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Report of the Executive Committee for 2013

1. Meetings

The IUCr sponsored the following meetings held during 2013:

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

Synchrotron Charge Density School, Chicago, USA, 23–29 March.

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

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

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

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

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

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

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

Zürich School of Crystallography – Bring Your Own Crystals, Zürich, Switzerland, 9–22 June.

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

XX Conference of Serbian Crystallographic Society, Belgrade, Serbia, 13–15 June.

International Workshop on X-ray Powder and Electron Crystallography, Rio, Greece, 2–6 July.

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

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

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

5th International Summer School on Crystal Growth, Gdansk, Poland, 4–10 August.

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

28th Meeting of the European Crystallographic Association, Warwick, UK, 25–29 August.

12th International Conference on Quasicrystals (ICQ12), Kraków, Poland, 1–6 September.

Advances in Static and Dynamic High-Pressure Crystallography, Hamburg, Germany, 8–11 September.

11th International Conference 'Biology and Synchrotron Radiation (BSR)', Hamburg, Germany, 8–11 September.

MISSCA 2013, Como, Italy, 9–12 September.

XXI Brazilian Crystallographic Meeting, Goiania, Brazil, 18–20 September.

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

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

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

School of Crystallization and Crystallography for Latin America (ECRISLA 2013), Florianopolis, Brazil, 14–25 October.

Fifth Moroccan School of Crystallography – EMC5, Oujda, Morocco, 23–27 October.

I Latin American Meeting on Crystallography and IX Annual Meeting of the Argentinian Crystallographic Association/V School of the Argentinian Crystallographic Association, Cordoba, Argentina, 29 October – 1 November/4–8 November.

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

12th Conference of the Asian Crystallographic Association (AsCA 2013), Hong Kong, People's Republic of China, 7–10 December.

Australasian Course in Macromolecular Crystallization 2013 (ACNC-13), Melbourne, Australia, 9–13 December.

The Executive Committee met in Leuven, Belgium, in August/September. The Finance Committee met in Leuven, Belgium, in March and August, to prepare its advice and recommendations on finances, establishment and staff matters.

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

editorial policy, pricing policy and subscription rates, approval of appointments of Editors and Co-editors, online-only publishing of journals, launch of *IUCrJ*, journals development, review of subtitles for *Acta* journals, status of *Acta B*, *Acta C* and *Acta E*, archival policy, Special Issues, open access, and other matters concerning the IUCr journals;

review of contract with Wiley for IUCr journals;

International Year of Crystallography (IYCr), IYCr Opening Ceremony, IUCr–UNESCO OpenLabs, summit meetings;

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, review of blackout period for 2014, young scientists' support, Visiting Professorship Scheme; inter-regional bursary fund;

cooperation with databases, Diffraction Data Deposition Working Group;

progress with Volumes A, A1, B, C, D, E, F, G and H 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;

proposals from National Committees for Officers of the IUCr and Chairs and members of Commissions;

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;

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

Crystallography in Africa, extension of scheme to other regions;

review of activities of Commissions, formation of new Commissions;

review of activities of Regional Associates;

review of reports of IUCr Representatives on other bodies.

Items concerning the Chester office were:

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

office premises;

risk analysis;

upgrading of office technology.

2. Publications

Volume 69 of *Acta Crystallographica*, Volume 46 of *Journal of Applied Crystallography* (*JAC*) and Volume 20 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

The year saw some fundamental changes to the journals. These were based on a journals development plan drawn up by the Journals Management Board and approved by the Executive Committee in December 2012.

Among the aims of the development plan is the extension and expansion of the scope of the 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 plan 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. A policy of closer interaction with IUCr's Commissions is also planned. The central premise of the development plan is that our journals should cater for all of the best science resulting from communities that are served by our Commissions, publishing original research articles as well as review articles in all areas covered by the Commissions. Each of the journals was assigned a dedicated Managing Editor so that these highly trained IUCr staff can be pro-active in the whole process of publications, community awareness and journals development.

	2008	2009	2010	2011	2012	2013
No. of submissions (all)	5765	7129	7033	7302	6628	4514
without Acta E	1919	2016	1905	1831	2023	2391
Rejection rate (%)	24	22	22	22	21	23
without Acta E	39	33	33	32	30	30
No. of published papers (all)	4795	5440	5431	5650	5330	3481
without Acta E	1239	1274	1318	1206	1283	1517
No. of open-access papers	3647	4245	4232	4571	4139	2177
without Acta E	89	79	119	127	78	213
No. of pages (all)	11295	12812	13156	12667	13307	12410
without Acta E	7034	7704	7961	7144	8136	9773

During 2013, a new journal subtitle for *Acta B*, *Structural Science, Crystal Engineering and Materials*, was introduced, new subtitles were approved for a number of other journals and a major plan for Special Issues to highlight the changes in scope of the journals was implemented. From 2014, the subtitle of *Acta A* changed to *Foundations and Advances* with the launch of a new Advances section. *Acta C* is now simply called *Structural Chemistry*. *Acta F* received the shortened subtitle *Structural Biology Communications* to provide a clear message that the journal was the home for structural biology papers that were best presented as Communications. It also signalled to the community that it was not solely a journal for crystallization or preliminary results. The changes in subtitles have been accompanied by a great deal of activity, with the journals publishing Special Issues relevant to their new subtitles, and also Lead and Feature Articles. Additional Main Editors were appointed during 2013–2014, including Marc de Boissieu (*Acta B*), Randy Read and Soichi Wakatsuki (*Acta D*), Bill Hunter (*Acta F*), and Andrew Allen and Janos Hadju (*JAC*), thus enabling our journals to have more than one Main Editor and as such enabling the scope of our journals to be widened. Much work remains to be done to transform the journals and make sure that authors appreciate the full range of publication choices.

While the strengthened teams of Main Editors, Co-editors and Managing Editors spearheaded these developments, ambitious plans for *IUCrJ* were put in place. The year 2013 saw the establishment of an Advisory Board (T. L. Blundell, P. M. Colman, J. B. Hastings, W. A. Hendrickson, B. Kobilka, Y. Ohashi, J. R. Schneider, W. G. Stirling and M. J. Zaworotko) and 20 Co-editors for the five broad sections of the journal. The objective of *IUCrJ* is to attract high-quality science papers of broad scientific significance from across all the scientific communities that use results obtained from diffraction methods. The goal for 2014 will be to publish 100 articles in *IUCrJ* covering as many aspects of structural methods development and applications as possible. The journal published its inaugural issue in January 2014 and has so far published nearly 40 papers. Many of the most important contributions at the Congress are being captured for the September and November 2014 issues of *IUCrJ*.

A final part of the development plan was the appointment of a Business Development Manager to work on the development and promotion of the journals. Jonathan Agbenyega took up this position in December 2013. Additional services to authors have been put in place. For example, facilitating promotional opportunities to authors for their articles is one of the areas that is being developed. While encouraging authors to submit their best work, we are undertaking to provide scientific commentaries (along the lines of News and Views articles in *Nature* or Perspectives articles in *Science*) on some of the outstanding articles that are published, and short Research News items are also being commissioned for distribution to the media.

In Spring 2012, Thomson Reuters announced that *Acta E* was to be de-listed from the *Science Citation Index*, giving a high self-citation rate as the principal reason for this action and also noting that the journal would not be reassessed until 2015. A detailed strategy for the re-launch of the journal was developed during 2013. *Acta E*, to be called *Crystallographic Communications* from January 2015, will be served by five Main Editors. Luc Van Meervelt (Belgium) joins Bill Harrison (UK), Helen Stoeckli-Evans (Switzerland), Edward Tiekink (Malaysia) and Matthias Weil (Austria) to complete the board of Main Editors. A highly reputable International Editorial Advisory Board consisting of Stuart Batten (Australia), Gautam R. Desiraju (India), Larry Falvello (Spain), Santiago Garcia-Granda (Spain), Judith Howard (UK), Simon Parsons (UK), Ian Williams (Hong Kong, People's Republic of China) and Chen Xiao-Ming (Guangzhou, People's Republic of China) will guide the journal. *Crystallographic Communications* will publish two article types: a longer format than at present (Research Communications) and a short format (Data Reports) that is similar to current articles.

Though the total number of pages published in 2013 was very similar to 2011, the total number of papers published in 2013 decreased significantly owing to a decrease in articles published in *Acta E* following its de-listing by the *Science Citation Index* in 2012. We note that the number of articles excluding *Acta E* was about 30% of the total in 2013 but made up about 80% of the published pages. The number of articles for all other journals represented an increase of about 15%, primarily owing to the increased attractiveness of *Acta D* (*Biological Crystallography*).

Three IUCr journals were included in the top five ranked crystallography journals, with *Foundations and Advances (Acta A)* having a five-year impact factor of 18.3, *Biological Crystallography* (*Acta D)* 7.5 and *Applied Crystallography (JAC)* 4.5. *Acta A*, *B* and *C*, and *JAC* had cited half-lives of >10 years. A total of 3.5 million downloads of journal articles were made from **Crystallography Journals Online** in 2013.

Very few open-access papers are published in *Acta 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 has generally been in the range 10–20%, with the highest proportions being in *Acta D* and *JSR*. Jonathan Agbenyega in consultation with other Chester staff has presented a strategy to deliver a near doubling of this by the end of next triennium.

At the end of 2013, more than 240 Editors and Co-editors worked on IUCr journals. The work of all these dedicated colleagues in ensuring the high standards of IUCr journals is highly appreciated. Their work was supported by the highly professional staff in Chester. The year marked the retirements of a number of editors as well as the appointment of replacement editors reflecting the broadening scope of our journals and emphasizing the scientific impact of crystallographic research in all of the mainstream science disciplines. We seek your support to create the equivalent of IUCr's *PNAS* (*IUCrJ*), while ensuring that all of our existing journals become the natural home for all of the best science resulting from communities that are served by our Commissions.

This report is based on the triennial report on the journals, which will be published as part of the General Assembly papers for the 23rd IUCr General Assembly, to be held in Montreal in August 2014. Detailed reports on individual journals can also be found in the General Assembly papers.

S. S. Hasnain, Chair

4.2. Commission on *International Tables*

International Tables for Crystallography is published by the IUCr in conjunction with Wiley. The series currently includes eight volumes designated A (and A1) through G. All eight volumes are available in print and online. A print edition of the Brief Teaching Edition of Volume A is available at a modest cost.

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

Additional information of a general type is included in Volumes B (*Reciprocal Space*) and C, which can be traced back to Volume II of the original series (1937) and Volumes II–IV of the series with red covers (1959–1974).

The other volumes of the series can be described as handbooks that cover more specific areas. These volumes are F (*Crystallography of Biological Macromolecules*), G (*Definition and Exchange of Crystallographic Data*), and the nearly finished ninth Volume H (*Powder Diffraction*).

Developments during 2013 include:

(1) Near completion of a new version of Volume A (edited by Mois Aroyo). The new electronic versions will include Seitz symbols [see *Acta Cryst*. (2014), A**70**, 300–302], which have been a topic of considerable discussion in the Commission during the last several years. The Editors of Volume E (Vojtech Kopsky and Danny Litvin) took leading roles in these deliberations.

(2) Very considerable development of the symmetry database (also edited by Mois Aroyo). This electronic resource simplifies discussion of non-standard space-group settings, which are often appropriate when phase sequences are being considered, and facilitates identification of group/subgroup/supergroup relationships. The Editor of Volume A1 (Ulrich Müller) is also involved in the development of this database.

(3) Planning for substantial revisions of Volumes B and C. These two volumes are the successors of Volume II of the original series (1937) and Volumes II–IV of the 'red' series (1959–1974). Over the years the two volumes have grown by accretion (especially C) to the point of being difficult to describe. Furthermore, many of the tables (*e.g.*, X-ray scattering factors) need no longer be printed, although having them available in an authoritative electronic form is important. The current editors (Gervais Chapuis, who was appointed for B in 2011, and Richard Welberry) are working closely together on very major revisions. The plan has been for B to focus on topics more related to its current title (*Reci-Reciprocal Space*) and for C to cover topics more connected to direct space, but it has become clear that such a simple division of topics is impossible.

(4) A revised edition of Volume D (editor André Authier) appeared online in late 2013 and will appear in print in 2014. It included one completely new chapter, new sections in two other chapters, and updates of a number of additional chapters.

(5) Retirement of Syd Hall as an editor of Volume G after the 2013 ECM meeting in Warwick, UK, during which a specialist workshop on building DDLm dictionaries and tools for CIF took place. Plans for the future are being discussed with Brian McMahon, who is the remaining Editor.

(6) Further work on Volume H on powder diffraction, which has gone from an outline to near publication during the triennium under the direction of Chris Gilmore, Henk Schenk and Jim Kaduk. Publication is expected during 2014. A novel feature will be the very extensive digital material that will be available with the electronic version. Many authors have included the raw diffraction data discussed in their chapters so that the reader may reproduce the data processing that is discussed.

(7) Planning of a new volume on XAFS. Editor Chris Chantler and Joint Main Editors Federico Boscherini and Bruce Bunker were appointed during the latter part of 2013.

(8) Discussions with the Commission on Magnetic Structures about a volume covering their field. As a preliminary step Danny Litvin's tables of magnetic (or black/white, or time-reversal) space groups have been published electronically by the IUCr (http://www.iucr.org/publ/978-0-9553602-2-0) and can be downloaded freely.

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

As mentioned above, Syd Hall [joint Main Editor of Volume G (*Definition and Exchange of Crystallographic Data*)] has announced his retirement from the Commission. Syd is very warmly thanked for his many contributions to the *International Tables* series and for his central role in developing the CIF format.

It is impossible to end this report without thanking the staff in Chester, and especially Nicola Ashcroft, for all that office does to help Editors and authors plan, produce and revise the volumes of this series. The people in Chester also create and maintain the web pages that explain and advertise the volumes.

C. P. Brock, Chair

4.3. Commission on Aperiodic Crystals

The Commission (CAC) 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, as well as the dissemination of research results to the greater scientific community.

Our central scientific activity in 2013 was ICQ12 – the 12th International Conference on Quasicrystals, which was held in Kraków, Poland, 1–6 September 2013. Janusz Wolny from AGH University of Science and Technology chaired the Conference. Over 160 participants from 22 countries attended, with many newcomers to the field of aperiodic crystals and a large group of young scientists. A special session was dedicated to celebrating the award of an Honorary Doctorate from AGH to Dan Shechtman, who was a distinguished guest of ICQ12. The scientific programme covered state-of-the-art advances in established aspects of quasicrystal research, as well as very new and exciting directions, such as the experimentally observed quasicrystalline thin films in perovskites, and the theoretically predicted quasicrystalline thin films in water and silicon. Altogether, 24 invited lectures and 32 contributed oral presentations along with 85 posters covered 16 diverse scientific sessions. Pedagogical tutorials on the mathematics (three talks) and physics (three talks) of quasicrystals aroused great interest as well. For more details, see http://icq12.fis.agh.edu.pl/. The Commission wishes to express its utmost gratitude to Janusz Wolny and his Local Organizing Committee for their excellent work. The next meeting, ICQ13, will be held in Katmandu, Nepal, in 2016, and organized by Hem Raj Sharma and An-Pang Tsai.

Our central educational activity – the 2nd International School on Aperiodic Crystals – was held at the University of Bayreuth, Germany, 7–12 April 2013. The school was organized by Marc de Boissieu, Andreas Schönleber and Sander van Smaalen, assisted by seven additional lecturers, and attended by 40 students (33 'young scientists' and seven 'senior scientists'). Participants came from universities and research institutes from 14 countries, including departments of condensed-matter physics, inorganic and general chemistry, materials science, and crystallography. The objectives of the school were to provide an overview of aperiodic order, of the basics of the mathematical description of both modulated structures and quasicrystals, and of physical properties and chemical understanding of aperiodic crystals, as well as a working knowledge of structural analysis of aperiodic crystals. It included morning lectures followed by hands-on afternoon tutorials, which greatly contributed to the success of the school. The Commission is grateful to the organizers and all the lecturers, and hopes that they will all agree to contribute their time also to the 3rd International School on Aperiodic Crystals, whose venue will be decided at the upcoming Commission meeting in August 2014. For more details see: http://old.crystal.uni-bayreuth.de/aperiodic_crys_school_2013/.

In addition to the above, ECM28 – the 28th European Crystallographic Meeting, which was held in Warwick, UK, 25–29 August 2013 – included two Microsymposia related to aperiodic crystals, a Keynote Lecture by Lukas Palatinus, as well as a Plenary Lecture on quasicrystals by Dan Shechtman. Finally, the series of *ad hoc* Workshops on *JANA2006* continued in 2013 with a number of workshops organized by Michal Dušek in Prague, Czech Republic.

In 2013 CAC integrated its web site with the highly popular and active web site of the special interest group (SIG) on aperiodic crystals of the European Crystallographic Association. The new joint web site is dedicated to all aspects of the crystallography of aperiodic crystals. It is maintained by Michal Dušek, and is now up and running and can be accessed at http://aperiodic.iucr.org/.

The Commission, with support from the Commission on Mathematical and Theoretical Crystallography, was successful in its nomination of Aloysio Janner and Ted Janssen for the 10th Ewald Prize. The two new laureates will receive the Prize at the Montreal Congress for *the development of superspace crystallography and its application to the analysis of aperiodic crystals*. The Commission wishes to congratulate Professors Janssen and Janner for this great achievement.

Two upcoming and important meetings for the Commission should be mentioned at this time. The first is the Montreal Congress, which will have a very good focus on aperiodic crystals, with 12 Microsymposia and 5 Keynote Lectures related to aperiodic crystals. There will also be a Plenary Lecture by Dan Shechtman, as well as the Ewald Prize ceremony with a lecture by Ted Janssen. The Commission is also planning a one-day satellite workshop, Introduction to Aperiodic Crystals, on 5 August, organized by the Commission Chair. For details see: http://www.tau.ac.il/~ronlif/CAC/IUCr2014-Workshop-Program.pdf.

The second meeting is Aperiodic2015, which will be held at the Břevnov Monastery in Prague, Czech Republic, 30 August – 4

September 2015. Michal Dušek and Lukas Palatinus will organize the meeting, and Vaclav Petricek will chair the International Programme Committee, which will be composed of the members of CAC. The Commission looks forward to this meeting, which is its flagship event, with great anticipation.

R. Lifshitz, Chair

4.4. Commission on Biological Macromolecules

Since 2013, one of the central activities of the Commission (CBM) has been to contribute to the organization and design of the Montreal Congress. We held numerous discussions about what kinds of Microsymposia and Keynote Lectures concerning CBM should be organized and which Chairs and speakers should be invited, and so on. With certain efforts, structural-biology-related crystallographers Tom Terwilliger, Hanna Yuan and Silvia Onesti were members of the International Programme Committee, two of them being current CBM members; they have been working hard and we look forward to having a well balanced programme for the Montreal Congress.

During 2013, I have written supportive letters on behalf of CBM for the following meetings:

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

2014 Kuo Symposium on 3D Cryo-EM Molecular Imaging and The 7th K. H. Kuo Summer School of Electron Microscopy and Crystallography, Shanghai, People's Republic of China, 26–30 September 2014.

Structural Biology: Using Synchrotron Radiation to Visualize Biological Molecules, Trieste, Italy, 2–6 June 2014.

Celebrating the International Year of Crystallography by encouraging Young People to Macromolecular Crystallography and Fostering International Collaborations, Turin, Italy, 16–17 October 2014.

Macromolecular Crystallography School 2014: From Data Processing to Structure Refinement and Beyond, Sao Carlos, Brazil, 8–16 August 2014.

47th Crystallographic Course – Structural Basis of Pharmacology: Deeper Understanding of Drug Discovery through Crystallography, Erice, Italy, 30 May – 8 June 2014.

We also had numerous discussions about the celebration of IYCr2014 among CBM members, and the following are summaries of these discussions.

Activities in People's Republic of China. The CCrS (Chinese Crystallographic Society) and CBM (there is a similar branch of CBM within CCrS, which I am also chairing) will focus on the following activities for celebrating IYCr2014:

CCrS will organize the writing and editing of *The History of Chinese Crystallography*.

CCrS will set up a museum for introducing and exhibiting crystallography for celebrating IYCr2014.

CCrS and CBM will have popular science exhibitions and activities to introduce crystallography to primary- and middle-school students (crystallization competitions, for example).

CCrS and CBM will hold a series of popular science summer lectures/tours in several cities of China to introduce crystallography and chemical and biological structures to the general public.

CCrS and CBM will hold an academic conference in Beijing, 25–26 October 2014, to celebrate IYCr2014. Local and national governments will participate in the activity with many different academic and governmental organizations taking part. This will be the highlight for the Chinese celebration of IYCr2014.

There will be many (more than usual) popular science lectures around China for crystallography and structural biology the whole year round.

Montreal Congress. The International Programme Committee is planning a series of public lectures as part of the Congress and Tom Terwilliger has volunteered a lecture in that series; he also tweets about the IYCr.

Worldwide PDB and RCSB PDB. The Worldwide Protein Data Bank (wwPDB) has created a 2014 calendar that illustrates how X-ray crystallography enables our understanding of biology at the atomic level. The calendar is available for download in PDF, ppt, and individual image formats from http://wwpdb.org/iycr2014.html. Christine Zardecki reports that the wwPDB are planning on sending printed copies to the Organizing Committee so they can be distributed at the Opening Ceremony at the UNESCO building. Two members of the wwPDB will be in attendance.

The RCSB PDB will promote IYCr stories and events on social media at https://www.facebook.com/RCSBPDB and https://twitter.com/buildmodels.

Activities at CNRS. Alberto D. Podjarny reports that CNRS is organizing a special meeting on 23 September 2014 entitled Highlights in Protein Crystallography in France, Germany and Switzerland for the IYCr, which will be held prior to the yearly Regional Meeting for the crystallographers of the Upper Rhine Valley.

Activities in Japan. Professor Kunio Miki is a Vice-Chair of the IYCr2014 Japan Initiative. In the field of structural biology, he has been appointed Chair of the Historical Review session at the 14th Annual Meeting of the Protein Science Society of Japan to be held in Yokohama, June 2014, where historical stories of protein crystallography will be presented from international and domestic viewpoints.

Activities in Poland. Professor Mariusz Jaskolski reports that he is in the process of designing a postage stamp commemorating IYCr2014 and that it is hoped that this will be issued through the Post Office in Poland, through the Polish Crystallographic Society.

On 11 April 2014 there will be the dedication of a Bronze Laue Memorial Plate on the school building in Poznan attended by Max von Laue. The ceremony will be connected with a one-day Laue Symposium, featuring a number of Laue-related talks, including biological macromolecular crystallography. The European Crystallographic Association and Professor Andreas Roodt are thanked for their support.

At the end of June, there will be the finals of the National Crystallography Olympiad. This again is a national event, coordinated by the Polish Committee of Crystallography.

Activities in India. Dinakar Salunke reports that, as in other countries, Indian crystallographers have also planned programmes for IYCr combining all disciplines of crystallography. As the IUCr President is from India, plans are on a really large scale. The release of a special postage stamp, a Special Issue of a journal and programmes for outreach in society have been planned. The annual National Conference is split into three at three different geographical locations. An International workshop-*cum*-discussion meeting on new frontiers of macromolecular crystallography is also planned and there will be a series of popular lectures by distinguished crystallographers in remote areas.

Activities in Brazil. Richard Garratt reports that activities that will be taking place in Brazil include the running of a CCP4 macromolecular crystallography course in April, held for the first time in Brazil. This follows on from a very successful course run in Uruguay

last year and hopefully will turn out to be a regular event helping to foster the use of crystallographic techniques in South America. Besides CCP4 it has sponsorship from the IUCr as well as CeBEM (The Center for Structural Biology of MercoSul). The latter is an initiative we set up in Brazil, Argentina, Uruguay and Paraguay several years ago and this also aims to grow structural biology (not just crystallography) in the region.

In May the Brazilian Biochemical Society will have a short session on the past, present and future of protein crystallography in Brazil.

Most importantly, in September, one of the IYCr2014 summit meetings will be organized in Brazil. The Brazilian meeting will be on Biological Crystallography and Complementary Techniques and will be held at the Brazilian synchrotron laboratory in Campinas. Hopefully we will have participants from many different countries in Latin America.

Activities in Spain. Dr Martin Martinez-Ripoll reports that in Spain there is a unique Commission to organize events for IYCr2014. The Commission, of which he is a member, has made no distinction between the different fields of crystallography, although wherever possible they have included exclusive events to highlight the importance of macromolecular crystallography. He has personally taken part (and will continue to do so) in several conferences and national broadcast programmes, as well as a strong outreach for younger people, including children.

In addition to the successful web page dedicated to crystallography (http://bit.ly/1cRPTnS), there is a special site devoted to the IYCr2014 (http://www.iycr2014.info/), Facebook (https://www.facebook.com/IYCr2014Spain) and Twitter (https://twitter.com/IYCr2014Spain). Most of the events organized in Spain are also announced on the general web page of the IYCr2014 (http://www.iycr2014.org/countries/spain).

Moreover, around the end of March 2014 a small book of about 15 chapters and coordinated by myself (*Through the Crystal: How Crystallography has Changed the World*) will be published (in Spanish) by the Spanish National Scientific Council (CSIC). Nearly 80% of its contents will be connected directly with macromolecules.

Activities in Australia. Professor Jenny Martin reports that she will be speaking about crystallography at a public seminar in Melbourne in March, and has already been interviewed by the national public broadcasting radio station ABC about IYCr. She is arranging for images of crystal structures to be on display at the National Science and Technology Centre in Canberra, and these images may then travel around Australia to the major cities and regions. In addition, she is organizing an Australian satellite of the IYCr/Agilent photo competition with a 'crystallographer's choice' prize decided by attendees at the CRYSTAL29 conference in April (of which she is programme coordinator). She advertises CRYSTAL29 and IYCr in her e-mail signature and tweets about IYCr.

Other events in Australia include:

Crystallography in the City – a crystal structure sculpture travelling exhibition;

Engaging with schools, National Science Week activities;

A crystal-growing competition (with RACI, coordinated nationally/internationally);

Public remote-access Australian Synchrotron data collection;

Explore the Crystals – the general public are invited to evaluate crystallization experiments posted online;

Crystal365 – tweeting and blogging one crystal structure per day.

Xiao-Dong Su, Chair

4.5. Commission on Charge, Spin and Momentum Densities

The Gordon Conference on Electron Distribution and Chemical Bonding chaired by Dr P. Macchi (University of Bern, Switzerland) and Professor W. Scherer (University of Augsburg, Germany) in Les Diablerets, Switzerland, 2–3 June 2013, attracted 101 participants, which is the highest participation since the beginning of the series in 1978. The theme of the 2013 conference was: Pushing the Limits of Experimental and Theoretical Charge and Spin Density Studies. It has been extremely successful in many aspects such as the high level and novelty of the scientific contributions and the strong interest of a broad audience to the individual discussion sessions. Two positive points are the large number of young lecturers (aged under 35) who provided nearly exclusively excellent talks and the participation of scientists from related scientific disciplines, where the electron or spin density distribution is apparently not the main focus of research, but is fundamental. For example, Professor Franz Giessibl (Regensburg, Germany) has attracted enormous interest by highlighting a way to achieve charge density distributions at subatomic resolution *via* AFM microscopy. Despite the success of this meeting, the Gordon Research Conferences have decided to discontinue this series at the end of 2013, mainly owing to insufficient participation over the last three conferences, which reflects the small size of our community.

One closed Commission meeting was held during the GRC in June 2013 with a large number of members and consultants, the organizers of the next conferences, Sagamore XVIII (C. Gatti, Italy) and ECDM7 (K. Woszniak and P. Dominiak, Poland) and Dr P. Nakashima (Australia), responsible for the QCBED charge density project.

The 8th International Conference on Inelastic X-ray Scattering (IXS2013) was held at the SLAC National Accelerator Laboratory, California, USA, 11–16 August 2013. This conference brought together 133 researchers from all over the world and provided discussion on electronic excitations by resonant and non-resonant IXS, phonons and molecular vibrations by high-resolution IXS, and ground-state electronic and magnetic structures by charge and magnetic Compton scattering. The oral and poster presentations included latest developments in experiment and theory, including XFEL as well as synchrotron results. Because of accelerated developments in this field, the IXS conference series has been changed to be held every two years, and then the next IXS conference (IXS2015) will be held in Taiwan in late 2015.

At the European Crystallographic Meeting (ECM28) in Warwick, UK, in August 2013, the field of charge and spin density was present through one Keynote Lecture (KN4) given by Professor D. Stalke (Goettingen, Germany) on chemical applications of charge density research entitled What a Synthetic Chemist Learns From Charge Density. Two sessions were organized by the special interest group SIG 2 on charge, spin and momentum densities research: (MS29) Getting More From Your Electron Density and (MS13) Charge and Spin Density Measurements of Materials. Another session (MS30) Beyond Harmonic Treatment was co-organized with SIG 9 on Crystallographic Computing and was really successful as it gathered approximately 60 participants despite the fact that the session was scheduled for the last day of the conference. The charge density field was also well represented at the young crystallographers satellite meeting by a Plenary talk given by Dr B. Dittrich (Goettingen, Germany) on the current state and future directions of invarioms.

Dr P. Nakashima (Monash University, Australia) is leading the IUCr project on electron distribution in the metallic bond by QCBED techniques and X-ray diffraction, jointly supported by this Commission and the Commission on Electron Crystallography. The

work is organized as follows: distribute the metals to the six different groups in Norway, Germany, the USA, Japan and Australia (two groups for each metal) and meet once a year (for three years). Au and Sn will be studied by students of Philip Nakashima.

The round-robin test on charge density studies using synchrotron radiation will be performed on manganese formate dihydrate, $Mn(HCOO)_2{\cdot}(H_2O)_2$, in collaboration with the Commission on Synchrotron Radiation, and involves three synchrotron groups at SPring-8 (Japan), APS (USA) and Soleil (France) and four groups working with conventional sources in France, Germany, the UK and Canada. Crystal batches were prepared this year at the LMI (Laboratory of Materials and Interfaces), Lyon University (France), for distribution to the different groups. The various measured data sets will be transmitted to Jacob Overgaard (University of Aarhus, Denmark) who will perform the charge density refinement on each data set in a systematic way in order to enable a valuable comparison.

B. Gillon, Chair

4.6. Commission on Crystal Growth and Characterization of Materials

In 2013 many members and consultants of the Commission had the chance to meet in person and exchange opinions. This happened on 12 August at the ICCGE-17 Conference in Warsaw, Poland. Although much work can be done *via* the internet, the chance to meet directly is really very important for the life of the Commission.

At the meeting, Koichi Kakimoto, Tatiana Bekker, Manuel Garcia Ruiz, Ewa Talik, Jiyang Wang, Abel Moreno, Thierry Duffar, K. Tsukamoto, Elias Vlieg and myself were present, and also Hanna Dabkowska as representative of the Executive Committee. These are the issues that were mainly discussed:

Welcome to the new members/consultants: Tatiana Bekker, Ewa Talik and Tom Keuch.

A report from Koichi Kakimoto about the situation concerning the preparation of the programme for the Montreal Congress and how the Commission could still help in the preparations.

The organization of the web site to show artificially grown crystals as the main contribution of the Commission to the celebration of IYCr.

Planning and discussion about the next crystal-growth schools to be organized. The first is in Costa Rica in January 2014, and then, as always, ISC2014 will take place in Granada, Spain. In 2015 there will be a school in Italy related to the European Conference on Crystal Growth. Then in 2016 there will be the international school connected with ICCGE-18 in Japan. It seems that the programme is very full, but other initiatives could be welcome. In particular, a school in Africa would be welcome, but at the moment there is lack of a local person to take charge of the organization.

The Commission decided to ask the IOCG Executive Committee to consolidate the organization of co-chaired symposia at the next IOCG Conference to strengthen further the connection between the two associations (the proposal was accepted).

Juanma Garcia-Ruiz and all Commission members with him congratulated Ewa Talik for the high level of the crystal-growth school organized in Gdansk.

During 2013 the Commission was busy helping with the organization of the Montreal Congress. Koichi Kakimoto was chosen to represent the Commission on the International Programme Committee (IPC). We then had discussions (by e-mail) in order to define the most interesting topics for microsymposia (MS) and brilliant scientists to suggest for Plenary and Keynote speakers. Finally, six MS proposals were prepared and one suggestion was identified for a Plenary and a Keynote speaker. We are very happy that the IPC finally accepted four of our MS proposals (the remaining two were combined with others, so that all of our ideas were actually accepted), and also our suggestions for the Plenary and Keynote speakers were accepted. I would like to congratulate all the Commission members and consultants for having found good proposals, and Koichi Kakimoto, who was able to transfer our enthusiasm and our ideas to the IPC.

2013 was also characterized by a lot of work in organizing events related to IYCr. In particular, the Commission organized a web site (http://www.iycr2014.org/participate/crystal-growing) to show people a photo gallery of artificially grown crystals. Together with the pictures, information is given on the crystal structure, growth method and possible applications. The scientific committee for the web site is composed of members/consultants of this Commission with important participation of member representatives of IOCG. All scientists and non-professionals are invited to submit their best crystal pictures: the number of pictures on the web site increases daily. The web site is intended for celebration of IYCr, but also as a permanent tool to diffuse crystallography in the coming years. I wish to take the opportunity to thank Brian McMahon for the extraordinary work that he did with us to set up the web site.

Moreover, most of the members/consultants are involved in the organization of national initiatives to celebrate IYCr.

In 2013, the IUCr supported the following schools/meetings that were important for the crystal-growth community:

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

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

46th Course of the International School of Crystallography, Erice, Italy, 30 May – 8 June 2013.

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

4th International School on Biological Crystallization (ISBC2013), Granada, Spain, 26–30 May 2013.

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

Meeting of the Italian Spanish Swiss Crystallographic Associations, Como, Italy, 9–12 September 2013.

Moreover, the Commission endorsed the Italian Crystal Growth Conference, Parma, Italy, 14–15 November 2013.

Also, 2013 was established in Poland as 'The year dedicated to Professor Jan Czochralski', and the Commission supported the successful application of the Polish Society of Crystal Growth to the Polish Parliament.

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

Finally, I wish to express what a great honour and pleasure it is to chair this Commission. I hope I am making my own contribution to all the work done up to now by the Commission to bring more understanding of the role of crystals and their influence on many aspects of life and technology.

A. Zappettini, Chair

4.7. Commission on Crystallographic Computing

Planning for the 2014 Computing School, as a satellite of the Montreal Congress, organized by Commission members Patrick Mercier and Harry Powell continued but this was subsequently cancelled owing to the low number of registrants.

Eight Microsymposia are planned for the Montreal Congress; most are co-sponsored with other Commissions:

MS-03 Maximum Entropy in Crystallography (with the Commission on Charge, Spin and Momentum Densities). This should feature any application of MEM to crystallography and new developments are particularly encouraged.

MS-19 Computational Methods for Charge Density Studies (with the Commission on Charge, Spin and Momentum Densities). New computational methods and approaches for charge density studies are especially desired.

MS-22 Improving Your Crystallography: Best Practices and New Methods. This session will present foundations and recent advances in how to determine macromolecular structures, covering best practices for data collection, data analysis and structure determination. It can include how to choose what crystal to use, how to optimize data collection, how to collect the data, how to monitor and adjust data collection based on radiation damage, as well as new methods and algorithms for structure determination.

MS-30 Data to Knowledge: How to Get Meaning From Your Result (with the Commission on Biological Macromolecules). Use of database information to exploit fully the results of a new structure determination. The session will cover ways to find out if structural features in a structure have been seen before, ways to identify binding sites, active sites, ligands, ions and other features in the structure.

MS-52 Remote Controls for Crystallography at Synchrotrons and Neutron Sources (with the Commissions on Synchrotron Radiation, Biological Macromolecules, Powder Diffraction and Neutron Scattering). The focus is on systems created to handle large numbers of samples from, for example, mail-in programs, automated sampling systems and high-throughput crystallography systems. The session should also include remote 'lab-to-lab' operation of instrumentation for data collection. Talks should focus on advances in technology for allowing remote data collection but should include practical information for users on the features of these remote systems and how they can use them.

MS-96 New Computational Approaches to Structure Solution and Refinement. New computational methods and approaches are especially desired here for all structural fields of crystallography.

MS-100 Beginner's Guide to Validation of Crystallographic Results (with the Commission on Biological Macromolecules). This is intended as a tutorial session on validation: what is validation, what are the key criteria for validation of small-molecule and macromolecular structures, how to interpret a validation result including expected values and how to identify what is an error and what is a an unusual feature, and what to do next if errors or unusual situations are found. A variety of software tools for validation and the tools provided by archives such as the PDB will be described.

MS-112 New Approaches to Crystal Structure Prediction (with the Commissions on Crystallography of Materials and Structural Chemistry). Methods and techniques that can be applied to either 'organic' and/or 'inorganic' structures are of interest here. Compare and contrast methods, predictions of stable compounds under ambient and non-ambient conditions, co-crystal stability, polymorph prediction and drug design, and related problems.

A suggestion was made to the Google team that is responsible for the appearance of themes on the main Google search web page for something to honour the 100th anniversary of X-ray diffraction. The emphasis seems to be on birthdays, national days and major holidays. They appear both globally and also focused on specific countries. For example, a previous Google 'Doodle' was for Rosalind Franklin's 93rd birthday (25 July 2013): http://www.google.com/doodles/rosalind-franklins-93rd-birthday. Perhaps others could write to proposals@google.com with crystallographic suggestions. Their web site https://www.google.com/doodles/about gives details.

R. B. Von Dreele, Chair

4.8. Commission on Crystallographic Nomenclature

Proposal for the addition of Seitz Notation for Symmetry Operations to the Symmetry Operations Subtables of International Tables for Crystallography Volume A. During the Madrid Congress, it was decided that the Commission on Crystallographic Nomenclature should try to establish a convention for Seitz notation that closely follows the already accepted crystallographic conventions for the description of symmetry operations. It was agreed that Seitz notation should not appear in the printed Volume A of *International Tables*, but could be added to the online versions of *International Tables*.

During 2013, the Commission discussed two proposals, one by D. B. Litvin and V. Kopsky, which was originally proposed in Madrid, and one by A. M. Glazer and M. Aroyo, the Editor of Volume A of *International Tables,* based on an idea also submitted by A. M. Glazer in Madrid, and differing by the symbols used.

The discussion was followed by an e-mail ballot, which gave the following result: (two members voted for both proposals).

	Yes	No	Abstain
Inclusion of Seitz symbols	35	0	1
Glazer and Aroyo proposal	33	2	1
Kopsky and Litvin proposal	4	29	3

Since the composition of the Commission changed slightly during the triennium, both the members originally appointed in 2011 and those appointed since were polled.

As a consequence, the Glazer and Aroyo proposal for inclusion of the Seitz symbols in the online version of Volume A of *International Tables* was adopted. A short paper describing the proposal has been submitted to *Acta Crystallographica* Section A for publication in the International Union of Crystallography section.

The other main nomenclature problem that was discussed in the course of 2013 was a proposal to use the symbol $\bar{2}$ instead of *m* with the argument that this notation is more consistent from a mathematical point of view and adds clarity to the relationships between rotations and rotoinversions. Although, in general, the arguments in favour of the $\bar{2}$ symbol were accepted, the vast majority of Commission members did not support the proposal because of the intuitiveness of the symbol *m*, its popularity and its long tradition of usage by the crystallographic community. Nevertheless, because of the pedagogical benefits of the symbol $\bar{2}$, it is recommended that the definition of *m* as $\bar{2}$ is emphasized whenever the opportunity arises.

A. Authier, Chair

4.9. Commission on Crystallographic Teaching

Since filing its last annual report, 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 157 'likes' (an increase of 80%). Our Twitter feed (@IUCrTeach) has 25 followers (up 92%). The Commission continues to increase activity on both social media outlets to disseminate better exciting findings and important information, particularly in the International Year of Crystallography and leading up to the Montreal Congress. We are also reviewing our web pages on the IUCr web site, examining resources for utility and audience, reorganizing content as appropriate, and updating information. Our objective is to make our communication channels and information more targeted and relevant to specific audiences.

The Chair (K. A. Kantardjieff) represents the Commission on the International Programme Committee for the Montreal Congress. The Commission is sponsoring three Microsymposia (MS):

Eric Reinheimer (USA) and Juanma Garcia-Ruiz (Spain) are Co-Chairing Spreading the Word. Introducing Crystallography to the Public (MS-68), which is scheduled on 10 August 2014 in the morning session.

Saulius Grazulis (Latvia) and Amy Sarjeant (USA) are Co-Chairing Crystallography Education and Training in the 21st Century: New Pedagogies, New Paradigms (MS-92), which is scheduled on 10 August 2014 in the afternoon session.

Clyde Smith (USA) and Tim Gruene (Germany) are Co-Chairing Crystallography Education and Training in the 21st Century: New Pedagogies, New Paradigms (MS-84), which is scheduled on 11 August 2014 in the morning session.

These MS will provide a platform for speakers to present on a wide variety of topics, from technology, to K-16 education and outreach, to community engagement, to 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 Commission has also agreed to co-sponsor the MS Beginners Guide to Validation of Crystallographic Results sponsored by the Commission on Crystallographic Computing. The Commission continues to explore effective strategies for education and outreach during the International Year of Crystallography, and its members are consulted as appropriate. The Commission Chair is working with all six MS Co-Chairs to write and submit a manuscript for *IUCrJ* based on content from MS-84 and MS-92 that reviews the current state of affairs in crystallographic teaching (how it spans the sciences and how advanced crystallography has become a bit too easy). A second manuscript will be devoted to outreach best practices.

During 2013, the Commission has reviewed and written supporting letters for several proposals of variable quality and made recommendations for workshops and summer schools focused on areas relevant to the discipline. Another application proposed establishment of an award for young scientists to be launched in 2014. These include:

(1) European Crystallography School, Pavia, Italy, August–September 2014.

(2) VI School of the Argentinian Crystallographic Association (AACr), Mar del Plata, Argentina, November 2014.

(3) 15th British Crystallographic Association/Chemical Crystallography Group Intensive Single Crystal Teaching School in X-ray Structure Analysis, University of Durham, UK, March 2015.

(4) 47th International School of Crystallography entitled Structural Basis of Pharmacology: Deeper Understanding of Drug Discovery through Crystallography, Erice, Italy, May–June 2014.

(5) Young Person's Prize in Crystallography, an annual award or prize for young people. The general idea behind the award would be to attract students receiving a scientific education to increase their own knowledge and contribute their ideas to crystallography and related scientific fields. It is suggested that the Commission evaluate where such an award might have the best impact.

The proposals we receive vary considerably in quality. Proposers often send in documents at the last minute, which are vague in details, missing supporting data, and/or do not justify the funds requested, and then proposers expect immediate response and automatic endorsement at full funding levels. The Commission this year has attempted to develop and implement more formalized rubrics for evaluating proposals, along with criteria and guidelines to be presented to those individuals or groups making proposals to the IUCr for support. These guidelines will enable proposers to make the best possible case in their request. Rubrics will enable the Commission to determine more easily whether the proposals meet the mission and goals of the IUCr, to compare and contrast the proposals, and to provide more useful feedback to the Executive Committee so that precious funds can be invested wisely and with maximum return. It is suggested that for all schools and workshops proposals a letter of support from the Commission should be required along with a second letter from the appropriate subject matter Commission.

Finally, the Commission is in the midst of scheduling a face-to-face meeting among members present in Montreal.

K. A. Kantardjieff, Chair

4.10. Commission on Crystallography in Art and Cultural Heritage

The web site http://www.crystaledges.org was inaugurated in fall 2013, and demonstrates connections between crystallography and, in particular, symmetry aspects and the arts as manifested in the Gothic Windows of the Medieval Cathedrals of Europe.

There was collaboration with Painton Cowen to extend and expand his web site (http://www.therosewindow.com), which contained over 500 Gothic Roses windows, to a larger number (over 1500 currently) and to include a rigorous description of the symmetry elements (and plane symmetry groups) contained in them. An example of the current status (still not public) may be found at http://www.therosewindow.com/TheRoseWindow2/Rose-1-Frame.htm.

An article entitled *The Beauty of Rose Windows and the Different Meanings of Symmetry* by Commission member C. Abad-Zapatero has been published [*Acta Cryst*. (2014), D**70**, 907–911].

E. Doorhyhée, Chair

4.11. *ad interim* Commission on Crystallography of Materials

Our *ad interim* Commission was approved at the meeting of the Executive Committee of the IUCr in Boston, USA, in July 2012. This is the newest and in many ways a unique Commission, covering a high-impact and deeply crystallographic topic that has not been covered by other IUCr Commissions.

The Commission has been actively involved in preparation for the Montreal Congress through participation in the International Programme Committee and the organization of 2 Keyonote Lectures and 2 Microsymposia:

Keynote Lecture: Michele Parrinello (ETH Zürich, Switzerland): Atomistic Modelling of Crystal Nucleation and Growth.

Keynote Lecture: Evgeny Antipov (Moscow State University, Russia): Impact of Crystallography on Design of Cathode Materials for Li-Ion Batteries.

MS-12 Crystallography and Physics of Low-Dimensional Systems: Fullerenes, Carbon Nanotubes, Graphene, Topological Insulators and Superconductors.

MS-104 Crystal Structure Prediction and Materials Design.

Our Commission has also co-sponsored a number of Microsymposia with other Commissions.

The conference New Approaches in Computational Materials Design was organized in Moscow, Russia, 13 December 2013, by A. R. Oganov (lecturers: M. Parrinello, A. R. Oganov, V. A. Blatov, V. I. Anisimov, S. Krivovichev, L. Chernozatonskii, A. Dzyabchenko, P. Sorokin, A. Lukoyanov). The conference was oversubscribed (~100 participants) and *Nature Materials* sent its Editor to attend the meeting. The programme and pdf files of the lectures are available at http://cdmlab.fizteh.ru/intconf/Programme.html.

The 7th Russian National Crystal Chemistry Conference was held in Suzdal, 17–21 June 2013 (Programme Chair E. V. Antipov) (http://www.icp.ac.ru/conferences/NCCC2013/1st-announcement.php).

Workshops to disseminate knowledge and technical skills.

The International Workshop on Thermoelectric Research and Thermal Management Technology, NIMS, Tsukuba, Japan, 28 June 2013, was organized by T. Mori, and two workshops on crystal structure prediction were organized by A. R. Oganov (http://uspex.stonybrook.edu/uspexworkshops.html):

Guilin University of Electronic Technology, Guilin, People's Republic of China, 3–8 August 2013.

Northwestern Polytechnical University, Xiquotean, People's Republic of China, 11–12 January 2014.

A. R. Oganov, Chair

4.12. Commission on Electron Crystallography

The year of 2013 witnessed the most exciting developments in biological electron microscopy in the past twenty years. Yifan Cheng and co-workers from the University of California at San Francisco solved a long-standing problem in single-particle cryo-electron crystallography that limited its resolution, *i.e.* specimen movement. Using Gatan's new K2 camera, this group was able to correct specimen movement by averaging subframes. This results in a much improved signal-to-noise ratio, yielding a 3.4 Å structure of the heat sensor TRPV1 channel. This is the first time that the structure of a ~340 kDa biological macromolecule without high internal symmetry has been determined at an atomic resolution, something that was previously only achievable by X-ray crystallography from well ordered crystals.

The Commission is committed to seek opportunities for and to take a leadership role in schools for electron crystallography and diffraction, including imaging. Various workshops, summer schools and symposiums on electron crystallography and microscopy were organized around the world, and the Commission was directly involved in the following.

In Asia: Electron Microscopy and Multiscale Modelling 2013 was held in Kyoto, Japan, 10–13 November 2013 (http://tem-defect.jp/emmm2013/index.html). The EMMM series is a biennial conference which was launched by the Commission in 2007 to bring together electron crystallography experts and scientists involved in materials modelling. It focuses on the link between methods of interrogating structures at the nano- and meso-scale using electron microscopy and diffraction, and the rapidly expanding field of multiscale materials modelling.

In Europe: a biennial workshop on Electron Crystallography of Membrane Proteins, Basel, Switzerland (http://2dx.org/workshop). The workshop dealt with methods to determine biological membrane protein three-dimensional structures from electron crystallography data for two-dimensional membrane protein crystals.

Commission members are also involved in organizing The Advances in Structural and Chemical Imaging meeting at CAMCOR in Eugene, Oregon, USA, 29–30 May 2013, and the 14th Frontiers of Electron Microscopy in Materials Science (FEMMS) meeting in Australia, 8–13 September, 2013.

Lian-Mao Peng, Chair

4.13. Commission on High Pressure

The Commission relied on its unusual size (ten members plus Chair) to maintain sufficient expertise throughout the broad range of different scientific disciplines – from biology through materials science and engineering to solid-state physics – that contribute to the interdisciplinary field of high-pressure crystallography.

The role adopted by the Commission in this multidisciplinary and dynamically evolving field is to facilitate and enable the exchange of new ideas and developments. The main tools available to the Commission to acheive this goal are annual workshops on high-pressure crystallography. The Commission also helps to shape a strong high-pressure programme at the triennial IUCr Congresses. In addition, Commission members and consultants are heavily involved in organizing summer schools dedicated to high-pressure crystallography.

Symposia and workshops. The 2013 Commission Workshop on Advances in Static and Dynamic High-Pressure Crystallography took place at DESY, Hamburg, Germany, 8–11 September 2013. The Local Organizing Committee was headed by Hanns-Peter Liermann (DESY) and Norimasa Nishiyama (DESY). The workshop covered the whole range of activities of the Commission and was attended by 93 scientists from 17 countries, as well as eight exhibitors. The scientific sessions included: (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: Nandini 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 Crystallography (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).

Travel grants for students and young scientists to participate in the workshop were made available through generous contributions from the IUCr, DGK and DESY. The meeting web site can be found at https://indico.desy.de/conferenceDisplay.py?confId=7443. The Commission held a closed meeting during the workshop.

Plans and preparations for the Montreal Congress. The Commission has been represented on the International Programme Committee by P. Dera. The Commission participated in the organization of ten scientific Microsymposia. The Commission was the primary sponsor of six of these Microsymposia and a co-sponsor with other Commissions for the remaining four (Inorganic and Mineral Structures; Neutron Scattering; Crystal Growth and Characterization of Materials; Structural Chemistry; Powder Diffraction): MS22 Phase Transitions in Functional Inorganic Materials and Minerals (Chairs:

Pam Thomas and Vladimir E. Dmitrienko); MS106 From Exo-Planets to Explosives: Ices and Other Molecular Compounds Under Pressure (Chairs: Werner Kuhs and Hiroyuki Kagi); MS39 High-Pressure Crystallography of Periodic and Aperiodic Crystals (Chairs: Vasily Minkov and Clivia Hejny); MS 41 Advances in Experimental Techniques and Data Analysis for Science at Extreme Conditions at Synchrotron and Neutron Sources (Chairs: Simon Redfern and Stanislav Sinogeykin); MS40 Electronic and Magnetic Phenomena at Extreme Conditions (Chairs: Karen Friese amd Karel Prokes); MS42 High-Pressure Solid-State Chemistry and Materials Synthesis (Chairs: Vladimir Solozhenko and Haozhe Liu); MS86 Multiferroics and Other Multi-Functional Materials: Synthesis, Properties and High-Pressure Behaviour (Chairs: Edmondo Gilioli and Lars Ehm); MS28 Non-Ambient Crystallographic Studies of Nanoporous Materials (Chairs: H.-C. Zhou and Stephen Moggach); MS37 Liquids, Amorphous and Nanocrystalline Solids at Extreme Conditions (Chairs: Yoshinori Katayama and Dennis Klug); MS38 Biomolecular Systems Under Pressure – in Memory of Roger Fourme (Chairs: Thierry Prange and Nick Brooks).

In addition to the above Microsymposia, the Commission proposed two Keynote Lectures. That to be given by L. Dubrovinsky was approved.

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 by 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 Chemsitry, CSC, of the IUCr 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 in the IUCr Working Groups on Database Users and on Diffraction Data Deposition.

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 the 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 for the period 2011–2014 and also Commissioning Editor of the *EMU Notes in Mineralogy*. In 2013, the EMU organized the school Minerals at the Nanoscale (Granada, Spain; main organizers: F. Nieto and F. Gervilla) and published Vol. 14 of *EMU Notes*: *Minerals at the Nanoscale* (Editors F. Nieto and K. J. T. Livi). The 2014 EMU school will focus on Planetary Mineralogy, and will be held in Glasgow, UK (main organizer: M. Lee); it has been supported within the Erasmus IP framework. A volume of *EMU Notes* related to the school is also in preparation.

CIMS was involved in the following meetings held in 2013:

2013 Goldschmidt Conference, held in Florence, Italy, 25–30 August. R. Oberti was Co-Chair of the theme The Cutting Edge in Mineralogy and Mineral Physics and a member of the Organizing Committee. The theme organized nine sessions, including GEOLIFE – Geomaterials for Environment, Technology and Human Activities, convened by R. Oberti [with R. Gieré (Freiburg, Germany), S. Quartieri (Messina, Italy) and R. Wogelius (Manchester, UK)]. A Special Issue of *Mineralogical Magazine* devoted to the same topic is in preparation. Another session within the scope of CIMS organized in the framework of the theme was High-Pressure Mineral Physics: A Key to Study Earth Dynamics, convened by P. Comodi (Perugia, Italy), L. Dubrovinsky (Bayreuth, Germany), T. Balic-Zunic (Copenhaghen, Denmark) and R. Caracas (Lyon, France).

O. Yakubovich, Co-Chair of Microsymposium MS-19, ECM28, Warwick, UK, 25–29 August 2013, also gave a talk in MS-18 entitled *A Polysomatic Series of Two-Dimensional Vanadates, Arsenates and Phosphates*.

CIMS has been involved in the organization of the following meetings.

The Montreal Congress; CIMS Chair J. Rocha attended the IPC meeting in Montreal on 6–8 May. In particular CIMS is organizing three Microsymposia:

MS-1, P. Thomas is chairing (with K. Sugiyama): Phase Transitions in Functional Inorganic Materials and Minerals;

MS-15, O. Yakubovich is chairing (with S. Pereira): The Role of Defects in Crystal Structure Formation, Organization and Stability;

MS-74, P. Mercier is chairing (with R. Peterson) Mineralogical Crystallography. Moreover, D. Pandey will deliver a Keynote entitled *The World of Perovskites: the Earth's Lower Mantle Material to Exotic Advanced Materials*.

J. Rocha is a member of the Organizing Committee of the conference SMARTER4, to be held in Durham, UK, 1–4 September 2014.

M. Nespolo and S. Krivovichev represent CIMS on the Advisory Committee of the 2014 Meeting of the International Mineralogical Association, to be held in Gauteng, South Africa, 1–5 September 2014, where CIMS is in charge of the Mineralogical Crystallography sessions.

R. Oberti is Co-Chairing the Organizing Committee of the 1st ECA European Crystallographic School: Reinforcing Foundations to Build the 2nd Century of Modern Crystallography to be held in Pavia, Italy, 28 August – 6 September 2014. This event is funded by Erasmus IP, and will be accompanied by talks open to the citizens to celebrate the International Year of Crystallography (IYCr).

G. Ferraris and R. Oberti are members of the Scientific Committees for the organization of two meetings to celebrate IYCr in Italy: (i) Impact of Crystallography on Modern Science, organized by the Accademia delle Scienze di Torino, to be held in Turin on 25 June, with a talk by Robert Huber, Nobel laureate 1988, entitled *Beauty and Fitness for Purpose: the Architecture of Proteins, the Building Blocks of Life* (R. Oberti will give a talk on the impact of crystallography and crystal chemistry on petrology and geochemistry); (ii) Challenges in Crystallography, organized by the Accademia Nazionale dei Lincei, to be held in Rome on 13–14 October 2014 (CIMS Chair, J. Rocha, will give a talk on *Materials and Crystallography*).

D. Pandey is Chair and M. Nespolo a member of the Programme Committee of the Workshop on Symmetry Relationships Between Crystal Structures with Application to Structural Phase Transitions, to be held in Varanasi, India, 27–31 October, 2014 (both are also lecturers).

CIMS supported the applications for financial funding by the IUCr of the following meetings to be held in 2014:

First ECA European Crystallography School, Pavia, Italy, 28 August – 6 September 2014.

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

XVIII International Conference on Crystal Chemistry, Diffraction and Spectroscopic Studies of Minerals, Yekaterinburg, Russia, 13–15 October 2014.

The CIMS nomination of D. Pandey for Co-editorship of *Journal of Applied Crystallography* has been approved by the IUCr Executive Committee.

J. Rocha, Chair

4.15. Commission on Magnetic Structures

The year has seen a great deal of software development in support of magnetic symmetry and various types of magnetic structural analysis, examples being *FULPROF*, JANA, the Bilbao Crystallographic Server and the *ISOTROPY* suite. As these tools continue to develop and interact, the importance of the pending magnetic CIF standard is growing.

In 2013, the Commission continued the difficult work of establishing standards for describing a magnetic structure, and for relating the three most common descriptions of a magnetic structure: the supercell description, the wave description and the representational (group-theoretical) description. If treated in a fully general way, these descriptions are entirely interconvertible. But a given magnetic structure may be much easier to describe in a non-general way using just one of them. The Commission is preparing a manuscript on this topic.

The book *Magnetic Group Tables*, authored by Commission member Daniel Litvin, and formally reviewed by the Commission, was published by the IUCr in 2013, and is made freely available at http://www.iucr.org/publ/978-0-9553602-2-0 as part of the celebration of the International Year of Crystallography.

Near the end of the year, the Commission created a new web site at http://magcryst.org, which, in addition to providing basic information about the Commission and its activities, provides a flexible means of advertising and supporting a variety of conferences and workshops. In addition to specific pages for events organized, sponsored or otherwise advertized by the Commission, we also provide an extensive list of other meetings where high-quality magnetic-structure research is to be presented (http://magcryst.org/meetings/).

In preparation for the International Year of Crystallography, the Commission has organized a three-day workshop on The Role of Magnetic Symmetry in the Description and Determination of Magnetic Structures (http://magcryst.org/meetings/cmsworkshop2014). This satellite meeting of the Montreal Congress will be held on 14–16 August 2014 at the Brockhouse Institute for Materials Research at McMaster University, which is located in the city of Hamilton near Toronto, Canada. In addition to addressing the theoretical foundations of magnetic crystallography, the workshop will include hands-on software tutorial sessions and a number of applications lectures that demonstrate the effectiveness of magnetic symmetry to simplify structural description and analysis. Eight of our Commission members and consultants participated in a video conference on *Google+ Hangout* on 10 October 2013 to plan this workshop.

Professor Wieslawa Sikora (AGH University of Science and Technology, Krakow, Poland) represented our Commission on the International Programme Committee (IPC) for the Montreal Congress. At the spring 2013 IPC meeting in Montreal, she was instrumental in the planning of an impressive array of lectures and Microsymposia related to magnetic crystallography (http://magcryst.org/meetings/iucr-congress-2014/). This will be an exciting and important Congress for researchers in this field.

Commission members gave featured presentations, developed workshop components, and organized or hosted workshops and Microsymposia at a variety of meetings in 2013. Some were not specifically organized under the auspices of the Commission, but substantially furthered its objectives of promoting magnetic neutron scattering and magnetic structure determination.

Flipper 2013: SCD with Polarized Neutrons, Grenoble, France, 23–25 January 2013 (Jane Brown).

11th TOPAS User Meeting, Gaithersburg, Maryland, USA, 20–21 April 2013 (Branton Campbell).

8th Polish Conference on Neutron Diffraction and Complementary Methods in Investigations of Condensed Matter, Chlewiska, Poland, 16–20 June 2013 (Wieslawa Sikora).

International Conference on Neutron Scattering, Edinburgh, UK, 8–12 July 2013 (Juan Rodriguez-Carvajal, Vladimir Pomjakushin).

Workshop on Resonant Elastic X-ray Scattering in Condensed Matter, Oxford, UK, 15–19 July 2013 (co-sponsored by the Commission).

European Crystallographic Meeting ECM28, Warwick, UK, 25–29 August 2013 (Harold Stokes, J. M. Perez-Mato, Vaclav Petricek).

Joint European Magnetic Symposia (JEMS 2013), Rhodos, Greece, 25–30 August 2013 (Vladimir Pomjakushin).

Master Class on Mott Physics Beyond the Heisenberg Model, Paul Scherrer Institut, Villigen, Switzerland, 26–27 October 2013 (Vladimir Pomjakushin).

FullProf School, Institut Laue–Langevin, Grenoble, France, 18–22 November 2013 (Juan Rodriguez-Carvajal).

Course on Magnetic Neutron Diffraction, September–December 2013, Ural Federal University, Yekaterinburg, Russia (Alexander Pirogov).

B. Campbell, Chair

4.16. Commission on Mathematical and Theoretical Crystallography

During 2013 the Commission (MaThCryst) organized three main activities.

The Society for Industrial and Applied Mathematics (SIAM) organized a Conference on Mathematical Aspects of Materials Science, Philadelphia, USA, 9–12 June 2013. Three Minisymposia on Mathematical Crystallography were organized by MaThCryst; in particular, Greg McColm (Commission consultant) and Massimo Nespolo (Commission Chair) who Co-Chaired the Minisymposia:

MS-9 Mathematical Crystallography: Geometric Foundations (http://meetings.siam.org/sess/dsp_programsess.cfm?SESSIONCODE=16322)

MS3-6 Mathematical Crystallography: Beyond Classical Crystal Symmetry (http://meetings.siam.org/sess/dsp_programsess.cfm?SESSIONCODE=16325)

MS-90 Mathematical Crystallography: Structure-Building Principles (http://meetings.siam.org/sess/dsp_programsess.cfm?SESSIONCODE=16326)

There is a photo gallery at http://www.iucr.org/gallery/2013/mathcryst,-siam.

Topological Methods in Crystal Chemistry and Materials Science, CECAM-HQ-EPFL, Lausanne, Switzerland, 9–13 September 2013. Organizers were Vladislav A. Blatov and Commission member Davide M. Proserpio. web site: http://www.cecam.org/workshop-869.html.

International School on Fundamental Crystallography, Glulechitza, Bulgaria, 30 September – 5 October 2013 (http://www.

crystallography.fr/mathcryst/bulgaria2013.php). Photo gallery at http://www.iucr.org/gallery/2013/mathcryst-bulgaria.

Planned activities include:

Fourth MaThCryst school in Latin America, La Plata, Argentina, 27 April – 3 May 2014 (http://www.crystallography.fr/mathcryst/laplata2014.php).

School on Topological Methods for Expert Systems in Materials Science, Samara Center for Theoretical Materials Science, Samara, Russia, 12–16 August 2014 (http://www.crystallography.fr/mathcryst/topos2014.php).

Montreal Congress Satellite Workshop on the Role of Magnetic Symmetry in the Description and Determination of Magnetic Structures, Hamilton, Canada, 14–16 August 2014, in cooperation with the Commissions on Magnetic Structure, Neutron Scattering, and Aperiodic Crystals (http://magcryst.org/meetings/cmsworkshop2014/).

Second South African School on Fundamental Crystallography, also Satellite meeting of the 21st Meeting of the International Mineralogical Union, Bloemfontein, South Africa, 25–29 August 2014 (http://www.crystallography.fr/mathcryst/SouthAfrica2014.php).

Workshop on Mathematical Crystallography, Symmetry Relationships Between Crystal Structures with Application to Structural Phase Transitions, Banaras, India, 27–31 October 2014 (http://www.crystallography.fr/mathcryst/index.php).

Thematic School on Electron Crystallography (Antwerp, Belgium, 2016).

Fifth MaThCryst School in Latin America, Quito, Ecuador, 2016.

Second Philippines Workshop on Mathematical Crystallography, (Philippines): this was originally planned for late 2014 but the organization was stopped by the flood that severely affected the country. We hope to realize it in 2015.

Publications. A Special Issue on Mathematical Crystallography is in press for *Acta Crystallographica* Section A, with Guest Editors Massimo Nespolo and Gregory McColm.

Other activities. Commission member Stephen Hyde has proposed a workshop on the manifold description of modulated structures and the use of differential geometry to describe crystal structures.

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 2014.

News from Commission members. Gregory McColm, University of South Florida, has joined the Commission as consultant and is proposed as a member for the next term.

M. Nespolo, Chair

4.17. Commission on Neutron Scattering

The activities of the Commission were marked by two main events in 2013. The first was the preparation of proposals for Microsymposia (MS) and Keynote Lectures (KNs) for submission at the spring 2013 meeting of the International Programme Committee, which was held in Montreal. Paolo Radaelli represented our Commission at this meeting, where certain of our proposals for MS and KNs were retained, while others were merged with related proposals by other Commissions, in particular with the Commission on Charge, Spin and Momentum Densities.

Paolo Radaelli was also one of the organizers of the second major event of the year, the International Conference on Neutron Scattering (ICNS), which took place in Edinburgh, UK, 8–12 July 2013. This Conference is held every four years and provides a unique opportunity not only for the neutron community to present the latest scientific and technical developments relating to neutron scattering but also for occasional neutron users to interact with professionals. Around 800 scientists from 34 different countries attended ICNS 2013.

The importance of crystallographic studies was highlighted throughout the Conference sessions, which addressed issues such as the structure of diverse materials, magnetism, biology, geosciences, engineering, energy research and cultural heritage, as well as neutron instrumentation. In addition, to mark the forthcoming International Year of Crystallography and to promote young scientists as the future of neutron research, a Young Scientists' Prize was awarded by the IUCr. Five members of the Commission attended more than 50 high-quality presentations by young scientists before awarding the prize to Elisa Wheeler of the ILL for her work on Probing the Magnetic Excitations of Frustrated Spinels, which was considered the best piece of research underpinned by crystallography.

ICNS 2013 also provided an opportunity for six members of the CNS attending the conference to discuss the Montreal Congress and the ongoing activities of the Commission relating to the IYCr. The involvement of regional neutron scattering associations in the organization of the IYCr was also discussed with members of the European Neutron Scattering Association and with the President of the Asia–Oceania Neutron Scattering Association (and former chair of the CNS), Professor Y. Fujii.

In keeping with the Commission's objectives to promote the use of neutron scattering, CNS members have been very active throughout 2013 in organizing and participating in crystallography-related workshops, schools and seminars. In April 2013, P. Langan organized the conference Frontiers in Neutron Structural Biology at the Oak Ridge National Laboratory's Spallation Neutron Source. He also participated in the 4th International Symposium on Diffraction Structural Biology (ISDSB2013) held in Nagoya, Japan, 26–29 May 2013. Shane Kennedy gave lectures on *Polarization in Neutron Beam Science*, and *Magnetically Induced Phase Transitions in Intermetallic Compounds* at the School on the Fundamentals of Neutron Scattering, Natal, Brazil, 2–14 September 2013.

At the 2013 Annual General Meeting of the American Crystallographic Association, which took place in Honolulu, USA, 20–24 July 2013, Garry McIntyre gave a talk on *Exotic Physics in Neutron Laue Diffraction*, and Thomas Proffen organized a two-part Microsymposium on Nanomaterial Structure from Diffraction Data, part I of which was on theory and modelling with part II covering experimental advances.

The Commission has given its support to the 6th AONSA Neutron School, Serpong, Indonesia, 12–17 October 2014, which will be sponsored by the IUCr.

Finally, the Commission has been and continues to be actively involved in a variety of activities aimed at preparing for the International Year of Crystallography in 2014. In this context, the Commission is currently co-organizing with the Commission on Magnetic Structures a workshop on the Role of Magnetic Symmetry in the Description and Determination of Magnetic Structures. This IUCr Congress Satellite Workshop will take place in August 2014 at the McMaster University in Hamilton, Canada, and will focus on the role of magnetic symmetry in the solution and refinement of magnetic structures. It will include lectures on the description of magnetic structures in terms of symmetry operators as well as hands-on tutorials on the solution and refinement of magnetic structures obtained by magnetic neutron diffraction.

M. T. Fernandez-Diaz, Chair

4.18. Commission on Powder Diffraction

2013 was a particularly active year on a number of fronts both for the Commission (CPD) and powder diffraction in general.

The 4th in the series of Accuracy in Powder Diffraction (APD) meetings was held at NIST in April 2013. These meetings are high-profile meetings held about every 10–15 years. Various CPD members past and present were involved in the organization and programme. Many thanks are due to Jim Cline (NIST), Jeff Post (Smithsonian Institution) and Ian Madsen (CSIRO) for the hard organizational efforts. I am sure that all those who attended will remember the evening visit to the Smithsonian 'Blue Room' to view the stars of the Gem and Mineral collection, and many thanks to Jeff for arranging it. Anyone who publishes structures from powder diffraction data in IUCr journals will be aware of some of the shortcomings of the powder CIF dictionary. Despite huge efforts by Brian Toby over many years, the single-crystal heritage of the CIF format continues to cause headaches. Discussions were held during 2013 on possible development paths to better support powder data now and in the future. The prospect of capturing the details of parametric refinements looks a little daunting in the current framework but the issue was one of many discussed with representatives of the IUCr journals during the APD meeting.

As expected, the programme for the Montreal Congress was front and centre of a number of months. Owing to an unusual combination of circumstances I was a stand-in during the IPC meeting in Montreal in May 2013. Together with Dave Billing at the meeting and Radomir Kuzel *via* e-mail, I am pleased to say that powder diffraction is well represented in the final programme with many joint sessions.

The excellent powder diffraction Erice school of 2011 is not forgotten. A valuable legacy was the videos of all the presentations given during the school, including some software-related sessions. During 2013 it became obvious that the commercial streaming service hosting the files had 'lost' some of the content, so efforts were made to retrieve and preserve what was left. In addition to those downloaded from the streaming provider, thanks are due to the Erice organizers for assistance in locating some of the missing files. Even greater thanks are due to Brian McMahon at the Chester office for his help in hosting the content and setting up the material on a new section of the CPD web site. The videos of the retrieved presentations (and Powerpoint slides of some of those that were lost) are now accessible both on the Schools and Workshops section of the CPD web site and *via* YouTube. It is intended that more educational content and links to external education material will be added in the future. To date, links to the slides of the Canadian Powder Diffraction Workshop and Patras Crystallography School have been added.

The usual business of considering applications for support for IUCr meeting sponsorship continued. For 2013 meetings there was a particularly strong showing from the Americas with three South American (Uruguay, Brazil and Argentina) and the APD meeting in the USA. The latter was the first USA-based meeting to submit an application for many years. Additional meetings were supported in Greece and Ethiopia, together with the Durham Powder Diffraction and Rietveld Refinement School held in early 2014. A number of applications were received from organizers of individual Microsymposia in larger international meetings. These did not fare well with the feedback from the Commission membership, the general feeling being that it would be an inappropriate use of limited funds.

P. Whitfield, Chair

4.19. Commission on Small-Angle Scattering

Commission meetings and communication. During 2013, Commission (CSAS) members communicated by e-mail or during personal meetings at national and international conferences. Virtually all CSAS members and consultants contribute to the various activity categories on an ongoing basis. What follows is a summary of highlights for 2013.

Commission activities. During 2013, Commission activities moved from a focus on the SAS2012 meeting of the previous year to planning for SAS-related activities at the Montreal Congress, and initial planning for SAS2015 to be held in Berlin, Germany, September 2015. CSAS activities also included planning for the International Year of Crystallography, IYCr2014.

Following the SAS2012 conference in November 2012, the SAS Commission Chair (and *Journal of Applied Crystallography* Deputy Editor) A. Allen worked with the Conference Chair, E. Gilbert, in 2013 to assemble a group of Guest Editors that included CSAS consultants, Y. Amemiya and D. Svergun, for a *J. Appl. Cryst*. Special Issue featuring a small number of selected papers associated with the conference. A proportion of the papers submitted were pre-selected for review and 24 papers were eventually accepted for publication, firstly in regular *J. Appl. Cryst.* issues in 2013 and 2014, then collected together in a Special Issue, just published in 2014. The Special Issue presents a good cross section of cutting-edge SAS papers to represent state-of-the-art in the field for IYCr2014. Furthermore, this select Special Issue publication presents a possible option for publication of papers associated with the SAS2015 and SAS2018 conferences, and beyond.

During 2013, CSAS members and consultants have continued to work with E. Gilbert in his role as a member of the International Programme Committee (IPC) for the Montreal Congress. Following discussion and suggestions from the Commission, an unprecedented number of SAS-related Microsymposia are planned for the Congress to mark IYCr2014. These include Microsymposia covering the following areas: SAS of biological macromolecules; SAS for magnetism and magnetic structures; grazing incidence surface techniques; simultaneous methods with SAS; *in operando* and structure evolution – from atomic to micrometre scale; industrial and technological applications of SAS; applications of anomalous SAXS. Other planned Microsymposia include a SAS component. Some CSAS members have been asked to Chair or Co-Chair Congress Microsymposia. Takeji Hashimoto has been invited to give the SAS-related Keynote Lecture *Applications of Small-Angle Scattering to Macromolecules and Polymer Physics*. An Open Meeting of the Commission is planned during the Congress to report on CSAS activities over the past three years.

Starting with the SAS2012 conference, discussions were initiated between the Commission and the SAS2015 Organizing Committee (Chair: D. Clemens). These continue into 2014 and will include the items discussed in last year's report on the SAS2012 Conference.

CSAS consultant D. McGillivray and CSAS chair A. Allen continued to explore ways to modernize and revise the Commission web page, and to link it with the 'SAS Portal' to provide a greater level of educational and reference information to SAS researchers. Changes are expected to be implemented in time for the 2014 IUCr Congress.

CSAS member P. Jemian and consultant D. McGillivray have continued work as part of the canSAS group. For some years, this group of SAXS and SANS beamline scientists, users and software developers 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. In 2013, the canSAS group released version 1.1 of the canSAS standard for storing one-dimensional (1-D) SAS data and metadata in XML files. 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 at http://smallangle.org. This work is ongoing.

Various CSAS members made plans during 2013 to mark the celebration of IYCr2014. These include active involvement in symposia and sessions at conferences to be held around the world during 2014, together with specific activities mentioned above and in the sections that follow.

Educational activities. CSAS members and consultants organized the following courses to improve awareness of SAS-related methods in 2013:

V. Volkov – annual lecture course to undergraduate and post-graduate students, Institute of Nuclear Physics and Physics Department, Moscow State University (MSU): Supra-Atomic Structures in Nanomaterials [now including X-ray free-electron laser (XFEL) opportunities for investigation of nanocrystals and macromolecules, as well as new approaches in SAS data treatment]; also lecture course on SAS methods, Physics Department, MSU, as part of a larger course on X-ray Methods for Investigation of Matter; training course on Investigation of Structure of Nanoscale Disperse Systems by Small-Angle Scattering Methods, also at MSU; training course on SAXS Instrumentation and Data Treatment for young students from Mordovia State University (Saransk, Russian Federation).

D. Svergun – educational lectures in 2013 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 of Local Organizing Committee and conducted SAXS beamline practicals for 13th SPring-8 summer school, July 2013, and for 7th AOFSRR (Asia/Oceania Forum for Synchrotron Radiation Research) Cheiron School, SPring-8, September/October 2013.

P. Jemian – assisted in courses on *Irena*, *Indra* and *Nika* software packages in *IgorPro* for SAS analysis given at the Advanced Photon Source, ANL and elsewhere.

Community-building activities. CSAS members and consultants served on various SAS-related committees, panels and editorial boards in 2013 (excluding the *J. Appl. Cryst.* SAS2012 Special Issue):

G. Kostorz – co-organizer and speaker at TMS Symposium on Scattering Methods in Materials Science (San Diego, California, USA); continued efforts to familiarize materials scientists with scattering methods; continued service as Co-editor for *Journal of Applied Crystallography*.

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

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

D. Babonneau – appointed regional representative to serve as a bridge with the French steering committee of IYCr2014.

N. Yagi – Plenary talks on time-resolved SAXS experiments at users' meeting of NSRRC, Taiwan (September 2013) and 11th International Conference on Biology and Synchrotron Radiation (Hamburg, Germany, September 2013).

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

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

D. McGillivray – Chair of Instrument Advisory Team for recently commissioned Kookaburra USANS instrument at ANSTO, NSW, Australia.

V. Volkov and the Institute of Crystallography (Moscow) – continued to consult in 2013 for various scientific and engineering institutes in Russia: National Research Centre 'Kurchatov Institute', Institute of Molecular Biology, Institute of Physical Chemistry, Institute of Elemento-Organic Compounds, Institute of Inorganic Chemistry, plus the Chemical and Physical Departments of Moscow State University.

N. Yagi – advisor for design of proposed LIX (High Brightness X-ray Scattering for Life Sciences) beamline at NSLS-II, Brookhaven Laboratory, New York, USA, attended beamline Advisory Team meeting, August 2013; also adviser for Advanced Soft Material beamline, SPring-8 (a dedicated SAXS beamline for industry-oriented polymer and soft materials science).

Organizational activities. In 2013 J. Trewhella and D. Svergun followed up on their previous work on publication guidelines for structural biology applications of SAS. A letter was sent in June 2013 on behalf of the Commission to the Editors of many of the high-impact journals that publish papers on structural applications of SAS. All responding Editors were positive regarding the guidelines outlined. Following a meeting of the Worldwide Protein Data Bank (wwPDB) Small-Angle Scattering Task Force Working Group on Theoretical Model Validation at Rutgers University, New Jersey, USA, in October 2013, Cell Press expressed an intention to adopt the guidelines if an easy 'table' form could be provided that would make it simple for authors, reviewers and editors to follow the guidelines. A proposed table is under development, following updates to the guidelines after review of the recommendations of the wwPDB SAS task force (see below).

At the SAS2012 Conference there was general support for the publication guidelines but a request was made for a mechanism for community input. To that end, a web site was established in 2013 that included the SAS2012 presentation material concerning the activities of the IUCr-supported publication guidelines and wwPDB SAS task force. This web site also accepts submissions (http://sas.wwpdb.org/) for comments and suggestions, and has been announced through the sa_scat discussion listserver: (http://mailman.iucr.org/mailman/listinfo/sa_scat).

Regarding wwPDB SAS task-force activities, a meeting report with recommendations of the task force was published in *Structure* [Trewhella *et al*. (2013), freely available for download at http://www.cell.com/structure/abstract/S0969-2126%2813%2900150-0]. Noting that the task force is focused on that subset of SAS relating to biomolecular structural modeling, the task force recommended:

a global repository to hold standard format SAXS and SANS data that is searchable and freely accessible for download;

options should be provided for including in the repository SAS-derived shape and atomistic models based on rigid-body refinement

against SAS data along with specific information regarding the uniqueness and uncertainty of the model, and the protocol used to obtain it;

criteria need to be agreed for assessment of the quality of deposited SAS data and the accuracy of SAS-derived models, and the extent to which a given model fits the SAS data.

It was the view of the task force that a SAS-data and model archive would be separate from but federated with the wwPDB.

At the meeting of the wwPDB Working Group on Theoretical Model Validation (October 2013), J. Trewhella gave a presentation on validation and assessment of SAS-derived biomolecular models. The recommendations of this workshop will be published and will feed into the work of the SAS task force – scheduled to meet next in May 2014 to advance discussions on:

the requirements for the recommended global repository, including the definitions of terms for data collection and for managing the data repository and model archive;

the criteria for assessment of the quality of deposited SAS data, the accuracy of SAS-derived models, and the extent to which a given model fits the SAS data;

communications with journal Editors on publication guidelines;

next steps required for implementation.

SAS Commission members and consultants served on several programme or organization committees for SAS-related conferences and workshops in 2013:

D. Babonneau – appointed Co-Chair: 3rd International GISAS meeting, 2015 (satellite conference of SAS2015 in Berlin, Germany).

D. Svergun – organizer and Co-Chair, 11th Biology and Synchrotron Radiation Conference (BSR), Hamburg, Germany, September 2013 (http://www.bsr2013.org), including visits to Petra-3 storage ring and the DESY FEL: mainly European attendance, but some from across the globe. SAXS presentations accounted for one-third of the conference and demonstrated how SAXS has become a key method in structural biology, and SAXS presentations proved highly multidisciplinary in their presentation. BSR2016 will be in Stanford, USA.

U.-S. Jeng and R. Serimaa – organizers of Microsymposium on Industrial and Technological Applications of Small-Angle Scattering at the IUCr Congress.

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 – continued development of *FitGISAXS* (software package for modelling and analysis of GISAXS data using *Igor Pro*; see http://theory.phymat.sp2mi.univ-poitiers.fr), and presentation of several invited talks on the quantitative analysis of GISAXS data, especially those from ion-sputtered surfaces and sputter-deposited thin films.

A. Allen – continued development of 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) intended for issue during IYCr2014; also continued contributing to ISO TC24/SC4 (Particle Size Committee) SAXS particle size (best practice) standard. A. Allen also contributed a chapter on heterogeneous materials for the new Voulme H of *International Tables for Crystallography*.

U.-S. Jeng – leading construction of new, dedicated, high brilliance, biological SAXS/WAXS NSRRC beamline at the new 3GeV synchrotron, planned to be operational in 2015.

P. Jemian – continued implementing goals of the canSAS 1-D standard in XML and supporting code packages and documentation. Working on coordinating goals of the canSAS standard for multidimensional SAS data within scope of 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

Different members of the Commission (CSC) have been active as organizers, tutors, lecturers or participants in most of the events endorsed by the Commission. In most cases they have sent informal reports to the Commission Chair evaluating the appropriateness of the Commission support. Topics covered ranged from non-covalent interactions, crystal engineering, dynamic structural science and photocystallography to proper crystallization.

The activities during 2013 have been mainly addressed to the contribution of the Commission to the Scientific Programme of the Montreal Congress, trying to obtain a strong and attractive programme in the chemical crystallography sector. Two Commission representatives were members of the International Programme Committee (S. E. Bourne and P. R. Raithby) and they collected proposals from the chemical crystallographic community together with those from Commission members. A total of 12 Microsymposia (MS) suggested by the CSC representatives, strictly related to CSC topics, were included in the Programme, together with three additional MS with shared interests; three Keynote Lectures and one Plenary Lecture are also directly connected to the concerns of the Commission. A couple of workshops, closely related to CSC topics, complete the offer for chemical crystallographers.

Regarding IYCr2014, the Commission exchanged several e-mails considering the possibility of organizing some events supported and organized directly by the Commission. Unfortunately, none of the proposals arrived to a proper conclusion, although most have been organized by members of the Commission on a national scale (videos, preparation of exhibitions, crystal-growth contests *etc.*).

Unfortunately, the expected reinforcement of potentialities between CSC and other Commissions through the existence of consultants from other Commissions on the CSC has not worked as smoothly as we had expected. Very limited interaction has been established with other Commissions and with scientists working in industry. We are convinced this system could put more energy into the running of the IUCr, and consequently a major effort should be made in the future to secure the interchange of initiatives, opinions and documentation among Commissions.

Some points still need to be addressed by the Commission. Earlier topics to be revisited are the contents of the IUCr *Online Dictionary* – work to be done in clear and close collaboration with the Commission on Crystallographic Nomenclature – and analysis of the convenience of an IUCr-supported International School on Structural Chemistry.

F. J. Lahoz, Chair

4.21. Commission on Synchrotron Radiation

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

bulk of the Commission's work is carried out *via* e-mail, with occasional face-to-face meetings held at selected conferences attended by sufficient of the Commission members.

The progress of synchrotron radiation and FEL-based user facilities and science continued at a rapid pace. In particular, the two operating XFEL facilities, LCLS in the USA and SACLA in Japan, are beginning to make very significant impacts in crystallography, especially in structural biology where the techniques of nanocrystallography and serial femtosecond crystallography are maturing. The past three years have seen these techniques advance from test experiments involving well known structures to the first determination of an unknown structure, *Trypanosoma brucei* cysteine protease cathepsin B (TbCatB) [Redecke *et al.* (2013), *Science* **339** (6116), 227–230]. These techniques are being supported by rapid technical advances in sample delivery, improving the hit rate (proportion of XFEL pulses that hit a crystal and produce diffraction data), detectors, data indexing and analysis software *etc.* In addition, novel crystallography techniques continue to be developed, such as the SLAC development of two colour laser pulses, and work continues at many institutions towards the goal of single-molecule imaging.

Demand for access to LCLS and SACLA is high and continues to grow rapidly, and new FEL sources are under construction or being planned. The European XFEL in Hamburg, Germany, is scheduled to begin user operation in 2017, the Swiss FEL project has a similar schedule, and the Pohang Accelerator Laboratory XFEL is under construction in South Korea and expected to start commissioning in 2016. Soft X-ray FEL facilities are also continuing to produce high-impact science, at facilities such as FLASH in Hamburg, Germany, and FERMI in Trieste, Italy.

The XFEL sources offer performance far in advance of today's storage-ring-based synchrotron-radiation facilities. Current XFEL sources offer peak brightness 9–10 orders of magnitude greater, pulse lengths 1000 times shorter, and much higher coherence than the best third-generation light sources. However, the development of storage-ring-based light sources is continuing, and promises to 'fill in' at least part of the large performance gap to the FEL sources. Several new high-brightness storage-ring facilities are in their final stages of construction and commissioning, led by NSLS II at Brookhaven National Laboratory, USA, MAX IV at Lund, Sweden, and the Taiwan Photon Source in Hsinchu, Taiwan; all offer significant brightness upgrades from current sources.

Proposed name change. In recognition of the increasing significance of free-electron laser sources to crystallography, the Commission proposes to modify its name to the Commission on Synchrotron and XFEL Radiation. This change was discussed and unanimously supported by Commission members in 2013.

The International Year of Crystallography. The synchrotron community in general has embraced the IYCr in a number of capacities. The synchrotron light source facilities are particularly supportive, with around 15 directly sponsoring the IYCr and all planning to host special events, dedicated sessions at their user meetings *etc.* In addition, many X-ray and synchrotron relevant conferences in 2014 are planning similar commemorative sessions, and some events were held in late 2013 as a lead-in to the IYCr. Two examples are: the Australia–France video link *Bragg Symposium – Crystallography for Life* hosted jointly at ANSTO in Australia and the ILL in France on 28 November 2013 (members of both the Synchrotron Radiation and Neutron Scattering Commissions were involved in planning this event); and the International Conference on Structural Genomics (ICSG) held in Tsukuba, Japan, in 2013 (Soichi Wakatsuki chaired the Organizing Committee), which included a special session on the 100th year of X-ray crystallography.

Commission member Jean-Louis Hodeau has been particularly involved in planning a number of European activities to celebrate the IYCr and the associated centenary of the Laue–Bragg discoveries. This includes events for the general public: Le Monde à l'Envers, 100 Ans de Cristallographie – ou Comment Voir le Cristal, la Matière, la Vie in France; and translating and producing crystallography-based games (e.g. Symmetry Mirror Rules), and exhibitions at the Opening Ceremony for the IYCr in Paris, France.

Montreal Congress. The Commission was represented by Richard Garrett on the International Programme Committee for the Montreal Congress. Following on from the Open Commission Meeting held at the Madrid Congress, where the participants suggested that more joint symposia be proposed for future Congresses, the Commission worked with a number of relevant Commissions to propose symposia for the Montreal Congress. The following Microsymposia were successfully proposed: High-Resolution Charge Density using SR, jointly proposed with the Commission on Charge, Spin and Momentum Densities (MS-CCSMD-7); Advances in Experimental Techniques and Data Analysis for Science at Extreme Conditions at Synchrotron and Neutron Sources, jointly with the Commission on High Pressure (MS-CHP-5); Applications of Anomalous Small-Angle X-ray Scattering to Soft Materials and Biomolecular Systems, jointly with the Commission on Small-Angle Scattering (MS-CSAS-2); Time-Resolved Spectroscopic Studies with Synchrotron Radiation and Free Electron Laser Sources, jointly with the Commission on XAFS (MS-CXAFS-1); XFEL Macromolecular Crystallography, jointly with the Commission on Biological Macromolecules (MS-CSR-1); X-ray, Muon and Neutron Studies of Magnetic Structure in Materials, jointly with the Commissions on Neutron Scattering and Materials Science (MS-CNS-5).

In addition, the Commission successfully proposed the following Microsymposia: Advances in X-ray FEL Coherent Scattering and Diffraction (MS-CSR-2); Advances in X-ray, Neutron and Electron Detectors (MS-CSR-3); and successfully proposed two Keynote presentations: *Future Light Sources and their Impact on Structure Studies* by Edgar Weckert (DESY) and *Use of Two Colour XFEL Modes for SAD/MAD Phasing and Improved Intensity Measurements for de novo Macromolecular Structure Determination* by Soichi Wakatsuki (SLAC).

In recognition of the increasing impact of the XFEL facilities in crystallography, and of the need to inform the world community of crystallographers of what is possible and how to access these sources, the Commission proposed and is organizing a one-day workshop on 5 August 2014 entitled Crystallography at XFEL Sources, which is WK-05. The aim of this workshop is to introduce Congress participants to the new capabilities of the XFEL sources, and to provide information and advice on how best to carry out a successful XFEL experiment.

R. F. Garrett, Chair

4.22. Commission on XAFS

At the beginning of 2013 the organization of the Commission (CXAFS) changed, with Chris Chantler (University of Melbourne, Australia) taking over responsibility as Chair.

During 2013 CXAFS put forth a strong proposal for its activities at the Montreal Congress; the goal of these activities – a wide-ranging list of Microsymposia and a one-day Tutorial for Crystallographers and Beginners – is to increase the appreciation and visibility of XAFS in the IUCr community. The proposal was discussed and approved at the meeting of the International Programme Committee held in

Montreal and attended by the CXAFS Chair. The programme of the Montreal Congress will include a record number of six Microsymposia (MS) related to XAFS; these Microsymposia are organized by CXAFS in collaboration with other Commissions. The one-day tutorial to be held on 5 August 2014 follows the very successful events held at two previous Congresses.

Another major activity was the preparatory work for the proposal of Volume I of *International Tables of Crystallography* dedicated to X-ray absorption spectroscopy. Following discussions within CXAFS it was agreed that topics to be included are (preliminary contents): XAS theory, experimental methods, processing of experimental data, data analysis, survey of packages in common usage for data collection and reduction, theoretical prediction and data analysis, data exchange and deposition, application, useful tables and definitions of XAS-related terms. The Commission believes that publication of this volume of *International Tables* will greatly strengthen the standing of XAFS in the crystallographic community, and also the reception and development of XAFS and the Commission work in the international XAS community.

Other CXAFS activities include the maintenance of the compendium of XAFS beamlines in the world, which is available on the Commission web site hosted on the main IUCr web server. While the Congress in the International Year of Crystallography was a key focus, the earlier sponsored International Symposium on Radiation Physics was a great success and the Proceedings in the 2014 January issue of *Radiation Physics and Chemistry* is an excellent sign of potential outcomes from support and sponsorship. It is important for this support to be seen as real by the wider communities and to look forward to joint workshops and international conferences over the next period.

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 2013 the Executive Committee approved sponsorship of various schools and meetings, mostly with financial support. Those held in 2013 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 2014, but approved in 2013, are listed below.

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

Southern Africa Powder Diffraction Conference and Workshop, Johannesburg, South Africa, 27–31 January 2014.

Powder Diffraction and Rietveld Refinement School, Durham, UK, 30 March – 3 April 2014.

Electron Crystallography School – Introduction to Electron Diffraction Tomography, Darmstadt, Germany, 7–11 April 2014.

Macromolecular Crystallography School 2014: From Data Processing to Structure Refinement and Beyond, Sao Carlos, Brazil, 8–16 April 2014.

RapiData 2014, Brookhaven, USA, 13 April – 2 May 2014.

International School on Fundamental Crystallography 2014 (ISFC 2014), La Plata, Argentina, 27 April – 9 May 2014.

Hot Topics in Contemporary Crystallography, Sibenik, Croatia, 10–15 May 2014.

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

Structural Basis of Pharmacology: Deeper Understanding of Drug Discovery Through Crystallography, Erice, Italy, 30 May – 8 June 2014.

International Expo/Sir Workshop, Bari, Italy, 10–13 June 2014.

1st International Symposium on Halogen Bonding (ISXB-1), Lecce, Italy, 18–22 June 2014.

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

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

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 Sub-committee on the Union Calendar that the authorities of the country in which the meeting is to take place guarantee free entrance of *bona fide* scientists from all countries.

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

Commission is required. Full details may be found at http://www.iucr.org/iucr/sponsorship/vp.html.

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

COMCIFS is charged with maintaining and developing the Crystallographic Information Framework (CIF) on behalf of the IUCr. The past decade has seen a great deal of effort expended on upgrading the set of standards that underpin CIF, with major emphasis on improving the language used to define data items in CIF dictionaries. This new language, DDLm, combines the best aspects of the previous DDL1 and DDL2 languages and adds a machine-readable way of specifying canonical mathematical relationships between data names. With these new standards now stabilized, the focus this year shifted towards implementation and creation of tools and dictionaries that leverage these standards. This year has seen a major step forward in this work, with the release of IUCr-funded software that can use the rich information in these new-style dictionaries, for example, to validate values in a CIF file. An intense and highly successful two-day workshop was held in Warwick, UK, in August to discuss the new standards and software. This was followed by a well attended one-day data management symposium immediately prior to the ECM.

Macromolecular developments. The Worldwide Protein Data Bank (wwPDB; http://wwpdb.org/) has established PDBx/mmCIF as the new standard format for data exchange and archiving in structural biology. Adopting PDBx/mmCIF will help address the challenges of ever greater numbers of PDB depositions, involving ever larger and more complex structures, often determined using multiple methods. (See: http://www.wwpdb.org/news/news_2013.html#22-May-2013.)

During this year wwPDB has released a completely new system for deposition and annotation of PDB entries. This new wwPDB deposition and annotation system uses PDBx/mmCIF for data processing and data exchange operations. As a result, the the new deposition system is able to support the deposition and processing of large structures as single PDBx/mmCIF files. This avoids the prior practice of dividing large structures into multiple PDB entries required to support the older record-oriented PDB format.

The wwPDB has convened a Working Group for PDBx/mmCIF Data Deposition (http://wwpdb.org/workshop/wgroup.html) that includes representatives from the major X-ray structure determination packages, and is chaired by Paul Adams. The Working Group has made recommendations about essential content extensions required for the deposition of large structures. PDBx/mmCIF files suitable for deposition can now be created with recent versions of the CCP4 (*REFMAC* 5.8) and *Phenix* (1.8.2) software packages. Both *Phenix* and CCP4 software packages support the above extensions for large structures.

To help facilitate the transition from PDB to PDBx/mmCIF format, the wwPDB has organized two PDBx/mmCIF workshops: the PDBx/mmCIF Data Exchange Format For Structural Biology (October 2013) at the Center For Integrative Proteomics Research, Rutgers, The State University of New Jersey, USA, and the wwPDB Workshop on mmCIF/PDBx for Programmers (November 2013) at the European Bioinformatics Institute, Cambridge, UK. The wwPDB has also created a new web site hosting PDBx/mmCIF resources at http://mmcif.wwpdb.org.

Interaction with other data management initiatives. COMCIFS has close links with the Diffraction Data Deposition Working Group (DDDWG) through participation of COMCIFS members in the DDDWG and the shared concern with metadata. COMCIFS has therefore appointed a small group that is available to advise the various IUCr Commissions as they embark on their own processes of metadata codification in line with the DDDWG's's recommendations.

In a related vein, as other scientific disciplines begin to formalize data archiving and transfer, overlap with IUCr definitions becomes likely. Harmonization of definitions is desirable to minimize the work required when translating or ingesting such foreign data files. NeXuS is a major emerging standard for raw data archiving at large-scale facilities, which overlaps significantly with imgCIF for single-crystal crystallography. A major step forward in 2013 was a joint decision of the NeXus International Advisory Committee and COMCIFS to work together on harmonized datanames, the result of which will be that raw data files written according to specific NeXus standards may be routinely read in by CIF software and *vice versa*. A draft standard and accompanying changes to CIF community software are already available. This work sets an important and promising precedent for collaboration and harmonization of data standards throughout the sciences.

Future plans. Over the coming year COMCIFS will initiate a review of the current core CIF dictionary and a group led by J. A. Kaduk will look at improving *checkCIF* handling of powder data files. Further software leveraging the new CIF standards is also under development by various COMCIFS members, and the long-awaited twinning dictionary will be published.

J. Hester, Chair

7. *IUCr Newsletter*

All issues of Volume 21 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, obituaries, 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 for issues 1, 2 and 3; Bill was responsible for issue 4. Patti Potter was responsible for layout and all phases of production and distribution.

Each issue devoted two pages to brief summaries of selected articles recently published in IUCr journals. All four issues contained coverage for the IUCr Congress. Issues 2, 3 and 4 contained articles pertaining to IYCr2014. Issues 1, 2 and 4 contained reports on the three Regional Associates.

Additional meeting and workshop reports were published covering activities in Australia, Belgium, Canada, Croatia, Italy, Poland, Singapore, the UK and the USA. Future meeting announcements included the Montreal Congress as well as meetings in Austria, Italy, Poland and the USA.

Distribution was done 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 went to several meetings, including the Regional Associates' annual meetings.

W. L. Duax, Editor, and **P. Potter**, Production Manager

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

In 2013, the cooperation between Oxford University Press (OUP) and the IUCr/OUP Book Series Selection Committee was quite productive.

A history book has been published:

Early Days of X-ray Crystallography, by André Authier, published 1 August 2013.

Three new volumes have been published in the *IUCr Texts on Crystallography* series:

18 – *Symmetry Relationships between Crystal Structures. Applications of Crystallographic Group Theory in Crystal Chemistry*, by Ulrich Müller, published 4 April 2013.

19 – *Small-Angle X-ray and Neutron Scattering from Solutions of Biological Macromolecules*, by Dmitri I. Svergun, Michel H. J. Koch, Peter A. Timmins and Roland P. May, published 8 August 2013.

20 – *Phasing in Crystallography. A Modern Perspective*, by Carmelo Giacovazzo, published 12 December 2013.

In addition, Monographs 19 (*Molecular Aggregation – Structure Analysis and Molecular Simulation of Crystals and Liquids*, by Angelo Gavezzotti) and 23 (*The Nature of the Hydrogen Bond*, by Gastone Gilli and Paola Gilli) have been republished in paperback.

A number of new books are in the production phase and others are in the pipeline. The Committee and the OUP editing staff reviewed a number of proposals and there are 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 2013 ACA Council consisted of Cheryl Stevens (President), Martha Teeter (Vice-President), George Philips (Past-President), S. N. Rao (Chief Financial Officer and Interim Treasurer), Jim Kaduk (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 ACA paid membership was 1574 by end of 2013.

ACA Honolulu. The highlight of the year is always the ACA Annual Meeting, which in 2013 was held in Honolulu from 20–24 July, and was attended by 767 delegates. The Programme Chairs were Allen Oliver and Jeanette Krause. This meeting continued the four-day format, featuring 20 oral sessions (263 talks) and three evening poster sessions with 291 presentations. The meeting was preceded by three workshops: Biological SAXS – Theory and Practice; Introduction to GSAS-II Crystallographic Analysis System; and Getting the Most out of the Cambridge Structural Database. There were four Transactions Symposia on various aspects of the role in crystallography of neutron and synchrotron sources: TR.01, chaired by Richard Gillilan, was concerned with Small-Angle Scattering; TR.02, chaired by Christine Dunham, focused on Supramolecular Assemblies; TR.03, chaired by Antonio dos Santos and Jonathan Hanson, featured Emerging Characterization Facilities and Tools; and TR.04, chaired by Christine Beavers and Simon Teat, was about Chemical Crystallography.

Four of the ACA's major awards were presented at the meeting in Honolulu. The first Bau Neutron Diffraction Award was presented to Tom Koetzle, the Fankuchen Award went to Richard Dickerson (as he was unable to attend, Alex McPherson presented a retrospective on Dickerson's career). The Trueblood Award went to Tom Terwilliger, and Eric Ortlund received the Etter Early Career Award. Finally, the third class of ACA fellows was approved and announced at the ACA banquet. New ACA Fellows inducted are Sidney Abrahams, Wim Hol, Jim Ibers, Alex McPherson, Keith Moffat and Alex Wlodawer.

The ACA Council undertook a number of important actions in 2013:

IYCr2014: Considerable discussion was devoted to the International Year of Crystallography 2014 (IYCr2014) and how the ACA could best support this initiative. Martha Teeter, the ACA Vice-President, is spearheading this effort. She has formed an *ad hoc* Committee to coordinate regional celebrations and activities, as well as provide ideas for IYCr2014. In addition, she has been working with the USNCCr and others to write a proposal to submit to the NSF.

The Task Force is considering a range of topics, including school outreach, media, web outreach, funding, and liaisons with politicians and with other scientific organizations. The ACA Council committed USD 12000 to fund activities related to IYCr2014 in North America. Of this amount, about USD 5000 will be allocated *via* a call for proposals with the balance used for Task Force projects, including a National Crystal Growth Contest.

ACA Journal. The ACA has agreed with the AIP (American Institute of Physics) to co-publish a new online journal titled *Structural Dynamics*. The AIP representatives to the Board of Managers are Mark Cassar and Chris McMahon, with Judy Flippen-Anderson and Soichi Wakatuski representing the ACA. The Editor is Majed Chergui with Thomas Elsaesser, George Phillips, Franz Pfeiffer, Gwyn Williams and Linda Young as Associate Editors. Journal topics include structural dynamics of molecular systems, biological systems, solid materials, liquids and solutions, and surfaces and interfaces studies using highly coherent sources; with a time resolution from femtoseconds to milliseconds; and spatial resolutions from 1 Å to 1 mm (see http://sd.aip.org).

Strategic planning. A strategic planning committee of Cheryl Stevens (Chair), Bill Duax, Judy Flippen-Anderson, S. N. Rao, Martha Teeter, George Phillips and Marcia Colquhoun met on 29–30 May 2013 at the AIP headquarters to discuss the mission of the ACA and analyze its strengths, weaknesses, opportunities and threats (SWOT). A list of action items resulted that include collecting information from ACA SIG members, succession planning, and developing an employee manual. Subsequent meetings to follow up on the action items were held on 20 July 2013 at the ACA meeting and 22 October 2013 at the fall Council meeting in Chicago.

By-Laws. Related to the strategic planning effort, Past-President George Phillips embarked on an effort to streamline and update the ACA By-Laws to eliminate inconsistencies, outdated items *etc.* that have accumulated over the years.

Latin American Division. At the ACA business meeting in Hawaii the members in attendance supported changing the ACA By-Laws to add Latin America to the areas authorized to form a national division. This was approved by a formal vote by the full membership. Areas currently authorized to organize as National Divisions are Canada, Latin America and United States of America.

Council meetings. The ACA Council has decided to try video-conferencing for their spring and fall meetings in future years in order to save money.

Summer schools. The ACA Summer Course in Small Molecule Crystallography for the period 2012–2015 alternates between Northwestern (odd years) and Notre Dame (even years). The next summer school will be held from 7–16 July 2014 at 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.

Future meetings. Upcoming ACA Annual Meetings include 2014 in Albuquerque, New Mexico, from 20–24 May with Christine Beavers and Petrus Zwart as Programme Chairs and Zoe Fisher and Kate Page as Local Chairs. The 2014 Award winners are John R. Helliwell (Patterson Award) for his pioneering contributions to the development of the instrumentation, methods and applications of synchrotron radiation in macromolecular crystallography, and D. Borden Lacy (Etter Early Career Award). The 2015 ACA Annual Meeting will be held in Philadelphia, PA, 25–29 July with Programme Co-Chairs Kraig Wheeler and Louise Dawe.

Elections. The fall 2013 elections results included Chris Cahill (Vice-President), Michael James (Canadian Representative), Ilia Guzei (Communications), Ed Collins (Continuing Education) and Peter Mueller (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 2013, including John C. Woolcock (16 May 1955 – 29 January 2013), Ray Davis (ACA President in 2003 and co-Local Chair for San Antonio 2002; 7 November 1938 – 29 May 2013), Charles Caughlan (Local Chair for the Bozeman meeting in 1964; 20 January 1915 – 25 April 2013), Jerome Karle (past ACA and IUCr President; 18 June 1918 – 6 June 2013) and Dave Rognlie (President and owner of Blake Industries; 26 November 1934 – 29 July 2013).

M. L. Hackert, IUCr Representative

9.2. Asian Crystallographic Association (AsCA)

AsCA Executive Committee Officers for the 2010–2013 term: President, Se Won Suh (Korea); Past-President, Mitchell Guss (Australia); Vice-President, Pinak Chakrabarti (India); Secretary-Treasurer, Alice Vrielink (Australia). The Council elected new AsCA Executive Committee Officers for the term 2016 term: President, Pinak Chakrabarti (India); Past-President, Se Won Suh (Korea); Vice-President, Jennifer Martin (Australia); Secretary-Treasurer, J. J. Vittal (Singapore).

Membership. The membership regulations in the AsCA Constitution were revised and new categories were adopted at the AsCA Council Meeting in Adelaide in December 2012: Category A (1 councillor with no vote), Category B (1 councillor with 1 vote), Category C (2 councillors with 2 votes), Category D (3 councillors with 3 votes), Category E (4 councillors with 4 votes), and Corporate/Affiliation (1 councillor with no vote). The current membership is as follows: Category B (Bangladesh, Indonesia, Malaysia, Mongolia, Pakistan, Philippines, Singapore, Sri Lanka, Thailand, Vietnam); Category C (China Taipei, Republic of Korea, New Zealand); and category E (Australia, People's Republic of China, India, Japan).

Financial report. The trustees of AsCA financial investments are 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 2 May 2014 are AUD 187 046.25.

Meetings. The full AsCA calendar normally runs as follows: no scientific meetings in IUCr Congress years and with alternating full and joint AsCA meetings in the other two years. In the past three years the Council met at the following occasions: Madrid Congress (2011); Joint AsCA/SCANZ meeting in Adelaide, Australia (2012); Full AsCA meeting in Hong Kong, People's Republic of China (2013).

Report on AsCA 2013. The most important activity during 2013 was the AsCA 2013 Conference in Hong Kong. At the 2011 AsCA Council meeting in Madrid, it was decided that the AsCA 2013 meeting would be held in Dhaka, Bangladesh. Owing to local political instability in conjunction with a national election, the Council decided to move the venue in late March 2013. Professor Ian Williams proposed that the meeting be held at the Hong Kong University of Science and Technology (HKUST), with new conference dates of 7–10 December 2013. The Chairs and Co-Chairs of the Local Organizing Committee (LOC) and International Programme Committee (IPC) were Ian Williams (People's Republic of China, LOC Chair), Takashi Kamiyama (Japan, IPC Chair), Zhi-Jie Liu (People's Republic of China, Area 1 IPC Co-Chair), J. J. Vittal (Singapore, Area 2 IPC Co-Chair), Alison Edwards (Australia, Area 3 IPC Co-Chair). Several workshops and a one-day Saturday Structural Biology Symposium were also organized. The attendance at the meeting, associated symposia and workshops totaled 413 individuals from 30 countries (Japan 97, People's Republic of China 56, Korea 47, Hong Kong 46, China, Taipei 31, Australia 30, India 25, United Kingdom 16, Singapore 10, USA 10, Thailand 8, Germany 5, Malaysia 4, New Zealand 4, Russia 4, Sweden 3, Switzerland 3, Italy 2, Austria 1, Bangladesh 1, Denmark 1, France 1, Indonesia 1, Ireland 1, Macau 1, Mexico 1, Netherlands 1, Pakistan 1, Poland 1, Vietnam 1). This was considered to be an excellent outcome given the very late change of venue and timing.

A special session on IYCr2014 was organized by Professor Ian Williams at the Hong Kong AsCA meeting to share the plans to celebrate IYCr in the AsCA regions. One of them is the recording of the AsCA history, which was well organized by Professor Sydney Hall. The report will be ready in the summer of 2014 to celebrate the IYCr. Many other activities are also being arranged by individual countries and through cooperations with IUCr.

The dates for the future meetings were decided. In 2015 the 13th Conference of AsCA (AsCA 2015) will be held as a joint meeting with the Indian Crystallographic Association, at Science City, Kolkata, India, 5–8 December 2015. Dr Pinak Chakrabarti (India) has been appointed as Chair of the LOC and Professor Alice Vrielink (Australia) as the Chair of the IPC. The IPC Co-Chairs are Catherine Day (New Zealand) (Area 1: Structural Biology), Ian Williams (Hong Kong) (Area 2: Chemical Crystallography), and Masaki Takata (Japan) (Area 3: Specialized Techniques). The 14th Conference of AsCA (AsCA 2016) will be held in Hanoi, Vietnam. Professor Duong Ngoc Huyen will be the LOC Chair.

J. M. Guss, IUCr Representative

9.3. European Crystallographic Association (ECA)

The link between IUCr and ECA functions well. The IUCr Representative 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 ECM in 2013 in Warwick.

The activities of the Special Interest Groups (SIGs) are reviewed from year to year. The number of individual members registered with SIGs has increased significantly in the last year. The ECA does a great deal to encourage individual members (IMs), including giving IMs more visibility at the ECMs. Two thirds of SIGs/GIGs now have their web sites active, one quarter have a mailing list. General Interest Groups (GIGs) follow similar constitutional rules as the SIGs. GIG1 – Young Crystallographers organized a very interesting Microsymposium in Warwick. GIG1 also had a one-day satellite meeting preceding ECM28 in Warwick, and this was a great success. GIG2 – Senior Crystallographers was very active at ECM28 in Warwick. The founding of a GIG for Teaching is emerging and others may be called into being in the future.

The ECA is aware of the general economic climate and that this might be presenting hardship to crystallographer colleagues at all stages of their careers as well as causing difficulty to attend an ECM. Thus the Executive Committee has launched a call for donations from those that can help other colleagues to attend the ECMs by contributing to their costs. The ECA Council has formally launched these ECA Scholarships; these are in addition to the ECA Student Bursaries for ECMs, which have been available for some time. Applicants have to have been an individual member for at least three years to qualify to apply for an ECA Scholarship to attend an ECM; detailed rules are made available. 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 ECMs.

The ECA places strategic importance and effort on the education of future generations of crystallographers at all levels. The ECA continues to provide financial support to conferences/workshops/schools within the ECA region. Whilst still being committed to give regular support to these local initiatives, the ECA also promoted a high-level European Crystallography School (ECS) for continuous, and rigorous, education in crystallography, initiated by the Italian Crystallographic Association. The plan is that this ECS will be held annually in a different European country. This initiative of a series of schools with an official commitment by the ECA is to have a direct involvement of the ECA through an *ad interim* Sub-Committee on Education (ECA-SE). The Executive Committee has worked out the guidelines that are available to all potential applicants for these European Crystallographic Schools. This proposal has been approved by ECA councillors. The First European Crystallography School will thus take place in Pavia, Italy, 28 August – 6 September 2014. ECS1 is directed to young researchers and PhD students involved in all different fields of structural sciences, 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 one of the most active contributors to the events of the IYCr. One can visit the http://www.iycr.org site to see all the numerous events organized in Europe, and in most of them active ECA members and officers are involved.

The ECA awarded the seventh Max Perutz Prize to Professor Randy J. Read for his contribution to the development and application of advanced statistical approaches to all stages of protein structure solution.

E. Boldyreva, IUCr Representative

9.4. International Organization for Crystal Growth (IOCG)

The most important event concerning IOCG (http://www.iocg.org/) in 2013 was its official meeting, the 17th International Conference on Crystal Growth and Epitaxy (ICCGE-17), Warsaw, Poland, 11–16 August. Ten general sessions and nine topical sessions were organized. The Conference was very successful (about 1200 participants) and very well organized. The week before the Conference, the 15th International Summer School on Crystal Growth (ISSCG-15) was held in Gdansk, Poland, with the participation of 120 students. Both the Conference and the School were supported by the IUCr.

Many members and consultants of the Commission on Crystal Growth and Characterization of Materials were involved in the organization of the Conference and the School, but I would like to underline in particular: the contribution of Ewa Talik, Chair of ISSCG-15; and the activity of Abel Moreno, Kullaiah Byrappa and Thierry Duffar, who respectively co-chaired as IUCr representative the sessions: Biological and Biogenic Crystallization, Industrial Crystallization Defect Formation/Elimination; it was the first time that sessions of the IOCG Conference were officially co-organized by IUCr representatives.

Moreover, the award of the 2013 IOCG Frank Prize to Katsuo Tsukamoto, consultant of this Commission, must be mentioned.

The new Executive Committee of the IOCG was elected and confirmed during the General Assembly of the IOCG in Warsaw. Roberto Fornari (Italy) was confirmed as President for the next triennium, Co-Vice-Presidents are T. F. Kuech (USA) and K. Kakimoto (Japan), the Secretary is H. A. Dabkowska (Canada), and the Treasurer is V. Fratello (USA). The members of the Executive Committee are J. M. Garcia-Ruiz (Spain), Y. Mori (Japan), K. Roberts (UK), M. Heuken (Germany), F. Puel (France), E. Vlieg (The Netherlands), Mu Wang (People's Republic of China), and J. De Yoreo (USA).

According to Roberto Fornari, the key issues for IOCG for the triennium 2013–16 will be:

Promotion and coordination of regional and topical meetings on crystal growth;

Support for the organization of ICCGE-18 and ISSCG-16;

Update of the IOCG web site and statistics of the visits/downloads;

Education – promotion of international and regional schools 'where the potential students are', and support for existing permanent educational activities;

Prizes – advertise the Laudise, Frank and Schieber Prizes and promote nominations;

Extend the number of national organizations – establish contacts to crystal-growth communities of countries with traditional activity as well as to new subjects of crystal-growth research and stimulate them to join IOCG;

Contacts to other international organizations – after the positive experience with IUCr and E-MRS in the past, IOCG should now seek new contacts with the MRS and the European Federation of Chemical Engineers – Working Party on Crystallization.

The next international meetings ICCGE-18 and ISSCG-16 (Chair K. Kakimoto, member of this Commission) will be held in Japan, respectively in Nagoya and Otsu, in 2016, and the 2019 meetings will take place in the USA. The Chair of ICCGE-18 accepted our proposal to continue the idea to co-organize three symposia in cooperation with IUCr representatives.

Both during the Executive Committee Meeting and the General Assembly, I was given the opportunity to underline the importance of the celebration of 2014 as the International Year of Crystallography.

Moreover, IOCG gave an important contribution for the organization of the web site on artificially grown crystals (http://www.iycr2014.org/participate/crystal-growing). Bogdan Ranguelov (Bulgaria), Kevin Roberts (UK) and Elias Vlieg (Netherlands) are part of the scientific committee of the web site as representatives of IOCG. Moreover, IOCG is helping to promote the web site.

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 2013, there was none of specific interest for crystallography.

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 with conferences and workshops, for example.

The ICSTI 2013 Annual Members' Meeting was held on 16–17 March 2013 in Hannover, Germany, hosted by the German National Library of Science and Technology – TIB. It was organized in conjunction with a Conference on Non-Textual Information on 18–19 March. Brian McMahon presented a lecture (http://www.nontextualinformation2013.de/images/Downloads/Brian_McMahon_lecture.pdf) and represented the IUCr.

The ICSTI Annual Congress and ICSTI business meetings for 2013 were hosted by the National Research Canada in Ottawa on 14–15 October 2013, along with the annual meeting of the WorldWideScience Alliance. In addition, ICSTI held a Workshop on Data and Non-Data Integration – A Journey Across Disciplines in the framework of the 2nd Annual CASRAI Conference, the central theme for which was Big Data: The Advance of Data-Driven Discovery. At the IUCr's suggestion John Westbrook of the RCSB agreed to present a talk at this Workshop and his presentation can be found at http://www.icsti.org/IMG/pdf/icsti-2013-v2.pdf. Unfortunately, owing to a prior commitment at The Royal Society, I was unable to attend.

A one-day consultation meeting convened by the ICSU Secretariat was held in Paris, on 25 September 2013, entitled Open Access to Scientific Data and Literature and Assessment of Research by Metrics. The IUCr Representative to ICSTI attended this meeting in order to represent ICSTI. ICSU had previously circulated a letter to its entire membership requesting information and opinions on open access and evaluation by metrics. The IUCr Representative to ICSTI submitted a document to the IUCr Past President summarizing the IUCr journals as a community driven ('learned society') publisher for authors and readers globally, who endorsed it and submitted it to ICSU. The Chair of the consultation meeting was Sir John Ball FRS, who is a member of the ICSU Executive Board. A report is in preparation. A notable point of principle was agreed of scientific data and literature ideally needing to be 'free for authors and free for readers' as an aim for science communication. The IUCr journals satisfy this principle *via* its suite of journal titles, *i.e.* combining some (*Acta B*, *Acta C*, *Acta D*, *Acta F*, *JAC* and *JSR*) as being free for authors [*i.e.* with no article processing charge (APC) but paid by subscribers] and some (*IUCrJ* and *Acta E*) as being free for readers (*i.e.* where authors or their research sponsors pay the APC).

I acknowledge with gratitude the close collaboration with Brian McMahon, R&D Officer of the IUCr, and with the IUCr journals Executive Managing Editor, Peter Strickland.

J. R. Helliwell, IUCr Representative

10.3. International Council for Science (ICSU)

The main activity during 2013 was the ISCU Meeting for Union Representatives held in Paris, France, 28–29 April 2013. The meeting was attended by 47 representatives from 22 Unions, the ICSU management and representatives from ICSU's Regional Offices in Africa, Asia and Latin America. Prior to the meeting each Union had been asked to provide information papers on its structure and activities during the past three years and planned activities for the coming three years. This gave a good overview of different Unions that are members of ICSU. During the evening prior to the start of the meeting I participated in an informal meeting of Representatives of Unions belonging to the Physical, Chemical and Mathematical Science cluster. The Unions IUPAC, IUPAP, IUMRS (Materials Research Societies) and IUCr face similar problems and it was useful to have this discussion, which also addressed the relation between ICSU and the Unions. There was interest in organizing joint activities that could involve engagement in IYCr activities.

The focus of the ICSU meeting for the Unions was to strengthen the engagement of the Scientific Unions in the implementation of ICSU's new Strategic Plan. The active participation of the Union Representatives was ensured through their participation in different break-out sessions. The first day was devoted to the discussion of the following three issues: Future Earth; Science Education; Communication between ICSU and the Unions. The Union Representatives were divided into three groups that discussed all three items. On the second day the break-out groups addressed: Urban Health; New Interdisciplinary Horizons; Open Access to Data and Information; IRDR (Integrated Research on Disaster Risk), with the possibility to participate in two of the break-out groups. The results from the discussions in the different break-out groups were reported *in plenum*, and carefully noted by the ICSU management. It was also very useful to have the opportunity to interact and establish contacts with representatives from ICSU's Regional Offices in Africa, Asia and Latin America.

The meeting was valuable in many aspects, it gave good insight into ICSU's strategic plan and created good contacts with other Union

members of ICSU, and it was also a good step in improving the relation between the Unions and ICSU.

S. Larsen, IUCr Representative

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

The CODATA–ICSTI Task Group on Data Citation Standards and Practices published a 75-page report, *Out of Cite, Out of Mind*, on current practices and policies across a range of scientific disciplines [*Data Science Journal* (2013), **12**, CIDCR1–75]. Material relevant to crystallography was contributed by Brian McMahon (BM) (as a member of the Task Group 2010–2012) and by BM and John Helliwell (JRH) during the Task Group sessions at the 2012 CODATA Conference in Taipei.

The CODATA–VAMAS Joint Working Group on the Description of Nanomaterials circulated a questionnaire to member organizations and convened a second Workshop in Paris, France, 30–31 May 2013. For the IUCr, the questionnaire was completed by JRH and by Daniel Chateigner (DC), who attended the Workshop. The outcome of the Workshop was the publication in October 2013 of a revised draft framework for a Uniform Description System for Materials on the Nanoscale (http://www.codata.org/workinggroups/Nanomaterials/Nanomaterials_Framework%20for%20Uniform_Description_System%203%20Oct%202013.pdf). While many scientific communities that work with nanomaterials are still in the early stages of formalizing nomenclature and other descriptive requirements, crystallographic structure is already well characterized by existing CIF dictionaries, and there is scope to extend the areas covered by CIF. For example, an early working draft of a materials properties CIF dictionary has been developed by DC and collaborators in the Materials Properties Open Database project.

Kathleen Cass retired as CODATA Executive Director at the end of July 2013, following a 12-year period during which she oversaw the development of many strategic initiatives and helped to increase the influence and visibility of the organization. We were pleased to welcome her successor, Simon Hodson, as a speaker at the COMCIFS Information and Data Management Symposium at University of Warwick in early August 2013. Dr Hodson was formerly Programme Manager of JISC's Managing Research Data initiative, and brought to the symposium both informed analysis of the role and nature of UK government funding for managing research data, and an enthusiasm for engaging the crystallographic community fully in the ongoing mission of CODATA.

J. R. Helliwell, IUCr Representative

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

COSPAR acts mainly as a body responsible for organizing biennial Scientific Assemblies, and the 39th COSPAR Assembly was held in Mysore, India, on 14–22 July, 2012, with over 1500 participants.

The previous (38th) Assembly of the Committee on Space Research took place on 18–25 July 2010 in Bremen, Germany, and the next will be in Moscow, Russia, 2–10 August 2014.

The International Year of Crystallography (IYCr) could provide an opportunity for stronger collaboration between the IUCr and COSPAR.

At the Mysore Assembly, I submitted information to the COSPAR Council about the (just announced) IYCr. A more detailed summary of IYCr activities will be presented in Moscow in 2014, the actual IYCr.

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 division of COSPAR for the IUCr, the Scientific Commission on Materials Science in Space (MSS Comission G) is 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 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 together 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 spacecraft, 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.

COSPAR co-sponsored the following meetings in 2013:

Atmospheric Correction of Earth Observation Data for Environmental Monitoring: Theory and Best Practices, Bangkok, Thailand, 4–8 November 2013.

High-Energy Astrophysics: An Advanced School for Asian Astronomers, Nanjing, People's Republic of China, 2–13 September 2013.

SCOSTEP School in Space Sciences, Nairobi, Kenya, 21 October – 1 November 2013.

Symposium on Cosmic Magnetic Fields: Legacy of A. B. Severny, Nauchny, Crimea, Ukraine, 2–6 September 2013.

12th IAGA Scientific Assembly, Merida, Mexico, 26–31 August 2013.

XXIII Festival d'Astronomie de Fleurance, Fleurance, France, 3–9 August 2013.

Table 1
Income and Expenditure Account (in Swiss Francs) for the year ended 31 December 2013.

	2013		*2012*	
Income				
Membership subscriptions		162 741		*164 497*
Sales				
Journals, back numbers and single issues	3 270 884		*3 517 553*	
Books	154 174		*170 232*	
Open Access Grant	—	3 425 058	*4 883*	*3 692 668*
Investment income				
Income from investments	3 803		*73 387*	
Bank interest	1 191		*1 164*	
Profit on disposal	69 575	74 569	*25 475*	*100 026*
Other income				
Royalties and copyright fees	7 712		*8 641*	
Advertising income	99 811		*203 806*	
STAR/CIF income	17 555	125 078	*6 845*	*219 292*
Total income		3 787 446		*4 176 483*
Expenditure				
Journals				
Publication costs	577 492		*540 815*	
Editorial expenses	263 581		*235 826*	
Technical editing	1 242 371		*1 317 250*	
Subscription administration	109 704	2 193 148	*108 212*	*2 202 103*
Books				
Publication costs	42 331		*29 576*	
Editorial expenses	46 507		*44 439*	
Technical editing	62 757	151 595	*80 250*	*154 265*
Newsletter				
Publication costs	16 392		*18 304*	
Editorial expenses	112 357	128 749	*104 367*	*122 671*
International Year of Crystallography		227 681		—
President's Fund and other Grants and Young Scientists' support		207 453		*188 160*
General Assembly and Congress costs		18 572		*30 646*
Committee meetings and expenses		116 985		*134 005*
Publications and journals development				
General	434 207		*531 979*	
Editors' meetings	7 809		—	
Promotion	119 420		*145 640*	
IUCrJ development	122 486		—	
STAR/CIF	24 198	708 120	—	*677 619*
Subscriptions paid		6 271		*3 901*
Visiting Professorship Programme		17 302		*6 211*
Administration expenses:				
Honorarium to General Secretary and Treasurer	6 820		*7 683*	
Audit and accountancy charges	59 739		*58 962*	
Legal and professional fees	2 512		*5 297*	
Travelling expenses	16 674		*13 203*	
Bank charges	8 327	94 072	*6 880*	*92 025*
Executive Secretary's office:				
Salaries and expenses	274 537		*265 221*	
Travel expenses of IUCr Representatives on other bodies	8 219		*10 603*	
Sponsorship of meetings	4 941		*4 884*	
President's secretary	4 853		*4 916*	
IUCr/FIZ agreement	(18 088)		(*16 252*)	
Bad debts	27 048	301 510	*811*	*270 183*
Depreciation		33 234		*29 795*
Total expenditure		4 204 692		*3 911 584*

Table 1 (continued)

	2013		*2012*	
Surplus of income over expenditure (before realized exchange losses)		(417 246)		*264 899*
Realized fluctuations in rates of exchange				
Exchange movement on trading activities		(5 643)		*72 597*
(Deficit)/surplus of income over expenditure (after realized exchange losses)		(422 889)		*337 496*
Movement in market value of investments in year		40 727		*24 999*
		(382 162)		*362 495*
Unrealized fluctuation in rates of exchange				
Exchange movement on trading activities	(18 387)		*10 765*	
Investment activities	(65 187)	(83 574)	(*13 102*)	(*2 337*)
Total recognized gains/(losses) relating to the year		(465 736)		*360 158*
Opening fund accounts at 1 January		5 062 278		*4 702 120*
Closing fund accounts at 31 December		4 596 542		*5 062 278*

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.

2013 International Reference Ionosphere (IRI) Workshop, Olsztyn, Poland, 24–28 June 2013.

29th International Symposium on Space Technology and Science, Nagoya, Japan, 2–9 June 2013.

COST Action ES1005, Training School for Students and Young Researchers: Towards a More Complete Assessment of the Impact of Solar Variability on the Earth's Climate, Thessaloniki, Greece, 10–15 March 2013.

6th European Conference on Space Debris, ESA/ESOC, Darmstadt, Germany, 22–26 April 2013.

H. A. Dabkowska, IUCr Representative

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 2012 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 2013 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 loss has arisen on the assets of the Union, in terms of CHF, amounting to CHF 89 217. In the accounts this loss has been assigned as a 'Realized loss' (CHF 5 643) and 'Unrealized loss' (CHF 83 574). The loss attributable to investment activities has been assigned to the General Fund and the overall loss attributable to trading activities has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 2013. It should be noted that this overall loss in CHF is not a real loss of money, but rather a loss on paper resulting from the accounts being expressed in CHF.

Investments are noted in the balance sheet at their market value at 31 December 2013.

The balance sheet shows that the assets of the Union, including the loss resulting from fluctuations in rates of exchange, have decreased during the year, from CHF 5 062 278 to CHF 4 596 542. The movement in market value of the investments was CHF 40 727 in 2013 (CHF 24 999 in 2012).

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 60 000 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 314 822, as compared with a deficit in 2012 of CHF 325 548. The administrative expenses were CHF 390 282 in 2012 as compared with CHF 371 514 in 2012. Of this amount, CHF 130 704 was charged to the publications of the Union.

The expenses of the Union Representatives on other bodies were CHF 8 219. The cost of the Finance Committee meetings held in 2013 was CHF 28 780, while the Executive Committee meetings cost CHF 35 727. The income from the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 18 088. The subscriptions from Adhering Bodies were CHF 160 000. Interest on bank accounts and investments credited to the General Fund was CHF 4 994.

Grants totalling CHF 18 572 were paid from the President's Fund in 2013.

The Journals Fund account for 2013 shows a surplus of CHF 659 194 before the transfer of CHF 385 000 to the other fund accounts, as compared with a surplus of CHF 799 078 in 2012 before the transfer of CHF 400 000 to the other fund accounts.

[1] The full audited accounts are available from the IUCr electronic archives (Reference ES0406).

Table 2
Balance sheet (in Swiss Francs) as at 31 December 2013.

	2013		*2012*	
Fixed assets				
Tangible fixed assets		40 994		*28 912*
Investments at market value		2 626 051		*2 716 611*
		2 667 045		*2 745 523*
Current assets				
Stock		119 459		*106 529*
Cash at bank and in hand				
Current accounts	115 221		*103 864*	
Deposit and savings accounts	1 542 174		*2 100 980*	
Cash with Union officials	18 237	1 675 632	*19 933*	*2 224 777*
Debtors, accrued income and payments in advance		428 093		*311 489*
Subscriptions due from Adhering Bodies		18 686		*22 880*
Total current assets		2 241 870		*2 665 675*
Creditors: amounts falling due within one year		(312 373)		(*348 920*)
Net current assets		1 929 497		*2 316 755*
Total funds		4 596 542		*5 062 278*

Table 3
Summary of Fund Accounts (in Swiss Francs) as at 31 December 2013.

	As at 1 January 2013	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 2013
					Trading	Investments	
Fund accounts							
General Fund	(2 462 640)	—	(314 822)	40 727	14 033	(65 187)	(2 787 889)
President's Fund	92 872	60 000	(18 572)	—	(689)	—	133 611
Journals Fund	5 004 474	(385 000)	659 194	—	(27 069)	—	5 251 599
International Tables	(513 389)	—	(38 057)	—	2 828	—	(548 618)
Publications and Journals Development Fund	1 006 838	25 000	(149 667)	—	(4 524)	—	877 647
Research and Education Fund	1 028 905	250 000	(452 436)	—	4 238	—	822 231
Ewald Fund	524 714	—	—	—	(2 691)	—	522 023
Newsletter Fund	42 360	50 000	(54 688)	—	(193)	—	37 479
General Assembly and Congress	338 486	—	(48 198)	—	(1 487)	—	288 459
	5 062 278	—	(417 246)	40 727	(24 030)	(65 187)	4 596 542

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 1 226 333 as compared with CHF 1 305 419 in 2012. 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 38 057, as compared with a deficit of CHF 19 418 in 2012. The net sales income was CHF 115 295 in 2013 as compared with CHF 128 287 in 2012.

The cost for the Union in producing the *Newsletter* in 2013 was CHF 54 688.

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.

CHF 155 924 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 17 302), Crystallography in Africa initiatives (CHF 33 501), 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 18 028) and IYCr costs (CHF 227 681) 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 2013 the cost of the International Programme Committee meeting was charged to this Fund (CHF 48 198).