Series

Because of an accidental fluctuation between two highly productive years (four books published in 2011, and four scheduled for 2013), the cooperation between Oxford University Press (OUP) and the IUCr/OUP Book Series Selection Committee did not produce any new book in 2012.

The four new books for 2013 are in the final stages of the production phase and others are in the pipeline. The Committee and the OUP editing staff reviewed a number of proposals and there are well established contacts with authors about possible new volumes.

The Committee is very interested in proposals for new volumes and encourages prospective authors to contact the Chair of the Committee (davide.viterbo@mfn.unipmn.it). 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.

**D. Viterbo**, Chair of Book Series Selection Committee

## 9. Regional Associates and Scientific Associates

### 9.1. American Crystallographic Association (ACA)

The 2012 ACA Council consisted of George Phillips (President), Cheryl Stevens (Vice-President), Tom Koetzle (Past-President), S. N. Rao (Chief Financial Officer and Interim Treasurer), Patrick Loll (Secretary) and Jamaine Davis (*ex officio*, YSSIG representative). David Rose served as the Canadian Representative, Bill Duax as Chief Executive Officer and Marvin Hackert as IUCr Representative. The paid membership of the ACA continued its recent decline, with about 1628 paid members by fall of 2012 compared to about 1700 paid members in the fall of 2011 and 1840 paid members at the end of 2010.

*ACA Boston*. The highlight of the year was the ACA Annual Meeting where 783 attendees met in Boston from 28 July – 1 August 2012. The Programme Chairs for this meeting were Bruce Foxman and Bruce Noll, with Peter Mueller serving as Local Chair and Ilia Guzei as Poster Chair. The Boston meeting featured a shorter four-day format with scientific sessions running from Sunday through Wednesday. In addition, four workshops were held: Refmac/Coot, organized by Paul Emsley and Garib Murshudow; OLEX2, organized by Ilia Guzei; Refinement of Nanoparticle Structures, organized by Thomas Proffen, Katherine Page and Reinhard Neder; and an outreach workshop for area K-12 teachers on Crystallography: World of Wonders, organized by Cora Lind and Claudia Rawn. The conference also featured an ACA Transactions Symposium in honour of Bruce Foxman and his 70th birthday on Transformations and Structural Oddities in Molecular Crystals, organized by Kraig Wheeler, Michael Hickey and Graciela de Delgado.

Five of the ACA's major awards were presented at the Boston meeting. The Buerger Award went to John Spence of Arizona State who spoke on The Future of Diffraction Physics in Crystallography, the Warren Award went to Paul Fenter of Argonne for his work on liquid–solid interfaces, the Supper Instrumentation Award was given to Ron Hamlin of ADSC for his efforts to advance the development of area detectors, the Etter Early Career Award to Emmanuel Skordalakes of the Wistar Institute and the University of Pennsylvania for his work on the structure of telomerase, and Daniel Nocera received the Elizabeth Wood Award for bringing science to the attention of a wider audience. His award was made in 2011, but he delivered his talk at the banquet in Boston.

A number of talks in Boston reflected on the history of crystallography, which was particularly appropriate since the UN had approved designating 2014 as the International Year of Crystallography earlier that month. Don Casper gave a Plenary Lecture on The History of Structural Biology, Jenny Glusker, Fox Chase Cancer Centre, reflected on 100 Years of Structure Determination, Sue Byram, Bruker AXS, described the Evolution of Small Molecule Crystallographic Instrumentation in North America, and Ron Hamlin Supper Award address: 2-D X-ray Detectors – What Do We Really Want and How Can We Build It? covered the development of X-ray detectors from film to the modern pixel-array detectors used today.

The ACA Council announced a number of important actions in 2012:

*Latin American Division*. The ACA Council suggested a change in its By-Laws to add Latin America to the areas authorized to form a 'national' division. Members in attendance at the business meeting supported the suggested By-Law change, paving the way for a formal vote by the full membership. Latin America would then have a member on the ACA Council in a manner similar to Canada.

*Strategic Planning*. The ACA Council has undertaken a strategic planning process. Members of this task force include Cheryl Stevens, George Phillips, S. N. Rao, Bill Duax and Judith Flippen-Anderson.

*Fellows*. The 2012 class of ACA fellows, whose names were announced at the banquet during the Boston meeting, include Donald Caspar, Dick Marsh, Virginia Pett, Jane Richardson and Thomas Terwilliger.

*New Journal*. The ACA is proposing to publish a new, online-only journal in partnership with the American Institute of Physics (AIP). The AIP, of which the ACA is a member society, would be responsible for the production side of the journal while the ACA would maintain full editorial control. The tentative title is S*tructure, Dynamics, and Kinetics*. [Note: the new journal was approved in 2013 with the name *Structural Dynamics*.]

*Summer Schools*. The ACA Council had approved a bid by Notre Dame and Northwestern to host the ACA Summer Course in Small Molecule Crystallography for the period 2012–2015. The next course will be given in June 2013 at Northwestern and organized by Amy Sarjeant and Charlotte Stern (Northwestern) and Allen Oliver (Notre Dame). No ACA course in macromolecular crystallography is currently approved, but it was noted that there are other macromolecular workshops that fill much of this void.

*Poster Prizes*. The ACA Council has decided to rename two of the ACA Pauling Poster Prize Awards to recognize the contributions of two highly respected crystallographers. The Pauling–Branson Award

recognizes the contributions of Herman Russell Branson, (1914–1995), one of the first African American physicists to make crystallography the focus of his research. The Pauling–Sundaralingam Award recognizes the ground-breaking crystallographic research on the stereochemistry of nucleotides and nucleic acids carried out by Muttaiya Sundaralingam (1931–2004).

*Future Meetings*. Upcoming ACA Annual Meetings include 2013 in Honolulu (20–24 July) with Jeanette Krause and Allen Oliver as Programme Chairs. The 2013 Award winners are Thomas Terwilliger (Ken Trueblood Award), Richard Dickerson (Isadore Fankuchen Award), Tom Koetzle (Robert Bau Award) and Eric Ortlund (Margaret Etter Award). The 2014 ACA meeting will be in Albuquerque, New Mexico, 24–28 May.

*Elections*. The fall 2012 elections results are Martha Teeter (Vice-President), James Kaduk (Treasurer), Graciela de Delgado (Communications), Kraig Wheeler (Continuing Education), Tom Terwilliger (Data, Standards and Computing Committee), plus new Chairs elected to head the 12 SIGs.

On a sad note, the ACA lost a number of outstanding members during 2012, including David Sayre (2 March 1924 – 23 February 2012) who won the 2008 Ewald Prize, R(obert) A(lan) 'Ray' Young (24 January 1921 – 13 June 2012), Hugo Steinfink (22 May 1924 – 25 August 2012), Louise Johnson (26 September 1940 – 25 September 2012) and Guy Dodson (13 January 1937 – 24 December 2012).

**M. L. Hackert**, IUCr Representative

### 9.2. Asian Crystallographic Association (AsCA)

AsCA Executive Committee Officers for the 2010–2013 term are: President, Se Won Suh (Korea); Past President, J. M. Guss (Australia); Vice-President, P. Chakrabarti (India); Secretary-Treasurer, A. Vrielink (Australia).

*Financial Report*. The trustees of AsCA are Professors M. A. Spackman, A. Vrielink and C. Bond at the University of Western Australia. All the funds are currently held as interest-bearing cash deposits in Australian dollars. The total funds as of March 2013 are AUD 176 404.80. The healthy financial situation permits the continuation of the support of early career researchers from developing countries to attend AsCA meetings.

*Meetings*. In the past the major (triennial) AsCA meetings have been held in a country without a large domestic crystallographic community with a view to fostering the development of crystallography throughout the Asian region. AsCA does not normally hold meetings in years with an IUCr Congress. The full AsCA calendar therefore runs as follows: Full AsCA meeting (2010) – IUCr Congress (2011) – Joint AsCA/local meeting (2012).

The most important activity of AsCA in 2012 was the joint AsCA'12/CRYSTAL-28 Conference, which was held in the Adelaide Convention Centre, Adelaide, Australia, 2–5 December 2012. A total of 456 delegates from 25 countries attended the meeting. There were 96 oral and 247 poster presentations. The talks were of a very high standard, equal or better than other international meetings of this kind. Three Plenary speakers were Professors Wayne Hendrickson, Xiao-Ming Chen and Henry Chapman. Professor Hendrickson, who played a key part in the development of protein crystallography, spoke of recent developments in methods of single anomalous dispersion phasing for macromolecular structures. Professor Chen presented data on metallo-organic lattices that have been engineered to selectively absorb compounds and gases. Professor Chapman presented the latest results from X-ray free-electron laser experiments on protein crystals. Three Keynote speakers, Professors Ringer, Welberry and Cole, addressed the state of the art in solid solutions, optoelectronics and diffuse scattering, respectively. AsCA thanks the efforts of Professor Ray Withers and the SCANZ Council, the International Science Advisory Committee led by Dr Jose Varghese, and the Local Organizing Committee (LOC) led by Professor John Carver.

Immediately following the AsCA'12/CRYSTAL-28 Conference, the Bragg Centennial Symposium was held on 6 December 2012 at the University of Adelaide to pay tribute to Lawrence Bragg and his father William Henry Bragg, who made pioneering and far-reaching contributions to the development of X-ray crystallography. A total of 333 delegates from 22 countries attended the symposium. William Henry Bragg was the Elder Professor of Mathematics at the University of Adelaide. William Lawrence Bragg was born in Adelaide and received his first degree from the University of Adelaide. November 2012 marked the centenary of the presentation of Lawrence Bragg's paper to the Cambridge Philosophical Society that defined his eponymous equation. The symposium speakers included Mrs Patience Thomson (younger daughter of Sir Lawrence Bragg), Dr John Jenkin (La Trobe University), Professor Anthony Kelly (University of Cambridge), Professor Brian Matthews (University of Oregon), Professor Anders Liljas (Lund University), Dr Thom Mason (Oak Ridge National Laboratory), Professor Colin Humphreys (University of Cambridge), Professor John Spence (University of California, Berkeley), Professor Wayne Hendrickson (Columbia University), Professor Tony Cheetham (University of Cambridge), Professor Jenny Martin (University of Queensland), and Professor Anthony Klein (University of Melbourne). Many Bragg-related papers presented at the Symposium have been published in January 2013 in the special Bragg Centennial issue of *Acta Crystallographica* Section A. AsCA thanks the efforts of Professor Steve Wilkins for organizing such a memorable symposium. [Steve Wilkins passed away suddenly on 25 March 2013. He will be sadly missed by the AsCA community.]

*AsCA 2013*. The venue for the 12th Conference of AsCA (AsCA 2013) was finalized by the AsCA Council Meeting in Madrid, Spain, in August 2011. AsCA 2013 will be held in Dhaka, Bangladesh, 1–4 December 2013. Professor Altaf Hussain is the Chair of the LOC and Dr Takashi Kamiyama is the Chair of the International Programme Committee. [A subsequent decision of the AsCA Council rescheduled this meeting. It is now due to be held in Hong Kong, 7–10 December 2013.]

*AsCA 2015*. The venue for the 13th Conference of AsCA (AsCA 2015) was finalized by the AsCA Council Meeting in Adelaide, Australia, in December 2012. AsCA 2015 will be held in Kolkatta, India, toward the end of November 2015. Pinak Chakrabarti is the Chair of the LOC and Alice Vrielink is the Chair of the International Programme Committee (IPC).

*AsCA 2016*. The venue for the 14th Conference of AsCA (AsCA 2016) will be finalized by the AsCA Council Meeting in December 2013. Representatives of Vietnam, New Zealand and Singapore expressed their interests to host AsCA 2016 in the AsCA Council Meeting in Adelaide in December 2012.

*Memberships*. In the AsCA Council Meeting in Adelaide in December 2012, six membership categories were introduced to the new AsCA Constitution as Category A (1 councilor with no vote), Category B (1 councilor with 1 vote), Category C (2 councilors with 2 votes), Category D (3 councilors with 3 votes), Category E (4 councilors with 4 votes), and Corporate/Affiliation (1 councilor with no vote). Border countries/regions keen to participate in the AsCA Council are welcome to join as Category A members.

*IYCr*. Professor Sydney Hall is organizing a detailed recording of the history of AsCA. Anyone wishing to contribute any information on AsCA's history should send details to Professor Hall. The report will be ready in the summer of 2014 to celebrate the IYCr.

**J. M. Guss**, IUCr Representative

### 9.3. European Crystallographic Association (ECA)

The link between the IUCr and the ECA is functioning well. The IUCr Representative is on the mailing list of the ECA Executive Committee. She attends on a regular basis the sessions of the ECA Council and of the ECA Executive Committee, and was a member of the Programme Committee of the two ECMs – Bergen, Norway, in 2012 and Warwick, UK, in 2013.

In 2012 the membership of the ECA Executive Committee was changed according to the regular rotation. The membership has a good country–gender–research-field balance. Every member of the Executive Committee has a well defined scope of duties and responsibilities and the work is very well organized. The spirit is highly democratic. Very good continuity is ensured by preserving some co-opted members from the previous term to share their experience. The present President of the ECA is Andreas Roodt (South Africa), the Vice-President Alessia Bacchi (Italy) and the Immediate Past President Santiago Garcia-Granda (Spain). The Secretary is Georgina Rosair (UK), the Treasurer Christian W. Lehmann (Germany) and the officers Udo Heinemann (Germany), Joke Hadermann (Belgium), Olga Yakubovich (Russia), Fermín Otalora (Education Coordinator, Spain) and Paolo Scardi (EPDIC Representative, Italy). Co-opted members from the previous term are Petra Bombicz (former Secretary, Hungary) and Radomir Kuzel (former Treasurer, Czech Republic).

The ECA successfully organizes many events, the annual ECMs being the most important. The ECMs in Bergen in 2012 and in Warwick in 2013 were very successful, and both related to the forthcoming IYCr. Very interesting special events, lectures and exhibitions were organized both in Bergen and in Warwick. Details can be found at the sites of both meetings (links from the ECA site).

As very interesting initiatives one can mention the organization of the two new General Interest Groups – GIG1 (Young Crystallographers) and GIG2 (Senior Crystallographers). The first has been in existence for a few years, is very active and has already organized several interesting events, including special Microsymposia at the ECM. The second is just starting, but the start is promising. An important initiative of the ECA is that not only young researchers, but also senior crystallographers if retired can register with a reduced registration fee at the ECM.

The ECA does a lot to encourage individual memberships and to encourage new countries to join the ECA. Olga Yakubovich is the officer responsible for this activity.

One should mention very high educational activity within the ECA. There are many annual schools and advanced study courses throughout Europe and outside it organized by the ECA. Special Microsymposia on teaching crystallography take place at the ECM, and are very well attended. Among others, one should mention a new initiative – the First European Crystallography School (ECS1) (28 August – 6 September 2014, Pavia, Italy). ECS1 is directed to young researchers and PhD students involved in all fields of structural science, and aims at diffusing and sharing the idea of crystallography as a unique discipline. The school will include lectures and practical sessions, as well as dissemination seminars open to the public, in order to increase the awareness and ignite an interest in crystallography among young students. Moreover, a series of satellite events will be organized to celebrate IYCr2014.

The ECA is also very active and successful in providing electronic platforms for disseminating information on various types of activity related to crystallography in general and the IYCr in particular. They can be well used by all the the IUCr community. Santiago Garcia-Granda is the contact person.

**E. Boldyreva**, IUCr Representative

### 9.4. International Organization for Crystal Growth (IOCG)

No formal meeting of the IOCG (http://www.iocg.org/) was planned or organized in 2012.

The IOCG President for 2010–2013 is R. Fornari (Germany), with Co-Vice-Presidents T. F. Kuech (USA) and E. Vlieg (The Netherlands); the Secretary is K. Kakimoto (Japan), and Treasurer V. Fratello (USA). The other members of the Executive Committee are H. Dabkowska (Canada), J. Derby (USA), T. Duffar (France), J. M. García-Ruiz (Spain), Y. Mori (Japan), K. Roberts (UK), P. Rudolph (Germany) and A. Voloshin (Russia).

The connection with the Commission on Crystal Growth and Characterization of Materials (CCGCM) is evident, as T. F. Kuech (USA), K. Kakimoto (Japan), T. Duffar (France), and J. M. García-Ruiz are also members/consultants of CCGCM.

At the end of 2010 the European Network of Crystal Growth (ENCG) was constituted. Part of the scope of ENCG is the organization of a European Conference on Crystal Growth (ECCG).

ECCG4 was held in Glasgow, UK, 17–20 June 2012, chaired by Kevin Roberts. This was an important event with more than 250 participants. Many members/consultants of CCGCM were involved in the organization of this conference.

The 17th International Conference on Crystal Growth and Epitaxy (ICCGE-17) will be held in Warsaw, Poland, 11–16 August 2013 [Chairs Stanislaw Krukowski (Poland), Roberto Fornari (Germany)]. Members and consultants of CCGCM are strongly involved in the work of the Programme and Advisory Committees of this meeting.

Moreover, for the first time, three symposia will be co-organized by members/consultants of CCGCM as IUCr representatives:

A. Moreno will co-chair symposium G03: Biological and Biogenic Crystallization;

K. Byrappa will co-chair G04: Industrial Crystallization;

T. Duffar will co-chair G07: Defect Formation/Elimination.

The 15th International School on Crystal Growth will be held in Gdansk, Poland, 4–10 August 2013, and will be chaired by Wojciech Sadowski and Ewa Talik, who is also a member of CCGCM.

Detailed information about both the conference and the school will be posted on the respective web sites (http://science24.com/event/iccge17/, http://www.ptwk.org.pl/pol/documents/ISSCG-15-1.pdf).

The next General Assembly of the IOCG will take place in Warsaw, Poland, during ICCGE-17.

**A. Zappettini**, IUCr Representative

### 9.5. International Centre for Diffraction Data

The Commission on Powder Diffraction maintains close links with the ICCD and also with the International X-ray Absorption Society (IXAS) (http://www.ixasportal.net/ixas/).

**P. Whitfield**, IUCr Representative

## 10. Representatives on Other Bodies

### 10.1. IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols (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. In 2012, there were none of specific interest for crystallography.

The following Technical Reports and Recommendations have been reviewed by referees chosen among IUCr members:

*Polymer Glossary*;

*Terminology of Polymers*.

**A. Authier**, IUCr Representative

### 10.2. 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. ICSTI increasingly liaises with CODATA concerning conferences and workshops, for example.

The winter ICSTI Workshop on Delivering Data in Science was organized by DataCite and held at ICSU, Paris, France, in February 2012. A detailed report on the Workshop by J. R. Helliwell and B. McMahon was published on the IUCr web site and in the IUPAC publication *Chemistry International* (http://www.iupac.org/publications/ci/2012/3404/cc1_050312.html).

The ICSTI Annual Congress and ICSTI Business Meetings for 2012 were held in Washington DC, USA, in October. The Congress was hosted by the USA National Library of Congress and was entitled Science, Law and Ethics (http://www.icstiannual.com/meeting-program/). The Congress focused on the importance of counterbalancing science, ethics and the law to ensure the healthy development of scientific innovation, globalized information sharing and technological advancement. The Congress was hosted by the Library of Congress, and featured research scientists, information scientists, lawyers, diplomats and other experts, who each provided the attendees with unique perspectives on the intersection of science, ethics and the law in today's global society. This was followed by a Workshop organized by Elsevier entitled Research Evaluation in Practice: Towards Sustainable Scientific Investments (see http://www.researchtrends.com/research-trends-seminar/). This focused on assessing research. Numbers of publications feature in some countries' research assessments; the impact of 'author pays' in an exclusively 'Open Access (for readers) publications era', namely that authors may not have funds to pay for publication of all of their research results, would impact on this and came out in the open discussion initiated by J. R. Helliwell.

The highlights of the ICSTI business meetings in Washington DC included:

(1) *The Living Publication* published in *ICSTI Insight*, authored by J. R. Helliwell, B. McMahon and T. Terwilliger, was highly praised by the ICSTI Executive Secretary Tony Llewellyn: 'the best *Insight* article ICSTI has ever had'.

(2) Achieving a break-even budget and projection for the next year for ICSTI.

(3) The tabling of a draft ICSTI risks analysis by the ICSTI Executive Secretary.

(4) The next Winter Workshop was confirmed as being in Hannover, Germany, 18–19 March 2013, and would be entitled Strategies for Non-Textual Information.

(5) At the Technical Activities Coordinating Committee (TACC) the topic of cloud data storage was covered in the talk from Microsoft.

The highlights of the Congress in Washington DC included:

(1) The views of science ethics presented by various research funding agencies in the USA [NIH (National Institutes for Health)], the European Community and Thailand.

(2) A presentation from the current Chair of CrossRef, Professor Linda Beebe, on the importance of linking data to literature.

(3) An update on the impressive WorldWide Science Alliance search tools now extended to various databases as well as allowing multilingual translation of queries and outputs.

Stimulated by the Research Council's UK (RCUK) Finch Committee Report into Open Access (see http://www.researchinfonet.org/publish/finch/), J. R. Helliwell initiated discussions within the ICSTI Executive Committee in Washington DC and then through the year by e-mail into one of the main recommendations of this Report – that 'Gold Open Access' was the 'strategic imperative' for the future of publications derived from publicly funded UK research. A major concern of this approach's focus voiced by J. R. Helliwell was the prospect of a policy shift from reader-pays subscriptions and hybrid open access to a system based on authors paying article processing charges (APCs). It is notable that, for example, the USA NIH does not show preference for Gold *versus* Green Open Access but accepts both for publications derived from its funding. In Professor Helliwell's view a core difficulty would arise in a completely Gold Open Access model for researchers firstly from those parts of the world with limited research funds and secondly for the unfunded work of researchers in the developed world. The average APC for journals seems to be around GBP 1500 per publication. Such APC fees for authors are indeed a widely recognized challenge and thus a policy of APC waivers for authors is often deemed essential.

J. R. Helliwell acknowledges with gratitude the close collaboration with IUCr's delegate to CODATA, Brian McMahon, and also with the IUCr Journals Managing Editor, Peter Strickland.

**J. R. Helliwell**, IUCr Representative

### 10.3. International Council for Science (ICSU)

There were no ICSU meetings with Union representation during 2012. An ICSU meeting for representatives of the Unions will be held in Paris, France, in April 2013. ICSU's strategic plan 2012–2017 (http://www.icsu.org/publications/reports-and-reviews/icsu-strategic-plan-2012-2017) was approved at the ICSU General Assembly held in Rome, Italy, in September 2011, which also elected Noble-Prize-winning chemist Professor Yuan Tseh Lee from Taipei as the new President of ICSU. Implementation of the Strategic Plan 2012–2017 was initiated during 2012. Strengthening the contacts with Union members is a component of the Strategic Plan in which environmental issues play a central role. The Strategic Plan also addresses the Universality of Science, which is of relevance for the IUCr.

**S. Larsen**, IUCr Representative

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

The major event for CODATA during 2012 was the biennial conference and General Assembly held in Taipei, 28 October – 2 November 2012. Both IUCr Representatives, B. McMahon (BM, outgoing) and J. R. Helliwell (JRH, incoming) attended.

*CODATA Conference*. The theme of the 23rd International CODATA Conference was Open Data and Information for a Changing Planet, with Keynote Lectures on Climate Change, Disaster Risk Evaluation and Open Data Access in Science. Plans within particle physics to use cloud storage for very large data sets (petabytes per year) are relevant to synchrotron X-ray facilities as a way to assist future inter-facility collaboration as well as access by users to their data. Sessions on access to data from the literature showed that several science disciplines are only now organizing such access, a practice which has been long established in crystallographic publishing. Panel discussion topics included Open Data Access and Ethics in Data. A new session at this CODATA conference featured Early Career Scientists.

IUCr was actively involved in two Data Mining Microsymposia sessions. JRH presented a talk, co-authored with BM, on Data Archiving in Crystallography and the Activities of the IUCr Diffraction Data Deposition Working Group. The second session was Chaired by JRH. Two talks were presented, and an impromptu panel discussion was convened to discuss various current perspectives on data mining. Scientific data and medical data featured in inputs from the audience as well as the perceived need for incentives for scientists to link data to their publications more than is currently practised.

Both IUCr Representatives participated in the sessions organized by the CODATA–ICSTI Task Group on Data Citation Standards and Practices (of which BM is a member). The Task Group will publish in early 2013 a report surveying current practices, and developing advocacy for closer integration between data deposition and the published literature.

A full meeting report is available at http://www.iucr.org/resources/data/meeting-reports/codata-2012.

*General Assembly*. There was a progress report by K. Ravio (ICSU Vice-President, Finland) of the ICSU review of CODATA, part of a regular review and evaluation process for ICSU's component and affiliate bodies.

The CODATA Strategic Plan 2013 to 2018 was reviewed by the General Assembly delegates and will be finalized by the Executive. A significant development was the recommendation to allow at-large (*i.e.* individual) members. Two new country members were approved (Finland and Mongolia).

The recently established (2011) Nanomaterials Standards collaborative project with ICSU, ISO and OECD was reported on and is chaired by John Rumble, formerly of NIST and past CODATA President.

A Working Group for Early Career Scientists was established for two years to help structure their work towards the establishment of a more permanent group.

The *Data Science Journal* is being reviewed, including possible links to a commercial publisher; the preferred funding model was 'Green Open Access' so as to retain the flexibility of reader or author payments, rather than 'Gold' with its restriction to author-only fees payment.

There was a resolution to investigate the use of an Open Knowledge Environment to promote the communication of CODATA's activities to the membership and world at large. The 2014 CODATA Conference was approved to be in New Delhi, India, in late October.

The General Assembly appoints or re-confirms Task Groups and Working Groups to further the objectives of CODATA. The Task Groups approved by the 28th General Assembly for 2012–2014 are as follows (those marked with an asterisk are continuations of existing Task Groups):

Advancing Informatics for Microbiology;
Anthropometric Data and Engineering*;
Data at Risk*;
Data Citation Standards and Practices*;
Earth and Space Science Data Interoperability*;
Exchangeable Materials Data Representation to Support Scientific Research and Education*;
Fundamental Constants*;
Global Information Commons for Science – GICSI/EU*;
Global Roads Data Development*;
Linked Open Data for Global Disaster Risk Research;
Octopus: Mining Space and Terrestrial Data for Improved Weather, Climate and Agricultural Predictions;
Preservation of and Access to Scientific and Technical Data in Developing Countries*.

The Officers of CODATA (terms of office in parentheses) are: President: Huadong Guo (People's Republic of China; 2010–2014); Vice-Presidents: Takashi Gojobori (Japan; 2010–2014), Fedor Kuznetsov (Russia; 2010–2014); Secretary General: Sara Graves (USA; 2012–2016); Treasurer: John Broome (Canada; 2012–2016). Ordinary Members of the Executive Board are listed on the CODATA web site at http://www.codata.org.

The 2012 CODATA Prize was awarded to Michael F. Goodchild, Emeritus Professor of Geography at the University of California, Santa Barbara, USA, for his outstanding achievements in geo-information science.

*Other activities*. An ICSU–CODATA Workshop on Description of Nanomaterials took place in Paris, France, 23–24 February 2012. It considered the development of systems for describing materials on the nanoscale. Present were representatives of International Scientific Unions (Reinhard Neder for IUCr), ISO Technical Committee 229 on Nanotechnology, industry, government, academia and the OECD. Since the workshop, a joint CODATA/VAMAS (Versailles Project on Advanced Materials and Standards) working group has been established to develop a White Paper setting out requirements for a description system for materials at the nanoscale, based on the needs of all scientific and technical disciplines. JRH will represent the IUCr on this Working Group.

A number of collaborative activities took place involving CODATA and the ICSU World Data System (WDS): joint sessions were organized at the International Conference on Planet Under Pressure, London, UK, March 2012, and within the framework of the Forum on Science, Technology and Innovation for Sustainable Development, 11–15 June 2012, in anticipation of the Rio+20 Summit.

CODATA is also actively seeking collaboration within the ICSU 'Future Earth' initiative for global sustainability, and continues to work to strengthen collaboration with GEOSS, the Global Earth Observation System of Systems.

A history of the first 45 years of CODATA, written by Gordon Wood and David Lide, was published and distributed at the General Assembly. This documents the continuous presence of IUCr throughout the whole period.

**J. R. Helliwell**, IUCr Representative, and **B. McMahon**, outgoing IUCr Representative

**Table 1**
Income and Expenditure Account (in Swiss Francs) for the year ended 31 December 2012.

| | 2012 | | *2011* | |
|---|---|---|---|---|
| **Income** | | | | |
| Membership subscriptions | | 164 497 | | *165 106* |
| Sales | | | | |
| Journals, back numbers and single issues | 3 517 553 | | *3 574 108* | |
| Books | 170 232 | | *124 251* | |
| Open Access Grant | 4 883 | 3 692 668 | *4 883* | *3 703 242* |
| Investment income | | | | |
| Income from investments | 73 387 | | *73 673* | |
| Bank interest | 1 164 | | *9711 123* | |
| Profit on disposal | 25 475 | 100 026 | — | *74 796* |
| Other income | | | | |
| Royalties and copyright fees | 8 641 | | *6 721* | |
| Advertising income | 203 806 | | *171 103* | |
| STAR/CIF income | 6 845 | 219 292 | *15 087* | *192 911* |
| **Total income** | | 4 176 483 | | *4 136 055* |
| **Expenditure** | | | | |
| Journals | | | | |
| Publication costs | 540 815 | | *527 215* | |
| Editorial expenses | 240 742 | | *276 231* | |
| Technical editing | 1 317 250 | | *1 265 121* | |
| Subscription administration | 108 212 | 2 207 019 | *104 225* | *2 172 792* |
| Books | | | | |
| Publication costs | 29 576 | | *37 183* | |
| Editorial expenses | 44 439 | | *33 211* | |
| Technical editing | 80 250 | 154 265 | *76 863* | *147 257* |
| *Newsletter* | | | | |
| Publication costs | 18 304 | | *86 614* | |
| Editorial expenses | 104 367 | 122 671 | *92 359* | *178 973* |
| President's Fund and other Grants and Young Scientists' support | | 188 160 | | *123 179* |
| General Assembly and Congress costs | | 30 646 | | *153 105* |
| Committee meetings and expenses | | 134 005 | | *92 922* |
| Publications and journals development | | | | |
| General | 531 979 | | *483 178* | |
| Editors' meetings | — | | *7 699* | |
| Promotion | 145 640 | 677 619 | *182 705* | *673 582* |
| Subscriptions paid | | 3 901 | | *14 219* |
| Visiting Professorship Programme | | 6 211 | | *12 542* |
| Administration expenses: | | | | |
| Honorarium to General Secretary and Treasurer | 7 683 | | *9 614* | |
| Audit and accountancy charges | 58 962 | | *56 575* | |
| Legal and professional fees | 5 297 | | *7 975* | |
| Travelling expenses | 13 203 | | *14 864* | |
| Bank charges | 6 880 | 92 025 | *5 759* | *94 787* |
| Executive Secretary's office: | | | | |
| Salaries and expenses | 265 221 | | *289 389* | |
| Travel expenses of IUCr Representatives on other bodies | 10 603 | | *5 979* | |
| Commission expenses | — | | *1 226* | |
| Sponsorship of meetings | 4 884 | | *7 612* | |
| IUCr/FIZ agreement | (16 252) | | (*15 457*) | |
| Bad debts | 811 | 265 267 | (*7 4989*) | *296 247* |
| Depreciation | | 29 795 | | *36 496* |
| **Total expenditure** | | 3 911 584 | | *3 996 101* |

**Table 1 (continued)**

| | 2012 | | *2011* | |
|---|---|---|---|---|
| *Surplus of income over expenditure (before realized exchange losses)* | | 264 899 | | *139 954* |
| Realized fluctuations in rates of exchange | | | | |
| Exchange movement on trading activities | | 72 597 | | (*71 566*) |
| Surplus/(deficit) of income over expenditure (after realized exchange losses) | | 337 496 | | *68 388* |
| Movement in market value of investments in year | | 24 999 | | (*53 250*) |
| | | 362 495 | | *15 138* |
| Unrealized fluctuation in rates of exchange | | | | |
| Exchange movement on trading activities | 10 765 | | *42 868* | |
| Investment activities | (13 102) | (2 337) | (*14 608*) | *28 260* |
| Total recognized gains/(losses) relating to the year | | 360 158 | | *43 398* |
| **Opening fund accounts at 1 January 2012** | | 4 702 120 | | *4 658 722* |
| **Closing fund accounts at 31 December 2012** | | 5 062 278 | | *4 702 120* |

All the income and expenditure related to continuing activities. Historic cost results would only differ from above by the profit on sale of investments. Separate Statements of Total Recognized Gains and Losses and Reconciliation of Movements in the Fund Account are not given, as the information is incorporated in the above.

### 10.5. 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 the creation of national and international organizations and specialist working groups.

COSPAR acts mainly as a body responsible for organizing biennial Scientific Assemblies, and the 39th COSPAR Assembly was held in Mysore, India, 14 June – 2 July 2012. 3489 abstracts were submitted (4488 in Bremen, 3780 in Montreal) with over 1500 pre-registered participants, including 238 supported participants. Dr Hermsen reviewed the budget update for COSPAR for 2012, noting continued projections for a satisfactory financial position for the next year.

The previous (38th) COSPAR Assembly was in Bremen, Germany, 18–25 July 2010, and the next will be held in Moscow, Russia, 2–10 August 2014.

The International Year of Crystallography (IYCr) could provide an opportunity for stronger collaboration between IUCr and COSPAR. At the Mysore Assembly, I submitted the information to the COSPAR Council about the (just announced) IYCr. As I was not present in person, Dr Valentina Shevtsova, the Chair of COSPAR's Scientific Commission on Materials Science in Space (MSS, Commission G) acted on my behalf. A more detailed summary of IYCr activities will be presented in Moscow in 2014, the actual IYCr. I am also planning to submit information about IYCr for publication in *Space Research Today*.

Most COSPAR activities are related to space topics (astronomy, astrobiology, geophysics, atmosphere studies, investigation of natural and artificial ecosystems, as well as space travel). The most interesting activity of COSPAR for the IUCr is the Scientific Commission on Materials Science in Space (MSS Commission G), chaired by V. Shevtsova (Belgium) and co-chaired by S. Amiroudine (France) and S. Yoda (Japan). This Commission coordinates fundamental experiments in materials and fluid sciences performed in space, utilizing reduced gravity for their objectives. This approach helps to understand emerging fields by recommending promising avenues for future research. It also facilitates exchanges of information on relevant scientific subjects.

*Advances in Space Research* (*ASR*, impact factor 1.178, http://ees.elsevier.com/asr/) is the official journal of COSPAR. It covers all areas of space research, including – but not limited to – space studies of earth surface, meteorology, climate, fundamental physics in space, materials physics in space, space debris, weather and earth observation of space phenomena. *ASR* also includes COSPAR's Information Bulletin, *Space Research Today*.

COSPAR's President for the period 2010–2014 is Giovanni Bignami (Italy) and the Vice-President is J. Wu (People's Republic of China). Members of the Bureau are: I. S. Batista (Brazil), K.-H. Glassmeier (Germany), A. Jayaraman (India), S. Sasaki (Japan), J.-P. St.-Maurice (Canada) and L. Zelenyi (Russia).

As discussed before, the IUCr would like to be involved with COSPAR in the organization of a public outreach/capacity-building symposium on the Importance of Crystallography in Past and Future Space Research (the subjects would cover search for materials applied in building spacecrafts, reports on crystallographic and crystal-growth experiments performed in space, and actual and future investigation of space debris by crystallographic methods). The timing and location of this potential meeting are being discussed.

The following is a list of COSPAR co-sponsored meetings in 2012:

20 Years of Progress in Radar Altimetry, Venice Lido, Italy, 24–29 September 2012;

Establishing Risk Levels for a Mars Sample Return Mission, Alpbach, Austria, 14–18 May 2012;

Remote Sensing of Global Water Circulation and Climate Change, Beijing, People's Republic of China, 15–26 October 2012;

International Colloquium and Workshop on Ganymede Lander, Scientific Goals and Experiments, Moscow, Russia, 4–8 March 2013;

Protecting the Earth and Planetary Protection Policy, Alpbach, Austria, 31 May – 1 June 2012.

I would like also to mention that the new, upgraded COSPAR web site is very informative.

**H. A. Dabkowska**, IUCr Representative

**Table 2**
Balance sheet (in Swiss Francs) as at 31 December 2012.

| | 2012 | | *2011* | |
|---|---|---|---|---|
| **Fixed assets** | | | | |
| Tangible fixed assets | | 28 912 | | *43 861* |
| Investments at market value | | 2 716 611 | | *2 390 156* |
| | | 2 745 523 | | *2 434 017* |
| **Current assets** | | | | |
| Stock | | 106 529 | | *135 659* |
| Cash at bank and in hand | | | | |
| Current accounts | 103 864 | | *54 833* | |
| Deposit and savings accounts | 2 100 980 | | *2 060 003* | |
| Cash with Union officials | 19 933 | 2 130 531 | *15 695* | *2 130 531* |
| Debtors, accrued income and payments in advance | | 311 489 | | *513 951* |
| Subscriptions due from Adhering Bodies | | 22 880 | | *13 162* |
| **Total current assets** | | 2 665 675 | | *2 793 303* |
| *Creditors*: amounts falling due within one year | | (348 920) | | (*525 200*) |
| **Net current assets** | | 2 316 755 | | *2 268 103* |
| **Total funds** | | 5 062 278 | | *4 702 120* |

## 11. Finances

Extracts from the full financial statements, namely the Income and Expenditure account, Balance Sheet and Summary of Fund Accounts, are given in Tables 1, 2 and 3, respectively.[1] For comparison, the figures for 2011 are provided in italics. The accounts are presented in CHF.

The ICSU exchange rates, based on the official UN rates, have been used in the preparation of these accounts. As a consequence of the many fluctuations in exchange rates during the year, the following procedure has been adopted for the accounts. Assets and liabilities in currencies other than CHF at 31 December 2012 have been translated into CHF in the balance sheet at the rate operative at that date. For the income and expenditure accounts, transactions have been translated into CHF by applying the rates appropriate to the individual dates of these transactions. As a consequence of the fluctuation in exchange rates, overall an apparent gain has arisen on the assets of the Union, in terms of CHF, amounting to CHF 70 260. In the accounts this gain has been assigned as a 'Realized gain' (CHF 72 597) and 'Unrealized loss' (CHF 2337). The loss attributable to investment activities has been assigned to the General Fund and the overall gain attributable to trading activities has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 2012. It should be noted that this overall gain in CHF is not a real gain of money, but rather a gain on paper resulting from the accounts being expressed in CHF.

Investments are noted in the balance sheet at their market value at 31 December 2012.

The balance sheet shows that the assets of the Union, including the gain resulting from fluctuations in rates of exchange, have increased during the year, from CHF 4 702 120 to CHF 5 062 278. The movement in market value of the investments was CHF 24 999 in 2012 (CHF −53 250 in 2011).

The following transfers were made from the Journals Fund: CHF 25 000 to the Publications and Journals Development Fund; CHF 250 000 to the Research and Education Fund; CHF 25 000 to the General Assembly and Congress Fund; CHF 50 000 to the President's Fund; and CHF 50 000 to the *Newsletter* Fund.

The following comments refer to figures in the full accounts.

The General Fund account shows a deficit of CHF 325 548, as compared with a deficit in 2011 of CHF 297 548. The administrative expenses were CHF 371 514 in 2012 as compared with CHF 390 072 in 2011. Of this amount, CHF 156 751 was charged to the publications of the Union.

The expenses of the Union Representatives on other bodies were CHF 10 603. The cost of the Finance Committee meetings held in 2012 was CHF 31 773, while the Executive Committee meetings cost CHF 108 082. The income from the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 16 252. The subscriptions from Adhering Bodies were CHF 161 922. Interest on bank accounts and investments credited to the General Fund was CHF 74 551.

Grants totalling CHF 29 594 were paid from the President's Fund in 2012.

The Journals Fund account for 2012 shows a surplus of CHF 799 078 before the transfer of CHF 400 000 to the other fund accounts, as compared with a surplus of CHF 900 129 in 2011 before the transfer of CHF 325 000 to the other fund accounts.

The cost of the technical-editing office has been divided between the Journals Fund and the *International Tables* Fund in percentages based on the staff time spent on each publication. The technical-editing costs for the Journals Fund were CHF 1 305 419 as compared with CHF 1 262 406 in 2011. The Journals Fund has also been charged with administration expenses as in previous years as shown in the General Fund.

The *International Tables* account shows a deficit of CHF 19 418, as compared with a deficit of CHF 67 737 in 2011. The net sales income was CHF 128 287 in 2012 as compared with CHF 92 913 in 2011.

The income for the Union in producing the *Newsletter* in 2012 was CHF 42 010.

In the Publications and Journals Development Fund account, the computing and promotion expenses are divided between the General Fund, the Journals Fund and the *International Tables* Fund. STAR/CIF costs, Special Issue costs, journal grants and web input costs are also charged to the Publication and Journals Development account.

[1] The full audited accounts are available from the IUCr electronic archives (Reference ES0403).

**Table 3**
Summary of Fund Accounts (in Swiss Francs) as at 31 December 2012.

| | As at 1 January 2012 | Transfers between funds | (Deficit)/ surplus of income over expenditure for the year | Increase in market value of investments | Fluctuations in exchange rates | | Balance at 31 December 2012 |
|---|---|---|---|---|---|---|---|
| | | | | | Trading | Investments | |
| **Fund accounts** | | | | | | | |
| General Fund | (2 108 756) | — | (325 548) | 24 999 | (40 233) | (13 102) | (2 462 640) |
| President's Fund | 70 941 | 50 000 | (29 594) | — | 1 525 | — | 92 872 |
| Journals Fund | 4 523 199 | (400 000) | 799 078 | — | 82 197 | — | 5 004 474 |
| *International Tables* | (485 539) | — | (19 418) | — | (8 432) | — | (513 389) |
| Publications and Journals Development Fund | 989 994 | 25 000 | (24 363) | — | 16 537 | — | 1 006 838 |
| Research and Education Fund | 956 375 | 250 000 | (194 370) | — | 16 900 | — | 1 028 905 |
| Ewald Fund | 516 096 | — | — | — | 8 618 | — | 524 714 |
| *Newsletter* Fund | (50 346) | 50 000 | 42 010 | — | 696 | — | 42 360 |
| General Assembly and Congress | 290 486 | 25 000 | 17 104 | — | 5 554 | — | 338 144 |
| | 4 702 120 | — | 264 899 | 24 999 | 83 362 | (13 102) | 5 062 278 |

In 2012, CHF 4883 was provided from this Fund as journal subsidies in connection with the Journal Grants Fund, which was set up to assist institutions that have difficulties in meeting the full subscription price.

CHF 154 249 for financial support to young scientists, to enable them to attend scientific meetings sponsored by the Union, was charged to the Research and Education Fund. Visiting Professorships (CHF 6211), crystallography in Africa initiatives (CHF 20 264) and inter-regional bursaries to enable young scientists from the region covered by one Regional Associate to attend the annual meeting of another Regional Associate (CHF 13 646) were also charged to the Research and Education Fund.

In 2007 a General Assembly and Congress Fund was established so that the costs associated with the General Assembly and Congress could be spread over the triennium. In 2012 this Fund received net income of CHF 17 104 and a transfer of CHF 25 000 from the Journals Fund.