

## Report of the Executive Committee for 2010

## 1. Meetings

The IUCr sponsored the following meetings held during 2010:

RapiData 2010, Brookhaven, USA, 11–16 April.

Powder Diffraction and Rietveld Refinement School, Durham, UK, 18–22 April.

Adsorption, Absorption and Crystal Growth, Gargnano, Italy, 18–23 April.

Third Annual School on Advanced Neutron Data Treatment using the FullProf Suite, Tenerife, Spain, 2–8 May.

Second International School of Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials, Granada, Spain, 24–28 May.

Diffraction at the Nanoscale: Nanocrystals, Defective and Amorphous Materials, Villigen, Switzerland, 24–30 May.

International Symposium of Diffraction Structural Biology (ISDSB 2010), Paris, France, 25–28 May.

Second Chemical Crystallography Workshop, Hamilton, Ontario, Canada, 25–29 May.

Structure and Function from Macromolecular Crystallography: Organization in Space and Time, Erice, Italy, 3–13 June.

Gordon Research Conference in Crystal Engineering, Waterville Valley Resort, New Hampshire, USA, 6–11 June.

Summer Schools on Mathematical and Theoretical Crystallography, Nancy, France, 21 June – 2 July.

ACA Annual Meeting, Chicago, USA, 24–29 July.

Fourteenth International Summer School on Crystal Growth (ISSCG-14), Dalian, People's Republic of China, 1–7 August.

Third K. H. Kuo Summer School of Electron Microscopy and Crystallography: International Workshop of 3D Molecular Imaging by Cryo-Electron Microscopy, Beijing, People's Republic of China, 8–12 August.

Sixteenth International Conference on Crystal Growth in conjunction with the Fourteenth International Conference on Vapor Growth and Epitaxy, Beijing, People's Republic of China, 8–13 August.

12th European Powder Diffraction Conference, Darmstadt, Germany, 27–30 August.

26th European Crystallographic Meeting (ECM-26), Darmstadt, Germany, 29 August – 2 September.

Structure Under Extreme Conditions of Pressure and Temperature, Oak Ridge National Laboratory, Knoxville, USA, 19–23 September.

International School on Aperiodic Crystals, Carqueiranne, France, 26 September – 2 October.

Modern Methods of Biocrystallography – BioCrys 2010, Oeiras, Portugal, 9–16 October.

IXS 2010 – Seventh International Conference on Inelastic X-ray Scattering, Grenoble, France, 11–15 October.

Tenth Conference of Asian Crystallographic Association, Busan, South Korea, 31 October – 3 November.

XII Seminario Latinoamericano de Análisis por Técnicas de Rayos X (Latin-American Seminar on Analysis by X-ray Techniques) – SARX 2010, Puebla, Mexico, 15–19 November.

First North African Crystallographic Conference – NACCI, Casablanca, Morocco, 23–26 November.

International School on Fundamental Crystallography, Montevideo, Uruguay, 29 November – 3 December.

Symposium No. 239 of Pacificchem 2010: Chemistry and Materials Science Under High Pressure, Honolulu, USA, 18–19 December.

The Executive Committee met in Darmstadt, Germany, in August and in Busan, South Korea, in October. The Finance Committee met in Copenhagen, Denmark, in March, and in Darmstadt 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 meeting, and in e-mail ballots, were:

editorial policy, pricing policy and subscription rates, approval of appointment of Editors for *Acta E*, approval of appointments of Co-editors, archival policy, Special Issues, open access, fraudulent submissions, facility information pages, and other matters concerning the IUCr journals;

approval of audited accounts for the previous year;  
review of Statutes and By-Laws; procedures at General Assemblies;

review of proposed revision to ICSU dues structure;  
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;

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

Journal Grants Fund;

cooperation with databases, establishment of Working Group of Database Users;

progress with Volumes A, A1, B, C, D, E, F and G of *International Tables* and development of associated software, approval of Volume H (Powder Diffraction), consideration of possible new volume on XAFS; appointment of new Editor for Volume C;

*IUCr Newsletter*;

*World Database of Crystallographers*;

promotional activities;

International Year of Crystallography – 2013;

Ewald Prize;

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

discussion of arrangements for Madrid Congress.

Other items dealt with in this way were:

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

IUCr web site;

collection of photographs;

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

crystallography in Africa;

Visiting Professorship scheme;

review of activities of Commissions;  
revision of General Statement of Principles for Commissions;  
establishment of *ad interim* Commission on Magnetic Structures;  
review of activities of Regional Associates;  
review of reports of IUCr Representatives on other bodies;  
relations with other Scientific Unions.

Items concerning the Chester office were:  
staffing requirements in the IUCr office in Chester;  
risk analysis;  
upgrading of office technology, provision of internet services.

## 2. Publications

Volume 66 of *Acta Crystallographica*, Volume 43 of *Journal of Applied Crystallography* and Volume 17 of *Journal of Synchrotron Radiation* 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-First General Assembly and International Congress of Crystallography [*Acta Cryst.* (2009), A65, 390–442].

## 4. Work of the Commissions

### 4.1. Commission on Journals

**4.1.1. Overview.** The total number of articles published in IUCr Journals in 2010 was 5431, which compares with 5440 in 2009 and 4795 in 2008. The number of pages published was 13 156, compared with 12 467 pages in 2009 and 11 295 pages in 2008. Of the total, 6879 pages were published electronically only.

In 2010, 724 pages were printed for *Acta Crystallographica* Section A (548 in 2009), 706 for Section B (790 in 2009), 1134 for Section C (1258 in 2009) and 1354 for Section D (1349 in 2009). Section E published 5195 electronic only pages (5108 in 2009) and Section F published 1684 electronic only pages (1319 in 2009).

The average lengths of Full Articles in Sections B, C, E and F increased to 9.8, 4.0, 1.3 and 4.5 pages, respectively. The average lengths of Full Articles in Sections A and D decreased to 9.8 and 8.7 pages, respectively. Average publication times were the same as 2009 for Sections C (1.9 months) and E (0.7 months) and increased for Sections A (5.7 months), B (5.2 months), D (5.1 months) and F (3.6 months). The rejection/withdrawal rates were: Section A (39%), Section B (40%), Section C (53%), Section D (22%), Section E (18%) and Section F (9%).

The number of Full Articles published in *Journal of Applied Crystallography* (*JAC*) in 2010 was 165 (131 in 2009). The number of pages increased from 1212 in 2009 to 1543 in 2010. The average publication time increased to 5.7 months. The rejection/withdrawal rate was 31%.

The number of Full Articles published in *Journal of Synchrotron Radiation* (*JSR*) in 2010 was 99 (107 in 2009). The number of pages decreased to 816 in 2010 (883 in 2009). The average review time decreased to 4.1 months and the technical editing time increased to 1.1 months; the overall publication time decreased to 5.2 months. The rejection/withdrawal rate was 26%.

The citation impact of IUCr Journals continued to be high, with the journals occupying three of the top six ranking positions in crystallography. The highlight was an impact factor of 49.9 for Section A. The primary cause of this record value was a single feature article by George Sheldrick entitled *A Short History of SHELX*, which was published in the January 2008 issue of Section A.

Another highlight of 2010 was the publication of the 100 000th article on **Crystallography Journals Online**. This online service has continued to be popular, with over 3 million downloads of journal articles in the year. The highest number of downloads was for Section E.

A Special Issue on Dynamical Structural Science was published in Section A. Papers presented at the CECAM/SimBioMa workshop on Structural Transitions in Solids were also published in Section A. Proceedings of the CCP4 Study Weekend on Experimental Phasing and Radiation Damage and a Special Issue on Neutrons in Biology were published in Section D. A Special Issue on the JCSG Pipeline: Technology and Dissemination was published in Section F. A Special Issue on Crystallography Education and Training for the 21st Century was published in *JAC* and a Special Issue on Synchrotron Radiation in Soil and Geosciences was published in *JSR*.

Informal meetings of the Commission on Journals were held in Chicago, USA, during the ACA meeting, in Darmstadt, Germany, during the ECA meeting, and in Busan, Korea, during the AsCA meeting.

Finally, I would like to thank the Section Editors and Co-editors for their work on the journals during 2010.

A survey of the contents of IUCr Journals is presented in Table 1.

### G. Kostorz, Chair

**4.1.2. *Acta Crystallographica* Section A.** In 2010, Section A published 724 pages in six issues as well as 320 pages of Abstracts for ECM-26 in Darmstadt, Germany. A 148-page issue on Dynamical Structural Science, containing 14 research papers on time-resolved crystallography, was edited by E. Collet and published in March 2010. Five research papers on Structural Transitions in Solids comprising 53 pages were edited by S. Leoni and published in September 2010. In addition to the Special Issues, Section A also published one Lead Article (33 pages on *Mode crystallography of distorted structures*) and a historical Feature Article [on *The birth of the European Crystallographic Committee (ECC) and of the European Crystallographic Meetings (ECMs)*].

674 pages were devoted to 68 scientific articles (Research Papers, and Lead and Feature Articles) and to 3 Short Communications. The number of submitted Research Papers, 47, was similar to 2009 (41) and 2008 (42). There were no very slim issues. The shrinking of Section A thus appears to have stopped. The average length of scientific articles was 9.8 pages. The average submission to publication time for research papers increased to 5.7 months. The proportion of withdrawn plus rejected manuscripts (39%) was the same as in 2009. The geographical distribution of the origins of the articles was 60% for Europe, 22% for the Americas and 18% for Asia–Australia. The impact factor for 2009 was a record value of 49.9 owing to a single publication as explained in the editorial of November 2010.

Section A covers all topics within crystallography, which may be defined as the science of the structure of matter at atomic resolution. The contents of the papers are diverse. The topics may be grouped somewhat arbitrarily into three categories: (i) structure determination with any radiation (phasing, refinement, charge density, aperiodic structures); (ii) structure properties (group theory, tensorial

**Table 1**  
Survey of the contents of IUCr journals.

*Acta Crystallographica*

Vol.	Year	Number of pages§	Number of papers	Full Articles†		Short Communications‡	
				Number	Average length	Number	Average length
A62	2006	528	58	43	10.1	15	6.2
B62		1138	127	119	9.3	8	3.1
C62		1450	447	446	3.3	1	8.0
D62		1571	191	178	8.6	13	3.5
E62		9843	3991	3978	2.5	13	1.7
F62		1300	345	338	3.8	7	1.6
A63	2007	510	66	47	9.1	19	4.4
B63		940	110	102	8.9	8	3.4
C63		1510	451	449	3.4	2	2.5
D63		1283	157	128	9.1	29	4.0
E63		8375	5181	5165	1.6	16	1.7
F63		1090	282	278	3.9	4	2.0
A64	2008	702	81	66	10.0	15	2.5
B64		791	91	82	9.3	9	2.9
C64		1197	332	328	3.6	4	2.8
D64		1294	152	135	9.1	17	3.9
E64		4261	3556	3527	1.2	29	1.3
F64		1187	302	293	4.0	9	1.7
A65	2009	548	56	43	10.3	13	8.2
B65		790	90	79	9.6	11	2.4
C65		1258	331	328	3.8	3	4.0
D65		1349	160	137	9.1	23	4.0
E65		5108	4166	4148	1.2	18	1.5
F65		1319	333	329	4.0	4	1.8
A66	2010	724	81	68	9.8	13	4.5
B66		706	73	71	9.8	2	6.0
C66		1134	284	280	4.0	4	3.0
D66		1354	167	148	8.7	19	3.6
E66		5195	4113	4091	1.3	22	1.5
F66		1684	377	368	4.5	9	1.6

*Journal of Applied Crystallography*

Vol.	Year	Number of pages§	Number of papers	Full Articles††		Short Communications‡‡		Short items§§	
				Number	Average length	Number	Average length	Number	Average length
39	2006	928	140	89	8.1	36	4.2	15	2.5
40	2007	1895	314	124	8.1	172	4.8	18	3.1
41	2008	1197	161	120	8.5	30	3.9	11	3.1
42	2009	1212	172	131	7.9	27	4.0	14	3.0
43	2010	1543	222	165	8.0	38	4.5	19	3.1

*Journal of Synchrotron Radiation*

Vol.	Year	Number of pages§	Number of papers	Full Articles		Short Communications		Short items§§	
				Number	Average length	Number	Average length	Number	Average length
13	2006	496	77	58	7.6	7	3.4	12	1.8
14	2007	535	76	64	7.8	2	2.0	10	2.6
15	2008	666	120	106	5.8	7	3.6	7	3.0
16	2009	883	132	107	7.5	12	3.8	13	2.4
17	2010	816	114	99	7.7	8	4.6	7	2.6

† Including Lead and Feature Articles for Sections A, B and D. ‡ Including Addenda & Errata, Letters to the Editor, IUCr Notices, Notes and News, Book Reviews, Books Received, Obituaries, Scientific Comments, Current Events and Editorials. § Numbered pages excluding contents pages. †† Including Lead and Feature Articles and Teaching & Education. ‡‡ Including Addenda & Errata, Computer Programs and CIF Applications. §§ Including Letters to the Editor, Laboratory Notes, Meeting Reports, Cryocrystallography Papers, IUCr Notices, Notes and News, Book Reviews, Books Received, Obituaries, Crystallographers, Commission Reports, New Products, Current Events and Editorials.

properties, crystal chemistry, topology); (iii) other forms of matter (diffraction physics, diffuse scattering, nanoscience, time-resolved studies, single-particle studies). These categories are on average of about equal importance, even though percentages vary from year to year. A few years ago, it seemed that electron diffraction was disappearing from Section A, but this trend has reversed with submissions belonging to categories (i) and (ii). Neutron diffraction is nearly absent. There is continued submission of manuscripts of macromolecular interest. Some referees would like to see all publications on macromolecular phasing methods in Section D while others applaud the choice of Section A.

Authors now use the electronic submission system almost exclusively. Some referees ask to receive the manuscript directly from, and send the report directly to, the Co-editor. Since Section A Co-editors handle relatively few but often rather long and difficult manuscripts, each of which presents its own characteristics and problems, the handling through Chester does not seem to facilitate operations as much as for other Sections. The electronic system works well enough for all operations a submission might require, but a direct contact with the author is easier when there is no appropriate form letter available.

The success of Section A is due to the combined efforts of many persons. The collaboration with the Editorial Office in Chester is extremely good, always efficient with very fast and competent answers to all questions. I thank in particular Nicola Ashcroft for her competent work and friendly communication. I also thank all the Co-editors, many of whom will retire in 2011, for their often difficult work and decisions.

**D. Schwarzenbach**, Editor of Section A

**4.1.3. Acta Crystallographica Section B.** The number of articles published in Section B decreased from 90 in 2009 to 73 in 2010; the number of pages decreased from 790 to 706. Until about July 2010 numbers of submitted and accepted articles were close to historical averages, but by August 2010 a decline could be discerned, which has continued into 2011.

The average length of a paper has continued to increase. For 2002–2006 the average was 9.1 pages per article but by 2010 the average was at an all-time high of 9.8 pages per article. The amount of supplementary material deposited also continued to rise. Some authors submitted CIFs for structures determined at many temperatures, pressures or degree of reaction, but included only some of the results in the standard table of experimental details. Other authors attached movies, extra and enhanced figures, and spreadsheets to their articles.

One Feature Article (*Polysomatic apatites*, Baikie *et al.*, 2010) was published; it was then downloaded more than 300 times.

The average time from submission to publication continues to hover at about five months, with authors' revisions accounting for a significant fraction of that time. The overall time seems quite short given the careful reviews written by many referees. The improvements in the submissions system developed in Chester have made handling manuscripts easy for all involved.

The Chester staff, and especially Jill Bradshaw, continue to turn accepted manuscripts into attractive, carefully edited journal pages. Jill negotiates tactfully, but firmly, with authors when figures need to be improved, and she has a real flair for layouts. The quality of the editing is very high. As a crystallographer wrote to us late in 2010: 'I think we can take great pride in the quality of *Acta B*.'

At the end of 2010 D. L. Dorset retired from the editorial board. We will miss his broad knowledge, his enthusiasm for good writing and his expertise in the area of electron diffraction.

**C. P. Brock**, Editor of Section B

**4.1.4. Acta Crystallographica Section C.** The strength of Section C is the rapid publication of high-quality studies of novel and challenging crystal and molecular structures of interest in the fields of chemistry, biochemistry, mineralogy, pharmacology, physics and materials science, for which a detailed discussion of the structures is presented that goes beyond reporting just the principal numerical and geometrical data.

In 2010, Section C published 284 papers (33 inorganic, 101 metal-organic, 146 organic and 4 communications) in a total of 1134 pages, which is down from the 331 papers (~14%) and 1258 pages produced in 2009 (~10%). In the same period, the number of submitted papers fell from 687 to 592 (~14%). The proportion of inorganic (12%), metal-organic (36%) and organic papers (52%) remains within the bands of previous years. The citation impact factor has increased from 0.56 in 2009 to 0.78, its highest value since 2006. Average publication times remained at 1.9 months. Approximately 53% of submissions to Section C in the past year were either subsequently withdrawn by the authors or rejected, which is consistent with the rate generally found over the last seven years. The average number of pages per article continues its upward trend – 3.6 in 2008, 3.8 in 2009 and 4.0 in 2010.

In 2010, Section C published fewer papers than in 2009 and this continues a longer term trend, which is a concern. In 2005–2007, Section C published around 440 papers annually, but this decreased to 332, 331 and 284 in the period 2008–2010. This correlates with the introduction of the new open-access format for Section E. One possible explanation for the decrease in submissions to Section C is the requirement for an extensive and detailed *Comment* section in Section C papers compared with the shorter discussion normally required in a Section E paper. The latter is attractive for authors whose language skills are limited or for those who do not wish to spend so much time on manuscript preparation. Compared with 15 or 20 years ago, authors of Section C papers are probably expected to write much more substantial discussions, so as to keep the journal's style distinct from Section E, but this may be having an effect on the popularity of Section C.

On the other hand, it is pleasing to see an increase in the number of quite substantial papers reporting several related structures in excellent detail, as well as a few manuscripts whose content extends beyond a routine structure report and includes less common aspects of an analysis or results from other techniques, while remaining briefer than what would be required for a Section B style paper. The increase in average paper length appears to be mainly a result of an increasing number of figures in papers.

The Notes for Authors emphasize clearly that the journal accepts reports of difficult or challenging structures not meeting all validation criteria, provided the presented structures are correct and unambiguous, and the difficulties and strategies used to treat them are scientifically discussed and properly documented. This is to avoid any misconception that the journal only accepts near-perfect structures.

The validation of structure-factor files has been introduced and is now an integral part of the *checkCIF* suite. This often reveals inconsistencies between the CIF data and the structure factors, which may result from incomplete updating of CIF data after a new refinement, uploading the incorrect version of the structure-factor file or a missed property in the refinement, such as twinning. The

submission system has been upgraded by the Editorial staff and now allows better tracking of activity during the review process.

A new initiative planned for the latter part of 2011 is the introduction of virtual issues of the journal. As the journal specializes in the rapid publication of papers, it does not lend itself easily to the production of Special Issues for which long lead times or the holding over of relevant submissions is required. Nevertheless, online publishing readily facilitates the creation of virtual issues, which can be used to bring together and highlight papers on specific topics that had been published over the preceding several months. The contents page of the virtual issue then provides suitable links to the original papers. Such virtual issues may focus on topics of current interest, such as twinned structures, polymorphs, metal-organic frameworks, particular classes of chemical compounds and so on. The virtual issue makes it easier for readers to find papers relevant to their field of interest, thus increasing the visibility and impact of those papers. The first virtual issue will focus on polymorphism.

I wish to thank warmly all the Section C Co-editors who have given generously of their time, expertise and effort during the reporting period, as well as the many reviewers and authors, without whom the journal could not exist. I am also grateful to A. J. Blake, Deputy Section Editor, for his assistance with the proofreading of manuscripts. The invaluable support of the Editorial Office staff is much appreciated, in particular the tireless efforts of Sean Conway, Mike Hoyland, Peter Strickland and the technical editors.

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

**4.1.5. Acta Crystallographica Section D.** Section D of *Acta Crystallographica* continues to play a key role in biological crystallography, focusing both on methods and on structural papers and the insights they bring to biology and chemistry. Structural biology is still expanding rapidly, and crystallographic studies have become integral to many areas of biology. As a result, many more journals now publish crystallographic results and Section D competes in a very large field for structural papers. On the other hand, with increasing automation, crystallographic methods are of intense interest and importance, and Section D is pre-eminent in this area. On average, about half of the papers published by Section D are methodological, with the remainder reporting structural results on biological macromolecules or their complexes. We are pleased that the journal does attract a steady flow of good-quality structural papers, at a rate of about 6–10 such publications per month.

The impact factor of Section D was 2.3, but it is expected that this will increase in 2011. A good impact factor is important in attracting more high-profile structural papers to the journal. Whereas the methodological papers are outstanding, and often very highly cited, an impact factor that is competitive with mainstream biological journals is essential for attracting the most significant structural papers.

The CCP4 Special Issue in April 2010 was focused on Experimental Phasing and Radiation Damage. We thank E. Garman, A. Pearson, C. Vornrhein and C. Ballard for their Guest Editorship of this Special Issue. A Special Issue on Neutrons in Biology was published in November 2010. This issue contains articles based on talks presented at the International Conference on Neutrons in Biology, held in Santa Fe, New Mexico, USA, in October 2009. We thank P. Langan for acting as Guest Editor for these articles.

The number of pages published in 2010 was very similar to 2009, as was the number of papers published: 148 full articles and 19 short articles were published. The total number of pages was 1354, with the average length of full articles being 8.7 pages. Publication times were

longer than in 2009, at an average of 5.1 months; the electronic submission system continues to work well.

Finally, we thank the many people who contribute to the success of the journal. We particularly wish to thank those Co-editors who step down in 2011 after their nine years of service: N. Chayen, S. Ealick, J. M. Guss, H. Holden, W. N. Hunter, M. Pusey and P. Timmins. They, together with our other Co-editors, have given much time and wisdom to shepherding papers through to acceptance. We also welcome as newly nominated Co-editors C. Bond, Z. Derewenda, J. Newman, R. Read and M. Schiltz. We also thank our authors and readers; the reviewers whose efforts are critical for maintaining quality; and Louise Jones and Simon Glynn for their efforts at the Editorial Office in maintaining superb production quality.

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

**4.1.6. Acta Crystallographica Section E.** 2010 has been another extremely busy year for the journal with over 5000 papers submitted. Fortunately, the revelation of frauds that clouded the second half of 2009 is now behind us and there have only been a few isolated incidents of submissions that raised concerns for Co-editors and Section Editors. Continued improvements to the validation procedures have been important in ensuring that problems such as element swapping are more readily identified and challenged. Thanks are once again due to Ton Spek and his collaborators for their continued excellent work with *PLATON* and *checkCIF*. We have also spent some time this year advocating the inclusion of structure factors amongst material required to be deposited for papers in any journal reporting small-molecule structures. This approach has worked very successfully for protein structures with data being deposited at the Protein Data Bank (PDB) and it would be a major advance if this could also happen with small-molecule and inorganic structures. A really positive development (February 2011) came with the checks on submitted structure-factor (.fcf) files, which have been a routine component of the submission process for some time, becoming an option in the *checkCIF* procedure. This will hopefully minimize the number of 'unexpected' alerts with which Co-editors have to deal. The most common problem found with structure-factor checking is that authors do not submit the .fcf file generated in the final refinement cycle, leading to a mismatch between the deposited data and the structure factors recalculated from the atomic model in the cif.

While the number of submissions to the journal increased by a small amount in 2010 (5128 compared to 5113 in 2009), the number of published papers has fallen very slightly with 4113 papers published in 2010 compared to 4166 in 2009. A feature of this reduction has been a significant drop in the number of articles submitted from China from 46.5% to 37.6% of the total, which might be correlated with the revelations of scientific fraud discovered in 2009. The original editorial alerting the scientific community to these problems attracted over 15 000 downloads. Fortunately, the fall in Chinese contributions has been compensated by increased submissions from Malaysia, Korea and the USA and, despite these variations, the open-access environment of the journal is now fully established and the future of the journal seems secure. Of the published manuscripts, 68% described structures of organic, 30% structures of metal-organic and 2% structures of inorganic compounds, which is a very similar situation to 2009. 38% of authors were from China, 12% from Malaysia, 8% from India, 5% from Pakistan and USA, 4% from Germany, 3% from Korea, and 2% from Turkey, Iran and Morocco, with smaller percentages from other countries. The percentage of papers withdrawn or rejected for a variety of reasons remains at 18%, and the journal's impact factor increased slightly to 0.41.

We have been particularly fortunate in the past year to recruit 18 new Co-editors to join the journal's hard-working team. A warm welcome to D. Albov, R. Banerjee, K. Biradha, L. Fabian, K. Fejfarova, J. Gallagher, L. Gomes, K. Haller, E. Herdtweck, A. van der Lee, S. Lindeman, M. Lopez-Rodriguez, J. Mague, P. McArdle, K. Mereiter, M. Nieger, P. Roussel and A. Yatsenko. The cohort of journal Co-editors now numbers 76 including the three joint Section Editors. We cannot over-emphasize the excellent work done by our Co-editors or thank them sufficiently. Without their commitment to what can be an extremely taxing job this journal would not exist. We are grateful also for the work of A. Bond, M. Czugler and L. Eriksson who retired as Co-editors during 2010. Jim Simpson will be stepping down as a Section Editor of *Acta E* at the Madrid Congress. He will, however, remain as a Co-editor. We are delighted to announce that the Executive Committee will be nominating Helen Stoeckli-Evans and Edward Tiekink as Section Editors of *Acta Cryst.* Section E at the General Assembly in Madrid.

Finally we are especially grateful for the excellent support that we receive from the staff in Chester, in particular Gillian Holmes, Sean Conway and Mike Hoyland for their constant help and support, and to Peter Strickland for his sound advice and continued guidance.

**W. T. A. Harrison, J. Simpson and M. Weil**, Editors of Section E

**4.1.7. *Acta Crystallographica* Section F.** In its sixth year of publication, developments continued to enhance the journal as a venue for rapid publication of structure, laboratory and crystallization communications on biological macromolecules. In 2010, 368 original science articles were published in 1684 pages. Importantly, 99 of those articles, more than a quarter, were structure or laboratory communications, a 70% increase over 2009. The average time from submission to publication, however, rose from 2.8 to 3.6 months.

There are several reasons for this increase in publication times. The number of pages rose by more than 25%, which matches the increase in publication time even though the number of articles published in 2010 represented an increase of only 13%. The increased number of structure or laboratory communications, which often take more time to review and process, could also be a contributing factor. A further reason could be closer editorial scrutiny, resulting from the discovery in 2009 that fabricated structures had been published in a number of important journals. The increase nevertheless runs counter to the expected impact that the special referee panel (covered below) was to have on publication times.

Progress on new developments continued in 2010. The utility *publBio*, designed to facilitate drafting of crystallographic publications and to speed editorial processing after submission, has gained popularity with authors. Much thought has been given to how best to build the user base for this utility, but it is not clear that all the answers have as yet been discovered.

The special referee panel began its work in 2010. It is composed of 30 experienced referees who have agreed to provide reviews at a rate of about one a month, to return each review within a two-week review period, and to respond to requests for reviews within two days. Each Co-editor is able to recruit a panel member for one of the referee reports for each submission edited. We believe this panel is the next step needed to assure continued progress in holding down publication times while maintaining high standards of quality. All reports indicate that the panel is returning reports of high quality, is doing so on a timely basis, and is much appreciated by the editorial board. With their concurrence, we plan to list the panel members and thank them in a future issue.

The October 2010 issue was composed of some 30 papers from the Joint Center for Structural Genomics (JCSG) led by Ian Wilson of the Scripps Research Institute. Structural genomics teams have come to recognize that both efficiency in preparation and impact of their work are enhanced when papers are published in topically related groups. The first example was a set of eight papers from the RIKEN-UK collaboration, published as a special section in the December 2009 issue. The JCSG Special Issue will be followed in 2011 by another devoted to work of the Seattle Structural Genomics Center for Infectious Disease. We anticipate future demand for special sections and issues from structural genomics and other groups. We note that the JCSG Special Issue was the primary contributor to the striking increase in structure and laboratory communications for 2010 and welcome this significant shift in the balance of papers we publish.

Finally, our impact factor was 0.551 for 2009. We have reason to hope, however, that the papers attracted by the 2010 Special Issue will have a beneficial effect on the journal's impact factor.

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

**4.1.8. *Journal of Applied Crystallography*.** Articles covering a wide range of topics were published in the journal in 2010. A Special Issue was also published. The issue, which contained 16 articles, covered the important topic of Crystallography Education and Training for the 21st Century, and was handled by Katherine Kantardjieff as Guest Editor.

The size of the journal increased markedly in 2010 – the number of full articles published was 165 (compared with 131 in 2009) and the number of pages was 1543 (compared with 1212 in 2009). There was also an increase in the number of manuscripts submitted (309 compared with 282 in 2009 and 258 in 2008).

The impact factor remained high at 3.0; the journal also had a five-year impact factor of 3.8 and a long cited half-life (>10 years). Publication times were slightly longer than in 2009 at 5.7 months. The average publication time for Short Communications was 4.5 months.

A number of Co-editors will retire in 2011; they include D. Chateigner, E. Dodson, S. E. Ealick, J. L. Hodeau, K.-I. Ohshima and T. R. Welberry. It has been a privilege and a pleasure to work with them. My sincere thanks also go to the many members of the crystallographic community who have served as reviewers of submitted papers, to the Co-editors for their hard work in overseeing the peer review process, and to the staff at Chester for an excellent job in preparing articles for publication.

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

**4.1.9. *Journal of Synchrotron Radiation*.** In 2010 a total of 114 papers were published, comprising 816 pages. This was slightly lower than in 2009, but remains higher than in recent years. One Special Issue was published, on the application of synchrotron radiation in the field of soil and geosciences, which included selected papers presented at the 2009 General Assembly of the European Geosciences Union. We continue to believe that the publication of selected papers from workshops in such Special Issues is an important service to the synchrotron-radiation community and have several planned for future issues of the journal.

The Facility Information pages also continued in 2010, providing an opportunity for synchrotron-radiation facilities to communicate important news and updates to the international community of synchrotron-radiation users. This year we were pleased to welcome new contributions from the Paul Scherrer Institut and the Photon Factory, with further facilities expected to join us next year.

A new category of paper was introduced towards the end of 2010: Beamline papers, which we hope will better serve the synchrotron-radiation community and provide a reference publication for users of beamlines at synchrotron-radiation facilities around the world. We expect the interest in this field will continue to grow as new facilities for the generation of radiation, including free-electron lasers, become operational.

The average review time for *JSR* papers in 2010 decreased from 4.4 months to 4.1 months, though the technical-editing time increased slightly to 1.1 months (0.9 months in 2009); this resulted in a slightly lower overall publication time of 5.2 months.

G. Ice, Å. Kvick and T. Ohta, Editors of *JSR*

#### 4.2. Commission on *International Tables*

The Editor of *International Tables for Crystallography Volume A (Space-Group Symmetry)*, M. Aroyo, has continued to work on the forthcoming sixth edition of the volume. Following the proposal that was approved by the Commission during the Osaka Congress, the text and data of the volume will be arranged in three main parts:

Part 1. *Introduction to space-group symmetries*. This part includes chapters on the topics treated in Volumes A and A1. Preliminary versions of about half of the material are available, namely, the general introduction to group theory, the chapter on crystallographic symmetry operations and their representations by matrices, the general introduction to space groups and their description in the tables, and the chapter on relations between Wyckoff positions for a group-subgroup pair of space groups. For various reasons, the authors of the chapters on coordinate-system transformations, reflection conditions, sections and projections of space groups, and subgroups and supergroups of space groups need more time to prepare their contributions. This will result in a delay to the production of the sixth editions of Volume A and the Brief Teaching Edition.

Part 2. *Tables of plane and space groups*. The new sets of plane-group and space-group tables are ready. For each plane- and space-group type the following symmetry items are listed: headline block with the group symbols, space-group diagrams, origin of the unit cell and asymmetric unit, symmetry operations, generators, general and special Wyckoff positions, reflection conditions and symmetry of special projections. The chapters that accompany the tabulated data, providing an explanation of the symbols and a guide to the use of the data, are in an advanced state.

Part 3. *Advanced topics in space-group symmetry*. The majority of the articles for this part have been ready since 2009. As mentioned in the previous report, the chapters on crystal lattices and lattice complexes have been substantially revised. The data listed for the normalizers of space and plane groups have been extended to include the chirality-preserving Euclidean normalizers. The chapter on point-group symmetries and physical properties of crystals has been modified considerably. Unfortunately, the planned article on magnetic space groups will probably not be included in the sixth edition owing to a request from the author.

The fifth editions of Volume A and the Brief Teaching Edition will be reprinted with corrections to replenish stock levels.

The second edition of Volume A1, *Symmetry Relations Between Space Groups*, edited by H. Wondratschek and U. Müller, was published in 2010. Compared to the first edition (2004), all detected errors have been corrected and several improvements have been introduced.

As in the first edition, Part 1 deals with group-theoretical aspects of space groups, group-subgroup relations and the underlying mathematical background. The new edition contains a more detailed discussion of the listed supergroup data and an extension of the theory to the minimal supergroups of space groups.

Two new chapters have been added:

(i) Chapter 1.6 gives instructions on how to relate crystal structures by group-subgroup relations and how to construct trees of group-subgroup relations for crystal structures that can be derived from a high-symmetry structure type (aristotype).

(ii) Chapter 1.7 describes the databases and computer programs of the publicly available Bilbao Crystallographic Server that are related to the subjects of this volume.

Part 2 contains the complete listings of the maximal subgroups for each plane group and space group, including their general positions and their generators, their conjugacy relations and the transformations to the conventional settings. The new edition contains procedures for the derivation of the minimal supergroups from the listed (complete) data on maximal subgroups.

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

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

U. Shmueli, the Editor of Volume B (*Reciprocal Space*), retired following the publication of the third edition of the volume in 2008. A successor has yet to be appointed.

The new Editor of Volume C (*Mathematical, Physical and Chemical Tables*), T. R. Welberry, is considering how best to bring the volume up to date for the fourth edition and plans to visit the IUCr Editorial Offices in Chester in early 2011 to discuss the volume further. The third edition will be reprinted with corrections to replenish stock levels.

The Editor of Volume D (*Physical Properties of Crystals*), A. Authier, reports that there have been no new developments with this volume in 2010. The volume has been reprinted with corrections to replenish stock levels.

A second edition of Volume E (*Subperiodic Groups*), edited by V. Kopský and D. B. Litvin, was published in 2010. A new feature of this second edition is the addition of Seitz notation: in the symmetry-operations section of each table of each subperiodic group, the Seitz notation of each symmetry operation is given below its geometric notation. Minor additions to the text and tables, and corrections of a few typographical errors, were also made.

Proofs for the second edition of Volume F, *Crystallography of Biological Macromolecules*, edited by E. Arnold, D. M. Himmel and M. G. Rossmann, are currently being prepared by the editorial office. There are 20 new articles and 25 articles have been revised. The new articles cover such topics as standard definitions for macromolecular crystallographic statistical indicators, expression of membrane proteins, protein engineering, radiation damage, detection of merohe-dral twinning, determining structures in the presence of merohe-dral twinning, low-resolution *ab initio* phasing, robotic crystal loading, whole-cell X-ray diffraction imaging and halogen interactions in biological crystal structures. There will also be articles on software in current use by macromolecular crystallographers and structural biologists, including software for electron microscopy. These enhancements should continue to make Volume F a key reference for macromolecular crystallographers and structural biologists.

Volume G (*Definition and Exchange of Crystallographic Data*), edited by S. R. Hall and B. McMahon, was reprinted with corrections

in 2010 to replenish low stock levels. The Editors continue to follow developments in the CIF infrastructure that will need to be reported in future editions, and a new CIF dictionary to be released in 2011 may provide an opportunity to update the online edition in advance of a new printed version.

The enhancement of **International Tables Online** by M. Aroyo and co-workers has focused on the development of a web server that provides access to symmetry databases and computer tools based on the space-group data from Volumes A and A1. The creation of the new web server (the *Symmetry Database*) is the initial stage of the long-term programme for the development of **International Tables Online** as discussed and approved by the Commission during the Osaka Congress.

The current databases and programs on the symmetry database server increase the variety and amount of crystallographic data from Volumes A and A1 that are available online, and provide access to: (i) the space-group data available in the XML-based databases; (ii) series of isomorphic subgroups, and (iii) data on minimal supergroups. The results of the initial stage also include the development of new computer tools for the study of group–subgroup and group–supergroup relationships: the transformation of a group to the basis of a subgroup; the development of procedures for left- and right-coset decomposition of a group with respect to a subgroup; Wyckoff-position splittings for a group–maximal subgroup pair; and the generation of isomorphic subgroups of higher indices. All these new features have been achieved either by the development of new databases containing additional data in a static form or by the development of software for generating specific crystallographic data that are not available in the static databases.

There are some problems at present with the speed of the programs for coset decomposition and Wyckoff-position splittings for isomorphic subgroups of relatively high indices. New versions of these programs that will allow calculations for isomorphic subgroups of indices higher than 50 are under development and testing.

A new volume on powder diffraction (Volume H) to be edited by C. J. Gilmore, J. A. Kaduk and H. Schenk is in the planning stage. New volumes on magnetic symmetry groups (by D. B. Litvin) and on EXAFS have been proposed. Because of the spread of information on space-group symmetry into other volumes in the series, C. P. Brock is considering expanding the scope of the Brief Teaching Edition of Volume A so that it would form an introduction to all those volumes in the series, and sections of volumes, that include information about symmetry groups.

The print volumes are selling well and the number of subscribers to **International Tables Online** continues to grow, in part due to a successful marketing campaign by Wiley. An advantage of the move to Wiley is that the IUCr journals and *International Tables* are now available from the same co-publisher.

H. Wondratschek (editor of Volume A1) and H. Fuess (former Chair of the Commission) have announced their retirement from the Commission. We thank them warmly for their many valuable contributions to the *International Tables* series.

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

C. P. Brock, Chair

### 4.3. Commission on Aperiodic Crystals

The Commission has continued actively to promote aperiodic crystallography in 2010, in organizing meetings and workshops as well

as in coordinating activities of and between the quasicrystalline and incommensurate structure communities.

As part of these activities, the Commission continued to promote aperiodic crystallography at national, regional and international meetings.

*International conferences.* The 11th Conference on Quasicrystals (ICQ11), Sapporo, Japan, 13–18 June 2010, was chaired by T. Ishimasa and Y. Ishii. More than 130 delegates from 19 countries attended the conference. A few talks on incommensurately modulated and composite structures were included in order to favour exchange within the aperiodic crystal community. Three satellite meetings were also organized before or after the conference: International Workshop on Strengthening of Magnesium Alloys by Application of Quasicrystal and Related Phases; International Workshop on Surfaces of Quasicrystals; and Mathematics of Quasi-Periodic Order. During ICQ11 it was decided that ICQ12 would take place in 2013 in Cracow, Poland, and would be chaired by J. Wolny.

Further to the activities associated with ICQ11, two Keynote Lectures and four Microsymposia were dedicated to aperiodic crystals at the 26th European Crystallographic Meeting, Darmstadt, Germany, 29 August – 2 September 2010.

A Special Symposium on quasicrystals honouring Distinguished Professor D. Shechtman on his 70th birthday was organized in Haifa, Israel, 12–13 January 2011.

The very important upcoming meeting for the Commission in 2011 is the Madrid Congress. There will be 3 Keynote Lectures and 6 separate Microsymposia in the area of aperiodic crystallography, which the Commission has helped organize. The two-day satellite meeting Aperiodic Crystals for Beginners will be held in Alcalá de Henares, 31 August – 2 September 2010. This satellite is aimed at giving an easy introduction to aperiodic crystals for beginners in the field.

*Schools and workshops.* The Commission has been active in the promotion of aperiodic crystals and, in particular, in promoting education in this field. Indeed, whereas aperiodic crystals are encountered in many different materials, this area of research remains difficult to tackle for the non-specialist.

The Commission has thus organized the first International School on Aperiodic Crystals, Carqueiranne, France, 28 September – 2 October 2010 (M. de Boissieu, G. Chapuis, S. van Smaalen). It gathered 54 participants coming from 19 different countries. This was the first school presenting in the same framework the structure determination and properties of aperiodic crystals. By alternating lectures and tutorials, the school was very much appreciated by the participants, as could be seen from the final survey. This was also a good opportunity for the different communities to interact better.

M. Duseck is organizing the Jana2006 *ad-hoc* workshops at the Institute of Physics, Prague, Czech Republic. The content and date of these specialized lectures is organized on demand. Seven *ad-hoc* workshops have been organized previously.

Two workshops on the mathematics of aperiodic crystals have been organized in 2010:

The ICQ11 satellite Workshop on the Mathematics of Quasicrystals, June 2010, with about 40 participants.

The Workshop on the Mathematics of Aperiodic Order, Korea Institute for Advanced Study, Seoul, Korea, 27 September – 1 October 2010, with about 50 participants.

*CIF dictionary.* Work has continued on updating the CIF dictionary for modulated structures. G. Madariaga is the Commission representative most involved, in cooperation with the Committee for the Maintenance of the CIF Standard. The CIF standard is available



at the IUCr web site. A new database for incommensurate structures is being implemented within the Bilbao Crystallographic Server.

*Web page.* The Commission maintains internet pages at the web site of the IUCr. A web site on all aspects of the crystallography of aperiodic crystals is maintained by the special interest group (SIG) on aperiodic crystals of the European Crystallographic Association. This is maintained by M. Dusek (Prague, Czech Republic), and it can be found at <http://www.xray.fzu.cz/sgip/aphome.html>.

**M. de Boissieu**, Chair

#### 4.4. Commission on Biological Macromolecules

The Commission has continued to support the vitality of the biological crystallography community, particularly through recommending and supporting IUCr proposals to hold meetings, workshops and schools. Numerous meetings of this type will be held in Asia, North and South America, and Europe in 2011. Commission member T. Terwilliger (USA) has been appointed as a member of the Working Group of Database Users in an effort to promote communication between the IUCr and the globally critical resources such as the Protein Data Bank that store and provide convenient access to biological structural data.

A central activity of the Commission has been to contribute to the design of the Madrid Congress. The biologically oriented portion of the International Programme Committee [H. Baker (New Zealand), P. L. Howell (Canada), M. Martínez Ripoll (Spain) and X.-D. Su (People's Republic of China)] has organized an exciting programme with topics ranging across the field of biological and macromolecular structure. A key highlight is that the three macromolecular crystallographers who received the Nobel Prize in Chemistry in 2009 for determination of the ribosome structure (V. Ramakrishnan, T. A. Steitz, A. Yonath) will each give a Plenary Lecture at the Congress. A large number of students are expected to attend and participate from all corners of the world, and the travel of many young scientists will be sponsored by the IUCr.

Regional meetings with biologically relevant content sponsored by the IUCr in 2010 included in April: the RapiData course (Brookhaven, USA); in May: International Symposium of Diffraction Structural Biology (ISDSB 2010) (Paris, France); in June: Structure and Function from Macromolecular Crystallography: Organization in Space and Time (Erice, Italy); in July: ACA Annual Meeting (Chicago, USA); in August: Third K. H. Kuo Summer School of Electron Microscopy and Crystallography: International Workshop of 3D Molecular Imaging by Cryo-Electron Microscopy (Beijing, People's Republic of China), 26th European Crystallographic Meeting (ECM-26) (Darmstadt, Germany); in October: Fundamentals of Modern Methods of Biocrystallography – BioCrys 2010 (Oeiras, Portugal); and in November: Tenth Conference of the Asian Crystallographic Association (Busan, South Korea), First North African Crystallographic Conference (Casablanca, Morocco). These meetings, schools and workshops provide tremendous value in training in and dissemination of novel scientific methods and in cross-fertilizing diverse scientific disciplines.

**E. Arnold**, Chair

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

The Sagamore meeting, the Gordon Research Conference (GRC) on Electron Distribution and Chemical Bonding, the European Charge Density Meeting (ECDM) and the International Conference

on Inelastic X-ray Scattering (IXS) are by tradition the major conferences of the charge, spin and momentum densities community (CSMD).

In 2010 the main activities were the Gordon Research Conference on Electron Distribution and Chemical Bonding (Mount Holyoke College, MA, USA, 11–16 July 2010), organized by D. Jayatilaka (Chair) and P. Macchi (Co-Chair), and the 7th International IXS 2010 Conference (Grenoble, France, 11–14 October 2010), organized jointly by the European Synchrotron Radiation Facility (ESRF) and the Politecnico di Milano, with M. Krisch and C. Dallera as conference Chairs.

The number of participants (92) at the GRC was at the same level as the previous meetings, though slightly less than in 2007. D. Jayatilaka and P. Macchi put together a very good scientific programme. The GRC meeting started with a session on the topic Electron Distributions in Chemistry: Meeting of Theory and Experiment on the evening of 11 July. For the remaining four days, the topics were: Electron Distribution and Interaction Energies; The Density and Crystalline Interactions; Electron Distributions in Biology; Topology or Orbitals: is Ecumenism Possible?; Chemical Bonds under Extreme Conditions; The Unpaired Electron Density; Measuring More: Developments in Instrumentation and Technique; Relativistic Effects in the Electron Density and the Chemistry of Heavier Metals. All sessions were very well organized, with about 20 speakers or discussion leaders who had never spoken before in this GRC series. Discussions were generally very intense and well attended. Some speakers were less than 30 years old, and for some this was their first participation or, at least, it was the first time that their research group had been invited to speak; however, it had not been possible to increase the number of women speaking at the conference. Four afternoon poster sessions were organized by P. Macchi. The next GRC will be chaired by P. Macchi in 2013, with W. Scherer as next Co-Chair. There was worrying news related to the time frequency of the conference: starting from the next meeting in 2013, meetings will have to be necessarily run on a biennial basis and this change will pose serious problems to our Commission concerning the schedule of the other usual CSMD meetings. As on the occasion of the previous conference, the GRC office was asked to consider the possibility of holding the next conference in Europe, since usually the majority of attendants to this GRC meeting come from Europe.

The 7th IXS conference was held in the WTC Conference Center in Grenoble, France. The IXS conference series customarily provides a forum for the presentation of novel results, discussion on present and future trends, and for an intense exchange between participants utilizing the various IXS techniques for a wide variety of different applications. The conference covered the techniques of electronic resonant and non-resonant scattering (in the soft and hard X-ray regime), emission spectroscopy, meV-resolved atomic dynamics, nuclear inelastic scattering, Compton scattering, and thermal diffuse scattering. The conference started with a visit to the ESRF on 10 October and continued on 11 October with two overview talks and a plenary talk on correlated electron systems in the light of X-rays and neutrons. Conference sessions were organized in ten themes: Correlated Electron Systems; 3D Transition-Metal Compounds; Magnetism, Superconductivity and Related Phenomena; Elements and Advanced Materials; Chemistry and Biology; Liquids; Glasses; Gas Phase Studies; Earth and Planetary Science; and New Scientific Frontiers. Two poster sessions were scheduled on 12 and 13 October in the late afternoon, where 84 posters were displayed and discussed. IXS 2010 attracted 162 participants from 61 different institutions from Europe (115; 49 of these from France), North America (23; 22 from USA and 1 from Canada) and Asia (24; 15 from Japan, 5 from

Taiwan, 2 from India, 1 from People's Republic of China and 1 from Korea). 33 participants were students. The decision on the host and location of the next conference, to be held in 2013, will be taken in 2011.

During August 2010 the European Crystallographic Meeting was held in Darmstadt, Germany. A Microsymposium on Charge, Spin and Momentum Densities for the Prediction of Physical Properties was organized by S. Pillet (Nancy, France) and J. Kozisek (Bratislava, Slovakia).

Planning of future projects, besides the currently running project on the Constrained Experimental Wavefunction started in 2005 and coordinated by D. Jayatilaka, has also been promoted by the Commission Chair on the occasion of the CSMD meeting at the 2010 GRC. One potential project, coordinated by P. Nakashima, would concern the dissemination of new differential quantitative convergent-beam electron diffraction (QCBED) techniques among a number of international groups to test their performance on a range of materials and to compare them with the current charge-density techniques. Another project would examine the pros and cons of the existing and developing charge-density databanks, while a third would involve the charge-density study of some organometallic compounds of medium-size crystals to compare the quality of data coming from different laboratories and the differences in chemical interpretations of the resulting static and dynamic densities, using the various available topological approaches.

The Commission, through some of its members, has participated in various forms in 2010 to the Deutsch Forschungsgemeinschaft (DFG) 1178 Project, which is a German-funded six-year project aimed at disseminating use of and expertise in the charge-density technique in chemistry laboratories, in particular in the field of metallorganic and organic chemistry, but also into materials science and pharmacology laboratories. The project, coordinated by D. Stalke and W. Scherer and involving more than 30 research groups, is close to completion and seems to have resulted in a surge of interest in charge density-applications and basic understanding.

An initiative, promoted by B. B. Iversen and funded by the Danish National Research Foundation, to establish an international Center for Material Crystallography (CMC) across four continents, started in 2010. It includes four university partners (B. B. Iversen, M. Spackman, D. Cremer, C. Gatti) and three large-scale facilities groups (M. Takata, SPring-8, Japan; B. Chakoumakos, ORNL, USA; P. J. Vicaro, APS, USA), and it is aimed at combining in a unique platform strong competences in synthesis, charge-density characterization and theoretical modelling to tackle some of the key challenges in materials science.

**C. Gatti**, Chair

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

In 2010 the members of the Commission collaborated actively but mostly *via* the internet. However, in August some of us had a rare opportunity to meet in person and exchange opinions about the future of crystal growth around the world.

The Sixteenth International Conference on Crystal Growth (ICCG-16) and the Fourteenth International Summer School on Crystal Growth (ISSCG-14), the main triennial meetings of the crystal growth community, took place in August 2010. For the first time, the meetings were held in the People's Republic of China and – with more than a thousand participants in total from around the

world – both venues were a great success. The conference organizers gracefully acknowledged the financial support of the IUCr. They also provided the Commission (CCGCM) with the room to hold our meeting (and lunch), which took place on 11 August. Ten Commission members and consultants were present at the meeting (H. A. Dabkowska, K. Byrappa, J. M. Garcia-Ruiz, K. Kakimoto, J. Wang, A. Zappettini, E. Vlieg, S. Baldochi, K. Tsukamoto, E. Talik). We also invited several observers representing different countries who were interested in the work of the Commission: D. H. Yoon (Korea), Z. R. Zytkeiwicz (Poland), S. Bocharow (Russia) and Mu Wang (People's Republic of China).

In 2010 the IUCr supported five meetings that were important for the crystal growth community:

Adsorption, Absorption and Crystal Growth, Gargnano, Italy, 18–23 April 2010 (chaired by A. Zappettini, CCGCM member) (<http://icg2010.imem.cnr.it>).

Second International School of Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials, Granada, Spain, 24–28 May 2010 (organized by J. M. Garcia-Ruiz, CCGCM member) (<http://www.iscgranada.org/>).

Sixteenth International Conference on Crystal Growth (ICCG-16), Beijing, People's Republic of China, 8–13 August 2010 (J. Wang, CCGCM member, was a very competent General Secretary) (<http://iccg16.tipc.cn/>).

The Fourteenth International Summer School on Crystal Growth (ISSCG-14), Dalian, People's Republic of China, 1–7 August 2010 (K. Tsukamoto, CCGCM consultant, was highly appreciated for his input into the innovative, experimental approach to the teaching of crystal growth) (<http://www.isscg14.org.cn>).

Gordon Research Conference on Crystal Engineering (Waterville Valley Resort, New Hampshire, USA, 6–11 June 2010).

At the Madrid Congress the Commission is represented by J. M. Garcia-Ruiz (as a Member of the the International Programme Committee). The Commission submitted six proposals, and we were granted five Microsymposia related to crystal growth topics (the highest number ever):

Wide Band Semiconductor and other Crystals Used in Optoelectronics (organizers E. Talik and E. Calleja);

Crystal Growth and Interface Phenomena at Nanoscale (organizers K. Tsukamoto and J. de Yoero);

The Growth and Morphology of Crystals (organizers A. Glikin and S. Lopez-Andres);

Biom mineralization and Biomimetic Materials (organizers G. Fallini and J. Gomez-Morales);

High-Throughput Crystallization and Polymorphic Search in Pharmaceuticals (organizers U. Griesser and S. Reutzel-Edens).

In 2010 the CCGCM received requests for letters of support for several local and international crystal growth meetings in 2011. All the proposals were well worth supporting, but some could not be supported owing to the time conflict with regional or international crystallographic meetings.

Two important meetings in 2011 have already received the support of the IUCr: 3rd International School on Biological Crystallization, Granada, Spain, 22–27 May 2011, and XVII International Conference on Crystal Chemistry, X-ray Diffraction and Spectroscopy of Minerals, St Petersburg, Russia, 20–24 June 2011.

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

Finally, it was my great honour and pleasure to chair this Commission for the last six years. I hope that all the work done here

will bring more understanding of the role of crystals and their influence on many aspects of life and technology.

**H. A. Dabkowska**, Chair

#### 4.7. Commission on Crystallographic Computing

The unexpected death in January of the Chair, L. M. D. Cranswick, overshadowed the Commission's activities this year. A. Thompson of the University of Oxford was appointed as Secretary to assist the new Chair, H. R. Powell. A. Thompson put some effort into putting together a Commission *Newsletter*, but suffered from a poor response from potential authors so this has been delayed until next year.

A number of the Microsymposia suggested by the Commission were adopted for the Madrid Congress; several joint symposia with other Commissions were also adopted. H. R. Powell represented the Commission at the International Programme Committee meeting.

Preparations for the Computing School in Mieres, Spain, continued, and a list of speakers was agreed. It became apparent at the end of 2010 that the accommodation in Mieres would not be ready for occupation by August 2011, so it was agreed that the venue be moved to Oviedo.

**H. R. Powell**, Chair

#### 4.8. Commission on Crystallographic Nomenclature

*Nomenclature issues.* The following topics have been discussed and will be on the Agenda of the Meeting of the Commission in Madrid:

(a) Definition of the term 'asymmetric unit'.

(b) Proposal to include Seitz symbols in Volume A of *International Tables*.

*Online Dictionary of Crystallography.* Various issues related to definitions in the Online Dictionary have been discussed, for instance relative to the definition of Brillouin zone. In order to enable an online discussion of topics, the Editor-in-Chief of the Dictionary, G. Chapuis, and the Administrator, B. McMahon, have set up an IUCr forum.

**A. Authier**, Chair

#### 4.9. Commission on Crystallographic Teaching

Following the idea of the importance of improving the teaching of the fundamentals of crystallography, during 2010 the Commission was involved in the organization of the The Zürich School of Crystallography – Bring Your Own Crystals, thanks to G. Chapuis, a very active member of the Commission.

In collaboration with the Commission on Mathematical and Theoretical Crystallography, a School of Fundamental Crystallography was held in Bloemfontein, South Africa, 12–16 April 2010, with Commission member M. Rademeyer as local organizer and lecturer.

Following the suggestion of the Executive Committee during the meeting in Osaka, the International School of Aperiodic Crystals was organized in September 2010 in Carqueiranne, France by the Commission on Aperiodic Crystals; G. Chapuis, on behalf of the Commission on Crystallographic Teaching, was one of the main organizers.

Commission member R. Baggio, together with his South American colleagues, organized a workshop at Buenos Aires, Argentina, on Structure Resolution from Single-Crystal Data; and thanks to its success another meeting is planned for 2011 in the southern village of Bariloche, at the Balseiro Institute (a renowned Physics Centre in

Argentina). The main subject of this school will be Powder Diffraction, from both X-ray and neutron sources, and its organization has been partially sponsored by the IUCr.

M. Weiss and P. Spadon were the Co-Chairs of a Microsymposium on Crystallographic Teaching during ECM-26 in Darmstadt, Germany, August 2010.

As the Commission representative on the International Programme Committee for the Madrid Congress, R. Baggio successfully proposed two Microsymposia:

Web-Based Crystallography Teaching: the Use of Modern Communication Methods to Teach Crystallography; Chair: K. Kantardjieff, Co-Chair: G. Chapuis.

Application of Crystal Structure Information in Chemical Education; Chair: L. Infante, Co-Chair: G. Battle (a joint proposal by the Commission on Crystallographic Teaching and the Commission on Structural Chemistry).

P. Spadon and F. H. Allen will be the Co-Chairs of a session dedicated to celebrate the almost 40 years of effort dedicated to crystallographic teaching by L. Riva di Sanseverino.

In October 2010 a Special Issue of *Journal of Applied Crystallography* (Volume 43, Part 5, Number 2) was published, with contributions from the successful 'Pre-Conference' Workshop organized in 2008 for the Osaka Congress.

This Special Issue provides a contemporary review of crystallographic education and training pedagogy and progress. Articles in this issue of the journal consider current and ongoing developments, the potential of utilizing Web 3.0 to provide practical experience, and the challenges we face in the next decade to not only educate and train the next generation of scientists, but also to renew an awareness and appreciation for crystallography and X-ray diffraction analysis as key underpinnings of modern science. As with previous Special Issues on this topic, the Commission hopes that this will provide ideas and useful material that its readers can adapt and adopt in teaching crystallography, and that the insights presented will continue to drive and stimulate discussion on teaching and education in crystallographic science.

**P. Spadon**, Chair

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

A Microsymposium on Crystallography in Art and Archaeology was part of the 26th European Crystallographic Meeting (ECM-26), Darmstadt, Germany, 29 August – 2 September 2010, with the following programme: E. Dooryhée: Introduction; J. M. Castera: Arabesques for Abu Dhabi – an Octagonal System; Y. Aboufadel: Classification of the Moroccan Ornamental Patterns Constructed by the 'Hasba' Method; J. Fabry: Quasiperiodic Symmetry in a Baroque Church in the Czech Republic; A. Haake: 'Bossenstein' – Unique Ornamentation of 'Weser-Renaissance'.

At the poster sessions of ECM-26, J.-M. Castera presented an entertaining practical on patterning and tiling using Zellij tiles.

Commission members A. Rafalska-Lasocha and A. Zürn participated in the International School Hubert Curien: 3rd Course in Structural and Molecular Archaeology on Non-Invasive Analysis of Painting Materials, Erice, Italy, 14–21 June 2010 ([http://www.nacho.ulg.ac.be/Summer\\_School.html](http://www.nacho.ulg.ac.be/Summer_School.html)).

A Workshop on X-ray Techniques in the Investigations of the Objects of Cultural Heritage, Krakow, Poland, 13–16 May 2010 (<http://www.heritagescience.pl/workshop>) included a one-day session dedicated to Around Rembrandt and his Workshop. This was the third in a series of meetings with the aim of bringing together

scientists from relevant disciplines with museum professionals (conservators and curators) responsible for the organization and preservation of art collections. A full report of the meeting may be found at [http://crysac.visual-chemistry.net/activities/2010\\_krakow\\_report.html](http://crysac.visual-chemistry.net/activities/2010_krakow_report.html).

**E. Doorhée**, Chair

## 4.11. Commission on Electron Crystallography

The main activities have been preparing for the Madrid Congress and finalizing work on *International Tables*.

The third K. H. Kuo Summer School of Electron Microscopy and Crystallography: International Workshop of 3D Molecular Imaging by Cryo-Electron Microscopy (<http://emworkshop2010.ibp.ac.cn/index.html>) was held in Beijing, People's Republic of China, 8–12 August 2010. The Summer School was supported by the IUCr, enabling nine young-scientist travel grants to be awarded.

Many of the Commission members have been involved in the 43rd Erice School on Electron Crystallography, organized by three members of the Commission: U. Kolbe, L. Meshii and A. Avilov. The School will be held in June 2011.

Some members of the Commission were involved in the EMMM11 conference, which was held in May 2011. This conference series was nucleated by the Commission, and seeks to bring scientists working in multiscale modelling together with scientists doing electron crystallography.

For the future, a number of workshops are planned:

(a) The Third Asian Electron Crystallography Workshop, provisionally in Japan.

(b) EMMM13, provisionally in Japan.

(c) The next Workshop on Precession Electron Diffraction, provisionally set for 2012.

(d) A School on Electron Crystallography organized by K. Balzuweit to be held in November 2011.

*Sub-committee on International Tables.* The Sub-committee has completed an extensive analysis of the contents of *International Tables* and the sections that need to be rewritten to reflect the substantial changes that have taken place (and continue to occur) in electron scattering. The details have been provided to the Commission on *International Tables*.

*Sub-committee on Dynamical Diffraction.* This Sub-committee has nothing to report.

*Sub-committee on Software for Electron Imaging, Diffraction and Crystallography.* This Sub-committee has nothing to report.

*Sub-committee on Software for Electron-Based CIF Entries.* The Sub-committee has prepared a partial list of CIF entries for electrons, and is continuing to discuss how to handle issues such as images.

*Sub-committee on Aberration Definitions.* This Sub-committee has nothing to report.

*Sub-committee on the Gjønnnes Medal.* This Sub-committee has nothing new to report: the next Gjønnnes Medal will be awarded to Professors A. Howie and M. Whelan for the development of the dynamical theory of diffraction contrast of electron-microscope images of defects in crystals, and other major pioneering contributions to the development and application of electron microscopy, diffraction and spectroscopy of materials.

The Commission's home page is maintained by the Chair, and can be found at [http://www.numis.northwestern.edu/IUCR\\_CEC](http://www.numis.northwestern.edu/IUCR_CEC).

**L. D. Marks**, Chair

## 4.12. Commission on High Pressure

The year 2010 has brought a number of new exciting and important developments in high-pressure crystallography. A new high-pressure beamline, SNSP, has been commissioned at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (USA) and has received the first beam. A similar state-of-the-art spallation neutron facility, J-PARC, also featuring dedicated high-pressure beamlines, has been commissioned in Tokai, Japan, and received the first beam in 2011. A new dedicated high-pressure beamline has also been commissioned at the Petra-III synchrotron in Hamburg, Germany. These significant investments in the shared high-pressure experimental infrastructure confirm that high-pressure crystallography is gaining an increasingly strong position among the solid-state sciences.

In addition to the new central facilities that have become available on the international scene, significant progress has been made in methodology development of both new and more established experimental approaches. One particular area that has attracted interest and attention is the exploration of amorphous and liquid structures at high pressure using total scattering techniques. Another important recent development is X-ray-based high-pressure imaging and computed tomography. Well established techniques, such as high-pressure single-crystal and powder diffraction, have also experienced significant advancements that now permit the collection of data at much higher pressure, with significantly shorter data-collection times and better accuracy.

*2010 Commission workshop in Gatlinburg, TN (USA).* The 2010 Commission workshop was held in Gatlinburg, TN, USA, near the site of the SNS at Oak Ridge National Laboratory, and was organized by C. Tulk (ORNL, USA). The workshop featured a Plenary Lecture delivered by J. Parise and ten scientific sessions on crystal structures and phase transitions, techniques for high-pressure studies, simple organic systems, geoscience and planetary science, theory and computations, chemistry, biological materials, amorphous, liquid, nano- and non-crystalline solids and magnetic and electronic phenomena at high pressure. The 2010 workshop was well attended (53 participants from 16 countries). 42 scientific abstracts were submitted.

The Commission held a closed meeting at the 2010 workshop, with P. Dera, I. Loa, F. Fabbiani, Y. Katayama and V. Solozhenko in attendance. The topics discussed included preparations for the Madrid Congress, plans for locations of the Commission workshops in 2012 and 2013, as well as changes in the Commission membership for the next triennium. The locations suggested for the next two Commission workshops are Tokai (Japan) and Hamburg (Germany).

*Plans and preparations for the Madrid Congress.* The Commission has been represented on the International Programme Committee for the Madrid Congress by F. Fabbiani. The Commission succeeded in having seven scientific Microsymposia approved, three of which were co-proposed jointly with other Commissions (Structural Chemistry, Powder Diffraction, Neutron Scattering and Synchrotron Radiation). In addition to the Microsymposia, the Commission proposed two Keynote Lectures, to be given by K. Hirose and E. Boldyreva, which have both been approved.

The summary of the approved Madrid Congress high-pressure programme is as follows:

MS5: Non-Ambient Powder Diffraction.

MS12: Non-Covalent Interactions in Molecular Crystals and Biomolecular Systems under Pressure.

MS19: Synthesis, Structure and Properties of Novel Materials at High Pressure.

MS40: Pressure-Induced Phase Transitions.

MS47: Advances in High-Pressure Techniques and Instrumentation.

MS60: Solid State Reactivity.

MS75: Liquids, Amorphous and Nanocrystalline Solids at High Pressure.

KN9: K. Hirose: High-Pressure Geoscience/Mineralogy (with Particular Reference to Post-Perovskite).

KN29: E. Boldyreva: Molecular Crystals at High Pressure.

**P. Dera**, Chair, and **I. Loa**, Secretary

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

Discussions amongst the members and consultants of the Commission (CIMS) were mainly performed *via* e-mail, but several members and consultants who attended the European Crystallographic Meeting held at Darmstadt met there in person. Other forms of communication were by other occasional meetings or conferences, or by using the web site. The latter is excellently maintained by M. Nespolo (<http://www.crystallography.fr/cims/>).

The Commission on Structural Crystallography (CSC) and CIMS maintain their links. A. Beatty is the representative of CSC in CIMS and the representative of CIMS in CSC is P. Mercier.

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

Strong links exist between CIMS and Special Interest Group 5 of the European Crystallographic Association (ECA-SIG5, <http://sig5.ecanews.org/>): M. Nespolo is the Secretary and the current Chair is F. Hatert. There are also very good relationships between CIMS and the European Mineralogical Union (EMU, <http://www.univie.ac.at/Mineralogie/EMU/>): H. Effenberger is the Secretary of EMU and R. Oberti is the current Chair.

CIMS was involved in the following meetings, held in 2010:

(i) III International Workshop on Layered Materials: Design and Function, Bochum, Germany, 14–15 May 2010 (<http://www.layeredmaterials.rub.de/>). G. Ferraris and W. Depmeier were members of the Scientific Committee.

(ii) Minerals as Advanced Materials II (MAAMII), Kirovsk, Russia, 19–25 July 2010 (<http://www.minsoc.ru/maam2010/>). The International Programme Committee included T. Armbruster, G. Ferraris and W. Depmeier. The latter and O. Yakubovich gave lectures. W. Depmeier organized the funding for 15 participants from Germany through grants from the Deutsche Forschungsgemeinschaft. A book with the results is in print.

(iii) Several members and consultants of CIMS attended the 26th European Crystallographic Meeting, Darmstadt, Germany, 29 August – 2 September 2010 (<http://ecm26.ecanews.org/>). P. Thomas gave a Keynote Lecture, H. Effenberger an oral contribution and M. Nespolo chaired a Microsymposium.

(iv) Several members and consultants of CIMS attended the 20th General Meeting of the International Mineralogical Association (IMA), Budapest, Hungary, 21–27 August 2010 (<http://www.ima2010.hu/>). G. Ferraris was convener of the session on Modularity and Modulation in Minerals and M. Nespolo of the session on Mineralogical Crystallography. T. Nagai gave an oral contribution in the session on Mineralogy of the Deep Earth.

(v) First North African Crystallography Conference (NACCI), Casablanca, Morocco, 23–26 November 2010 (<http://naccl.univ.ma/>). A. Thalal, who is President of the Moroccan Crystallographic Association (AMC), was a member of the Organizing Committee.

CIMS has supported the application for financial support by the IUCr for the following meetings planned to be held in 2011:

(i) XVII International Conference on Crystal Chemistry, X-ray Diffraction and Spectroscopic Studies of Minerals (CCXRDS), St Petersburg, Russia, 20–24 June 2011 (<http://onlinereg.ru/ccxrds/>).

(ii) Symposium on X-ray Techniques for Materials Research – from Laboratory Sources to Free Electron Lasers, at the EMRS Spring Meeting, Nice, France, 9–13 May 2011 (<http://www.emrs-strasbourg.com/>).

(iii) Second SMARTER Crystallography Workshop, Aveiro, Portugal, 23–27 May 2011 (<http://smarter.web.ua.pt/>). J. Rocha chairs the Organizing Committee and is also a member of the Scientific Committee.

Some additional personal achievements:

W. Depmeier acted as a member of the International Programme Committee for the Madrid Congress. Following his presentation at ECM-25, W. Depmeier gave three lectures in Austria (Vienna, Graz and Salzburg) covering the topic Minerals as Advanced Materials. A new mineral was named after him, and he also became an honorary member of the Russian Mineralogical Society.

G. Ferraris is series editor of the *EMU Notes* (<http://www.minersoc.org/pages/EMU-notes/EMU-notes.html>). He has also been appointed a member of the Accademia Nazionale dei Lincei (<http://www.lincci.it/>).

C. Cahill served as the 2011 Programme Chair for the annual meeting of the American Crystallographic Association. He also gave an invited lecture at MAM-10: 5th IUPAC Sponsored International Symposium on Macro- and Supramolecular Architectures and Materials, Ocho Rios, Jamaica, 15 August 2010.

O. Yakubovich worked as an Associate Editor of *The Canadian Mineralogist*.

P. H. J. Mercier is the organizer of a full-day Rietveld Session at the 60th Annual Conference on Applications of X-ray Analysis (<http://www.dxcidd.com/11/index.htm>).

D. Yu. Pushcharovsky published the following book: *Geology of the Earth's Mantle*, by Yu. M. Pushcharovsky and D. Yu. Pushcharovsky, Moscow, GEOS, 2010, 138 pp. He continues to act as associate editor of *European Journal of Mineralogy*, and was among the organizers of a festival of sciences in October 2010, where he gave an introductory talk.

D. Pandey has been nominated as Editorial Advisory Board Member of *Zeitschrift für Kristallographie*. He is organizing one CIMS-sponsored Microsymposium for the Madrid Congress.

**W. Depmeier**, Chair

#### 4.14. Commission on Mathematical and Theoretical Crystallography

*Scientific activity in 2010.* During 2010 the Commission (MaTh-Cryst) organized four main activities.

A School on Fundamental Crystallography was held at Faculty of Natural and Agricultural Sciences of the University of the Free State, Bloemfontein, South Africa, 12–16 April 2010. The School was organized in cooperation with the Commission on Crystallographic Teaching and was supported by the University of the Free State. The School was attended by 43 participants from ten institutions and six countries. Participants ranged from Masters students to post-docs, while lecturers were from South Africa, France and Spain. This School served as a sort of canvas for the following Schools, whose content will be based on the Bloemfontein School. Details of the School can be found at the School web site (<http://www.crystallography.fr/mathcryst/SouthAfrica2010.php>) and a selection of photographs are available at the IUCr web site (<http://www.iucr.org/gallery/2010/fundamental-crystallography/>).

Two summer schools, which ran one after the other, were organized at the Faculty of Sciences and Technology of the Université Henri Poincaré, Nancy 1, France, 21 June – 2 July 2010. The first day was an optional day devoted to introducing or revising fundamental concepts, which was, however, attended by the majority of the participants. During the next four days a School on Topological Crystal Chemistry: Theory and Practice was held, where the theory and practice of topological packages (TOPOS, Systre, 3dt) were presented. A weekend intermission followed, when participants attended an intensive preparation for the next School on Irreducible Representations of Space Groups (28 June – 2 July). The Schools were attended by 56 participants (49 for the first school, 31 for the second) from 18 countries and were sponsored by the IUCr, the ECA, the French Crystallographic Association, the Scientific Council of the Université Henri Poincaré, Nancy 1, the Région Lorraine and the Communauté Urbaine Grand Nancy, and supported by Special Interest Group No. 5 (Mineral and Inorganic Crystallography) of the European Crystallographic Association. Abstracts of the poster presentations and didactic material are available from the Schools' web site (<http://www.crystallography.fr/mathcryst/nancy2010.php>).

Satellite Conference of the XXVI European Crystallographic Meeting, Darmstadt, Germany, 27–29 August 2010. The satellite included three sessions: (1) Foundations of Aperiodic Structures made Comprehensible (in cooperation with the Commission on Aperiodic Crystals); (2) Introduction to Quaternions and Geometric Algebra and Their Applications in Crystallography; (3) Mathematics of Minimal Surfaces. During the third session, participants could manipulate concrete three-dimensional models of minimal surfaces, partly from the collection originally at Marburg University. The satellite was attended by 27 participants from 11 countries. Details of the conference, abstracts of posters and contributed presentations and PDF versions of the presentations can be found at the satellite web site (<http://www.crystallography.fr/mathcryst/darmstadt2010.php>).

A School on Fundamental Crystallography, based on the canvas of the School in Bloemfontein, was held at the Chemistry Faculty of the Universidad de la Republica in Montevideo, Uruguay. The School was sponsored by the University of Uruguay (through Facultad de Química, CSIC and CINQUIFIMA), the IUCr, PEDECIBA and ANII (Uruguay), the American Crystallographic Association and the ICDD. A total of 50 participants from Argentina, Brazil, Chile, Colombia, Mexico and Uruguay with backgrounds in structural biology, mathematics, chemistry, physics, materials science and mineralogy attended the week-long event that also counted 30 poster presentations from all the mentioned countries; there was allowance for significant interaction among attendees who shared an intense eight hours per day of lectures, with coffee and lunch breaks and two social events on Monday and Thursday evenings, where the typical 'candombe' music was played and danced by local artists and participants and enjoyed by everyone. Collected abstracts of the poster presentations are available from the conference web site (<http://www.crystallography.fr/mathcryst/montevideo2010.php>) and a selection of photographs are available at the IUCr web site (<http://www.iucr.org/gallery/2010/fundamental-crystallography-montevideo/>).

*Scientific Activities in 2011 and later.* Planned activities include, at present:

A School on Fundamental Crystallography in Mahdia (Tunisia) was planned in April 2011 but the recent events in the region obliged us to move it to a future date – most likely late 2011 (see <http://www.crystallography.fr/mathcryst/mahdia2011.php>).

A Workshop on Crystallographic Software at the Tokyo University of Science, Tokyo, Japan, was planned for May 2011 but has had to be postponed until December 2011 because of the tsunami; the aim of the Workshop is to give participants a detailed introduction to the theory and approaches behind the packages that will be presented, not a blind-user approach (see <http://www.crystallography.fr/mathcryst/tokyo2011.php>).

A Workshop on Mathematical Crystallography in Manila, the Philippines, 2–6 November 2011 (see <http://www.crystallography.fr/mathcryst/manila2011.php>).

Other activities under discussion:

A workshop in India, under the responsibility of Commission consultant D. Pandey (dates to be fixed);

A contribution to an American meeting for which W. L. Duax, former IUCr President, has promised to help MaThCryst to obtain logistic help in North America, where the Commission has more difficulties to affirm its presence;

A School on Graph Theory in Crystallography and Crystal Chemistry, after the publication of the book with the same title, currently in preparation by J. G. Eon, W. Klee, J. Rutherford and B. Souvignier [The original project concerned only the first three authors but following the passing away of J. Rutherford (September 2009), B. Souvignier kindly accepted to take over. Oxford University Press, which will publish the book in the IUCr/OUP Book Series *Monographs in Crystallography* has agreed to provide copies to participants of the school at a reduced price.];

A Workshop on the Manifold Description of Modulated Structures and the Use of Differential Geometry to Describe Crystal Structures, proposed by Commission member S. Hyde;

A book entitled *Geometric Algebra in Crystallography*, currently under consideration in the IUCr/OUP Book Series *Monographs in Crystallography*;

A School on Fundamental Crystallography in Uberlandia, Brazil (probably October 2012), which will be the natural successor to the school held in Montevideo in 2010.

**M. Nespolo**, Chair

#### 4.15. Commission on Neutron Scattering

An important part of the activity of the Commission (CNS) during 2010 concerned the preparation of the proposals for Microsymposia and Keynote Lectures for the Madrid Congress. The Commission was represented on the International Programme Committee by V. Aksenov. The Programme has been upgraded and refined based on synergies with other Commissions having similar scientific interests.

In the landscape of neutron sources, several advances in neutron scattering capabilities over the past year must be recognized around the world. At the SNS in the USA there are now 13 operating instruments, six in the user program and seven being commissioned in particular advanced powder and single-crystal scattering capabilities.

The Material and Live Science Experimental Facility at JPARC in Japan took a major step forward with the completion and opening of the user programme for ten instruments, of which five are dedicated to diffraction techniques. The characteristics of these new instruments were presented at the 26th European Crystallographic Meeting, Darmstadt, Germany, in an interesting lecture by T. Kamiyama.

Moreover, at JPARC the power level of 200 kW was reached in December 2010. OPAL in Australia operated seven neutron beam instruments for 173 days in 2010, two more will be commissioned in 2011 and four more are scheduled for completion in 2013.

The CARR reactor of the China Institute of Atomic Energy (CIAE) achieved first criticality on 13 May 2010 and the 15th anniversary of the Hanaro research reactor (Korea) was celebrated by a special symposium in November.

In Europe, the ILL at Grenoble, France, continues with the second phase of its Millennium Programme and is preparing a new impetus, with the 2020 Vision Meeting attended by more than 300 people to set priorities for future development of instruments and infrastructure. In 2010 Poland joined the ILL, and India agreed to sign up for 2011, facilitating access to neutron techniques for an already mature community. In the UK the Phase Two Instruments Project at the ISIS second target station has been launched with the aim of building four new instruments together with the necessary advanced detectors, electronics and software. The neutron source Heinz Maier-Leibnitz (FRM II) in Munich completed the 25th cycle since its commissioning in 2004. The FRM II reactor was available on 203 days in 2010 and reached 100 per cent availability compared to the planned operational time. The ten-year programme for renovation of the IBR-2 reactor (Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia) has been finished. The first fuel elements were installed in the core on 17 December 2010.

The CNS has the conviction that in order to take real advantage of these technical advances, an important and sustained effort has to be deployed for the education of new users in the skills of neutron scattering. Consequently, during 2010 the Commission has continued to support the vitality of the neutron scattering community, particularly recommending and supporting IUCr proposals to hold meetings, workshops and schools, but also through the active participation of members of the CNS in different meetings devoted to the future development of the use of neutrons in crystallographic areas. More than 30 dedicated events took place during 2010, including regular school series and workshops shared with other techniques, in particular X-ray diffraction. Major occasions for exchange within the neutron crystallographic community were the American Conference on Neutron Scattering in Ottawa, Canada, the 26th European Crystallographic Meeting in Darmstadt, Germany, and the Asian Crystallographic Association Conference (AsCA 2010) that was held in Busan, Korea.

In cooperation with the Asia–Oceania Neutron Scattering Association (AONSA), the Commission is putting forward a proposal to the International Council of Science (Asia Pacific region) to develop training and scientific collaboration in the Asia–Oceania region. This would be the next level of training for promising young scientists to acquire experience with neutron methods beyond short training courses.

The Erwin Felix Lewy Bertaut Prize is awarded by the European Crystallographic Association (ECA) and the European Neutron Scattering Association (ENSA) to young European scientists in recognition of notable experimental, theoretical or methodological contributions in the investigation of matter using crystallographic or neutron scattering methods. In 2010, the Prize Committee decided to award the Erwin Felix Lewy Bertaut Prize to Tom Fennell, a scientist from the Institut Laue–Langevin, Grenoble, France, for his pioneering work to characterize spin ice materials and demonstrate the existence of a Coulomb phase therein.

Recently, the formation of a Commission on Magnetic Structures has been proposed, and the CNS is supportive of this and has proposed some of its future members. The purpose of this new Commission would be very precise and focused, *i.e.* to promote and establish some standards in the description and the reporting of magnetic structures. We encourage that specialist groups to achieve a

consensual standard, but the CNS will maintain a great interest in magnetism. Neutron diffraction being the main technique for the determination of magnetic structures, we trust that the two Commissions will work together in the forthcoming years.

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

#### 4.16. Commission on Powder Diffraction

*Commission meetings.* The Commission (CPD) held its 2010 meeting during the EPDIC/ECM meeting in Darmstadt, Germany.

The untimely passing of L. M. D. Cranswick was felt in many quarters. One of his more public activities was as Chair of the Commission on Crystallographic Computing and organizing the software fairs at IUCr Congresses and elsewhere. This responsibility now passes to people with less exposure to powder diffraction software and techniques. It was communicated to the new Chair of the Commission on Crystallographic Computing that the CPD would help the new fair organizers with the powder diffraction content if required.

The seeming decline in education in powder diffraction techniques was discussed at length once again. Crystallography overall has been suffering in this regard but powder diffraction is especially vulnerable. If taught at all during crystallography courses, it is usually mentioned in passing and rarely are practical issues raised. One of the strengths of powder diffraction, *i.e.* simplicity in data collection, can also be one of its weaknesses with inexperienced operators. Even crystallographers experienced in single-crystal techniques taking over responsibility for powder instruments can run into trouble with powder diffraction as a seemingly 'simple technique'.

Although tackling declining knowledge of crystallography in the developing world continues to challenge the community there still remain opportunities in the developing world for expanding the base of crystallography. Powder diffraction is an important technique in many resource-based industries, and basic instrumentation can be simpler to maintain and operate than many analytical techniques, so it is a good place to start. Consequently the CPD is hoping to organize a workshop to be held in South Africa in 2013.

It was decided that the 2011 CPD meeting will take place during the Madrid Congress with a smaller get-together with the members present at the powder diffraction crystallography school at Erice, Italy, in June.

*Madrid Congress Programme.* The International Programme Committee meeting was held in May 2010. The CPD was fortunate in being allowed to send three representatives to the meeting: P. Whitfield, R. Cerny and N. Masciocchi. Given the need for cooperation with the other Commissions to maximize impact on the programme, the additional 'bodies' were very useful during simultaneous negotiations with multiple Commissions. We were very pleased to be able to sponsor jointly two Microsymposia with the newest Commission, the Commission on Crystallography in Art and Cultural Heritage. The methodology used during selection limited the CPD's direct involvement to 12 Microsymposia, three Keynotes and an evening session, but powder diffraction will play a significant role in many others that we could not officially support. Consequently, powder diffraction will have a greater presence in Madrid than in recent Congresses.

*Meeting sponsorship and other support.* 2010 proved an unusually quiet year with regard to applications for support for IUCr sponsorship with only three requests received. The CPD also provided a letter of support for the Erice Powder Diffraction School for an application to the ECA. The powder diffraction community lost a valuable resource when the funding for the CCP14 web site ended.

The CPD unanimously supported an application by R. Cernik to EPSRC in the UK to restore the CCP14 funding.

*Projects.* There was some discussion at the CPD meeting about potential future projects. The issue of refinement residuals was raised as a problem area, but we were unable to frame the issue in such a way as to be suitable for a stand-alone project. This subject will be revisited in the future.

The CPD would like to see more resources available to scientists wishing to learn powder diffraction crystallography. While there are three excellent textbooks that have been published or revised recently, in the absence of a topical university course, textbooks appear to offer little traction to many younger scientists (and some older ones as well), who turn first to the web and e-mail when faced with a new problem. To address this, the CPD is looking into ways in which material from tutorials and workshops can be captured and presented as web content.

*CPD meeting in 2012.* The issue of the accuracy and reliability of crystal structures determined using powder diffraction data has been around for a number of years. The recent publication of dubious structures from powder and single-crystal data give this some impetus. The CPD has decided to organize a workshop in 2012 entitled Accuracy in Structure Solution from Powder Diffraction Data. It is to be held as a satellite to the ECM in Bergen, as opposed to EPDIC, to open attendance to non-powder specialists (*i.e.* not preaching to the converted). The crystallographic databases have an obvious stake in structures being correct and reliable so one or more of them are expected to be involved at some level.

*International Tables Volume H.* Under the guidance of C. J. Gilmore of the IUCr Executive Committee, progress towards a volume of *International Tables* dedicated to powder diffraction is moving along steadily. An outline of the contents has been distributed and J. A. Kaduk and H. Schenk have agreed to join C. J. Gilmore as joint Main Editors.

**P. Whitfield**, Chair

## 4.17. Commission on Small-Angle Scattering

*Commission meetings and communication.* As in previous years, the Commission (CSAS) members communicated by e-mail or during personal meetings at national and international conferences. During the year, routine communications were accomplished by e-mail.

*Activities.* J. Trehwella was a member of the International Programme Committee for the Madrid Congress and has coordinated with the CSAS members to propose the following SAS-focused Keynote Lecture and CSAS-sponsored Microsymposia:

Keynote Lecture by I. Torriani on X-ray Diffraction and Small-Angle Scattering for the Study of Polycrystalline Materials, Polymers and Soft Matter.

MS: Industrial Applications of SAXS and SANS to Hard Materials, chaired by R. Knott and co-chaired by A. Craievich.

MS: SAXS/SANS, Total Scattering and the Nanostructure Problem, chaired by S. Billinge and co-chaired by M. Avdeev.

MS: Standardization, Validation, and Automation in Modern Biological Small-Angle Scattering, chaired by J. Perez and co-chaired by M. de Oliveira Neto.

MS: Biological Neutron Scattering and Deuteration, chaired by T. Forsyth and co-chaired by J. Krueger.

MS: Powder Diffraction and Complementary Techniques, chaired by P. Chupas and co-chaired by M. Milanesio.

MS: Complementary Biophysical Methods: Adding Value to Protein Structure, chaired by N. Cowieson and co-chaired by D. Beckett.

J. Trehwella is also a member of the Scientific Programme Committee of SAS 2012, to be held in Sydney, Australia, 18–23 November 2012, and with D. McGillivray will be assembling the full Scientific Programme Committee for that meeting.

As a Consultant of the Commission, D. I. Svergun was involved in the discussion of topics for the Madrid Congress. He and several Commission members are also members of the Advisory Committee for the next SAS meeting in Australia (2012). The CSAS has provided advice on a series of issues in connection with the planning of the SAS 2012 conference.

*Educational activities.* The Commission members are very active in promoting the small-angle scattering techniques and in contributing to research schools and workshops.

R. Serimaa gave a lecture on the application of SAXS and WAXS methods in studies on natural polymeric materials at a Finnish Bioregs graduate school autumn seminar, Espoo, Finland, 11 November 2010.

N. Yagi was involved in the 4th AOFSSR (Asia/Oceania Forum for Synchrotron Radiation Research) Cheiron School at SPring-8, 9–18 October 2010, acted as a member of the local organizing committee and conducted beamline practice on SAXS. N. Yagi was also involved in the 10th SPring-8 Summer School, 24–27 July 2010, where he acted as a member of the local organizing committee and conducted beamline practice on SAXS.

J. Trehwella, N. Yagi, D. I. Svergun, and J. S. Pedersen gave lectures at the EMBO Practical Course on Solution Scattering from Biological Macromolecules at EMBL Hamburg, Germany, 25 October – 1 November 2010.

V. V. Volkov was involved in the preparation of material for a 32-hour lecture course on Supramolecular Structures in Nanomaterials as a further development of the course of lectures on X-ray and neutron small-angle scattering. The lectures were given to the students of the Scobel'syn Institute of Nuclear Physics of Moscow State University.

V. V. Volkov was involved in an updated six-hour training course (practicum) for students of the Physical Department of Moscow State University. The topic of the training is the determination of the shape and size distribution function of nanoparticles from small-angle scattering data. In total, 19 students were involved.

I. Torriani gave lectures on SAXS characterization of materials at a Materials Research Workshop for young researchers sponsored by the National Research Council and the Brazilian Crystallographic Association in Vitória, Espírito Santo, Brazil, 31 July – 2 August 2010.

I. Torriani gave a Plenary Lecture on Structural and Functional Aspects of Disordered Regions in Polymers and Biopolymers during the VI Meeting of the Argentinian Crystallographic Association, Buenos Aires, Argentina, 13–15 October 2010.

D. I. Svergun gave many educational lectures in 2010.

J. S. Pedersen was part of the Organizing Committee of the 10th European Summer School on Scattering Methods Applied to Soft Condensed Matter, Bombannes, Gironde, France, 12–19 June 2010. He also presented lectures on Instrumentation, Resolution Effects and on Model Fitting and Simulation Techniques at the School.

J. S. Pedersen also educates undergraduate and graduate students in the small-angle scattering techniques by his lectures at Aarhus University in the courses (1) Biophysical Chemistry 2, (2) Protein Biophysics and (3) Physical Chemistry of Soft Matter.



Course (1) also includes hands-on applications of SAS to protein samples.

J. S. Pedersen also gave additional educational lectures.

*Community-building activities.* R. Serimaa participated in the Max IV support meeting, 30 September 2010, in Lund, Sweden.

R. Serimaa has also been a board member of the Finnish Synchrotron Radiation Users Organization. (SAS is one of the main methods recognized to be important for the Finnish users community and this organization has tried to promote Finnish participation in Max IV.)

N. Yagi participated in the NSRRC SAXS interest group meeting at NSRRC (National Synchrotron Radiation Research Center), Hsinchu, Taiwan, 20–22 October 2010, and gave a talk on Application of Small-Angle Scattering on Dynamics of Biological and Material Samples at SPring-8.

A. Allen continues to serve on the SANS beam-time allocation committee at the NIST Center for Neutron Research.

I. Torriani gave a Plenary Lecture on Structural and Functional Aspects of Disordered Regions in Polymers and Biopolymers during the VI Meeting of the Argentinian Crystallographic Association in Buenos Aires, Argentina, 13–15 October 2010.

I. Torriani offered training and support to newly hired staff at the SAXS2 and SAXS1 beamlines of the Brazilian Synchrotron Facility (LNLS), prior to handing over the coordination of those facilities to a new LNLS group.

The group of V. V. Volkov has given several lectures of educational and community building character.

D. I. Svergun continued as a deputy Chair of Working Group V (Complementary Methods) of the European INSTRUCT initiative.

D. I. Svergun also gave several lectures for the benefit of expanding the SAS community.

G. Kostorz gives occasional invited talks on scattering methods in materials science and continues to serve as Co-editor for the *Journal of Applied Crystallography* and Editor-in-Chief of the IUCr journals. He has given advice on organizational and publication matters for the forthcoming SAS conferences.

J. S. Pedersen continued to support new users at his laboratory's SAXS facility at Aarhus University, Denmark, from the universities and research institutes in Denmark, Scandinavia and the rest of Europe. He also continued to train students and post-docs in the SAS technique in Aarhus.

*Consultant activities.* The Institute of Crystallography and V. V. Volkov continued to provide consultancy in 2010 for about 20 scientific and engineering institutes in Russia, in part from the Institute of Molecular Biology, Institute of Physical Chemistry, Institute of Elemento-organic Compounds, Institute of Inorganic Chemistry *etc.* In total, about 380 samples of polymers with inorganic nanoparticles, liquid crystals, magnetic fluids, complexes of DNA with transition metals and proteins in solution (proteins from the flu virus, chaperonin, alpha-crystalline, bacterial aldolase and many more) were investigated.

I. Torriani coordinated a proposal for implementation of a high-throughput protein characterization and crystallization platform at the National Laboratory for Biosciences, within the Brazilian Synchrotron Facility, which was approved by the São Paulo State Research Foundation in August 2010 and is now being implemented.

D. I. Svergun is a member of the Scientific Advisory Committee, Diamond, and is a reviewer for the beam-time proposals for GKSS (Geesthacht).

J. S. Pedersen is a reviewer for the beam-time proposals for GKSS (Geesthacht) and the Bragg Institute, ANSTO, Australia.

*Organizational activities.* R. Serimaa headed the organization committee of Seventh Nordic Workshop on Scattering from Soft Matter, Department of Physics, University of Helsinki, Finland 27–28 January 2010.

I. Torriani collaborated with the 20th LNLS User's Meeting (22–23 February 2010), organizing and coordinating the Structural Biology and Macromolecular Chemistry sessions.

The group of D. I. Svergun co-organized a BioSAXS course, Copenhagen, Denmark, in January 2010 (Commission Chair J. S. Pedersen was among the speakers).

D. I. Svergun organized an EMBO Practical Course on Solution Scattering from Biological Macromolecules in Hamburg, Germany, 25 October – 1 November 2010. There were over 140 applicants, of which 20 were selected as full participants and six for lectures, representing over 20 countries from Europe and overseas. Three participants from industry were accepted. A team of 15 lecturers and tutors, including several Commission members (N. Yagi, J. S. Pedersen, J. Trehwella), conducted the Course.

In 2010, the International Rusnanoprize in the field of nanodiagnostics was awarded to L. Feigin and D. I. Svergun for their scientific achievements in the field of SAXS and the Hecus firm (Graz, Austria) for fabricating SAXS equipment.

*Technical activities.* In the area of the development of requirements for the presenting of biological macromolecule small-angle scattering data in publications, a document has been prepared with initial input from the Trehwella and Svergun laboratories and provided to the Chair of the Commission for distribution to members for comment and suggested revisions. This (revised) document will provide a starting point for discussion at the Madrid Congress and SAS2012 with the intent of working toward a set of community-agreed standards that would be available to journal Editors in order to ensure SAS publications in this rapidly expanding area are of a standard and quality that will support the continued strong impact of the technique.

An international round robin exploring the potential of glassy carbon as a SAXS (and possibly SANS) intensity standard reference material was completed in 2009. On the basis of the results, plans moved forward in 2010 to develop an intensity reference material (see below). This is likely to be certified for SAXS but not, for the time being, for SANS.

Following the successful issue in 2008 of three nanoparticle Reference Materials: NIST RMs 8011, 8012 and 8013 (for, aqueous suspension – for use primarily in biological research applications), NIST is currently preparing an Ag nanoparticle Reference Material (both for biomedical and for environmental health and safety applications). SAXS/USAXS measurements will provide informational size values for Ag, and the potential for supplying certified size values is currently under discussion.

A research paper on glassy carbon as a potential SAXS intensity standard has been published [F. Zhang, J. Ilavsky, G. G. Long, J. Quintana, A. J. Allen & P. R. Jemian (2010). *Metall. Mater. Trans. A*, **41**, 1151–1158].

A prototype NIST standard reference material for SAXS intensity calibration, based on glassy carbon, is under development in 2010–2011. If successful, production and release of the standard is envisaged for 2012 or 2013.

In 2010, NIST efforts to pursue development of a standard reference material for small-angle X-ray wavelength calibration have turned from a conventional diffraction standard (*e.g.* silver behenate) to the proposed fabrication of a nano-engineered diffraction grating artifact, which should have a stable long-term, perhaps unlimited, shelf life. Work is ongoing.

In 2010 A. Allen contributed to a second draft of a possible ISO TC24/SC4 (particle size committee) SAXS particle size (best practice) standard. Activities remain ongoing.

I. Torriani worked on the design of experiments for researchers from the University of Buenos Aires, Argentina, involved in bio-remediation for environmental studies. Graduate students and post-doctoral visitors stayed for several weeks in Brazil funded by a Brazil–Argentina Programme from the Ministries of Education from both countries (March 2010).

In 2010, D. I. Svergun's group provided the community with a new release of *ATSAS*, a program package for SAS data analysis. Web access to several new programs was established.

**J. S. Pedersen**, Chair

#### 4.18. Commission on Structural Chemistry

The activities of the Commission (CSC) in 2010 were mainly focused on the preparation of a strong scientific programme for the Madrid Congress. Three members of the International Programme Committee are related to the interests of the CSC (R. Kuroda, L. R. Nassimbeni, T. N. Guru Row), and the CSC has collected and submitted a list of 18 possible titles for Microsymposia, together with potential names for Chairs and Keynote speakers. Out of these, 12 Microsymposia strictly related to the CSC have been selected for the final programme, covering all the areas of structural chemistry. The organization of joint Microsymposia with other Commissions has also been promoted.

The proposal for a Satellite Meeting for the Madrid Congress has also been submitted with the endorsement of the CSC, namely Categorizing Halogen Bonding and Other Noncovalent Interactions Involving Halogen Atoms, chaired by P. Metrangolo and G. Resnati.

Regarding other activities, the CSC has been asked to contribute a member to the IUCr Working Group of Database Users; A. Bacchi has joined the Working Group, which started its activity in October 2010. In this context, the CSC has also set up a stable connection with the Cambridge Crystallographic Data Centre by inviting one representative of the CCDC to join the list of consultants. E. Pidcock has accepted to serve as consultant for the CSC.

As a general comment, it seems that the exchange of consultants between related Commissions, initiated by the CSC together with the Commission of Inorganic and Mineral Structures (A. Beatty and P. Mercier) and extended also to the Commission on Crystallographic Teaching (P. Mueller), is really working very well, providing, especially for the former case, an effective sharing of information and opinions, particularly useful in the process of evaluating support for schools and meetings, and in setting up the scientific programme for International Crystallographic Conferences, first of all the Madrid Congress, where synergy between Commissions can strengthen the programme.

The addition to the consultants of a scientist working in industry is also being considered by the CSC, in order to improve the potentially significant links between pure and applied research that are traditionally strong in the field of structural chemistry.

In 2010 the web site of the CSC has been updated and harmonized to the new format published on the IUCr site.

Some points still need to be addressed by the CSC, mainly a stronger effort to link with the Commission on Crystallographic Nomenclature in order to improve the contents of the IUCr Online Dictionary service. Some tentative suggestions have been made in this context, but Commission members did not enter into a complete evaluation of the potential contributions to the dictionary from the CSC.

During 2010 a number of scientific events related to structural chemistry have been supported by the CSC:

2nd International School of Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials, Granada, Spain, 24–28 May 2010.

Gordon Conference in Crystal Engineering, Waterville Valley Resort, Waterville Valley, NH, USA, 6–11 June 2010.

2nd Canadian Chemical Crystallography Workshop, McMaster Analytical X-ray (MAX) Diffraction Facility, McMaster University, Hamilton, Ontario, Canada, 25–29 May 2010.

**A. Bacchi**, Chair

#### 4.19. Commission on Synchrotron Radiation

The aim of the Commission is to promote access and awareness of crystallographers worldwide to the world's synchrotron-radiation (SR) facilities. To this end, the Commission promotes, in a broader sense, the development of crystallographic instrumentation technology and standards, and 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 Commission is very pleased to note the tremendous progress made by several XFEL projects, including the European XFEL and FLASH in Hamburg, Germany, LCLS in Stanford, CA, USA, and SACLA in Harima, Japan, which successfully lased at 1.2 Å wavelength on 7 June 2011, as well as ERL projects at CHESS in Ithaca, NY, USA, and KEK in Tsukuba, Japan. These triggered many new projects for building FEL facilities in many countries. The initial scientific outputs from the LCLS have been enormous and transformative, and have already affected the courses of new developments in various fields, including crystallography, scattering, spectroscopy and imaging. Detector developments were also accelerated in preparation for these next-generation light sources as well as by new demands from the storage-ring-based light sources.

S. Pascarelli, a consultant of the Commission, has played an important role as a member of the International Programme Committee of the Madrid Congress to promote synchrotron-related topics and speakers. We have placed particular emphasis on featuring the recent spectacular progress in LINAC-based light sources, and are organizing Microsymposium 37: X-ray Lasers and Other New Frontiers in Synchrotron Applications to Structural Science, in which the most up-to-date science and technology developments will be presented. Other important areas include detectors and instrumentation, coherence, inelastic X-ray scattering, materials under extreme conditions, surface and interface, combined methods, structural biology, cultural heritage *etc.*

As reported last year, we continued the preparation of a workshop on quality control and standardization of XAFS experiments in collaboration with the Commission on XAFS, the International X-ray Absorption Society and the Japanese XAFS society. The purpose of this workshop, which we named Q2XAFS (Improving the Data Quality and Quantity for XAFS Experiments), is to establish international standards for XAFS experiments and data analysis with well defined quality control. This topic has been discussed for more than ten years but some difficulties have been experienced in finalizing the proposal and implementing it in practice. During the Q2XAFS workshop, we will learn from the experiences in small-molecule crystallography and protein crystallography in establishing similar international standards. Our intention is to establish a set of standard protocols for experiments, data analysis and verification. We will make special efforts in approaching editors of relevant international journals, including those of the IUCr, and ask them to implement such protocols and verification as part of the requirement for publi-

cation. To this end, we will be compiling a Special Issue of *Journal of Synchrotron Radiation* with manuscripts prepared by the key participants, including the final proposal and scientific highlights from the workshop. After exploring several possibilities for the workshop venue, we decided to hold the meeting at the Photon Factory and scheduled it for 11–12 April 2011. Unfortunately, owing to the devastating earthquake on 11 March 2011 and the subsequent Fukushima nuclear reactor crisis, the meeting has been postponed to December 2011. The Commission on XAFS is planning to have Microsymposium 77: XAFS Instrumentation: Automation, Standardization and Validation of XAFS Experiments at the Madrid Congress in Madrid, and we intend to take advantage of this Microsymposium to discuss the subject matter and prepare for the December meeting in Tsukuba.

The Commission continued the discussion from the previous year on the recognition of beamline scientists in various forms, which is a long-standing issue in this field: as the technique matures it becomes less and less frequent to acknowledge the scientists who have developed and operate the methods/instruments. We considered establishing a new section on beamlines in the *Journal of Synchrotron Radiation*. In consultation with the IUCr President S. Larsen, P. Zwart, Z. Dauter and S. Wakatsuki have proposed a format for such brief publications in *Journal of Synchrotron Radiation*, which has been implemented.

The Commission supported the requests for financial support for several conferences: the International School/Conference on Resonant Elastic X-ray Scattering in Condensed Matter, Aussois, Savoie, France, 13–17 June 2011, and the VIII holding of the School on Crystallography and X-ray Diffraction, Havana, Cuba, 21–26 November 2011. It also continued to support the RapiData course on automated data collection at NSLS, Brookhaven National Laboratory, 3–8 April 2011; in particular, the Commission recommended to the organizers that they support the participation of Latin-American students.

The fifth AOFSSR (Asia Oceania Forum for Synchrotron Radiation Research) workshop was held in Pohang, Korea, 5–9 July 2010. R. Garrett continues his role as treasurer of AOFSSR and together with other Commission members contributed to the activities of AOFSSR. The next AOFSSR workshop will be held in Bangkok, Thailand, 24–28 October 2011. Commission member Shih-Lin Chang joined the organization as an executive member from April 2011.

As reported last year, C. Nave played an active role in the preparation of the 6th Radiation Damage Conference, which was held in March 2010 in Stanford, CA, USA. The next biennial meeting is scheduled to be held at the Diamond Light Source, UK, 14–16 March 2012, to continue discussions on fundamental processes of radiation damage in biological samples, implication for structure interpretation and exploitation of radiation damage in structural determination as well as evaluation of radiation damage in XFEL ‘diffract and destroy’ experiments. Another Special Issue in *Journal of Synchrotron Radiation* will be prepared from talks at the 2012 workshop.

The Commission will promote and be actively involved in various activities during the 100th year of X-ray crystallography and International Year of Crystallography 2013. The next International Conference on Structural Genomics (ICSG) will be held in Tsukuba, Japan, in 2013 (dates to be decided) and organized by S. Wakatsuki as Chair of the Organizing Committee. Although the scope of the meeting is very wide, protein crystallography is certainly one of the most important aspects of structural genomics and proteomics projects. We intend to include special sessions on the 100th year of

X-ray crystallography in ICSG 2013. The 4th Workshop on XFEL Science will be held in Cairns, Australia, 29 August – 2 September 2011. This is primarily an Asia–Oceania workshop and focuses on the proposed scientific programmes of the new XFEL facilities, in particular the SACLA facility currently being commissioned at SPring-8. R. Garrett is a member of the Organizing Committee. We will also encourage synchrotron facilities to highlight the achievements of crystallography and the contribution of synchrotron radiation to this field.

**S. Wakatsuki**, Chair

#### 4.20. Commission on XAFS

*Commission meetings and communication.* Discussions among the steering committee members occurred during the Biology and Synchrotron Radiation (BSR) Conference in Melbourne in February 2010. Moreover, the Chair communicated with Commission members by e-mail and during personal meetings at other conferences or in correspondence or visits to laboratories. For example, in order to progress with the document on XAFS nomenclature, the Chair met C. T. Chantler at Melbourne University (Australia) and at Chimie-ParisTech (Paris, France), and P. Glatzel at ESRF (Grenoble, France).

*Contribution to IUCr Online Dictionary.* The Working Group on XAFS Nomenclature (WG), created in 2009, has drawn up several versions of a document with definitions of XAFS-related terms in order to contribute to the *IUCr Online Dictionary*.

In 2010, an Advisory Committee (AC) was created to review definitions. Members are C. Brouder, D. Creagh, J. Garcia, C. Natoli, J. Penner-Hahn, R. Sarangi and E. I. Solomon. AC members have sent detailed reports, indicating comments, corrections and, in some cases, proposing alternative definitions to the XAFS Commission Chair, who transmitted anonymous reports to P. Glatzel.

The WG has prepared a revised document taking into account nearly all suggestions. P. Glatzel, the WG Coordinator, has also consulted F. Neese, F. de Groot, A. Kotani and S. Huotari concerning some definitions, and their valuable contributions have been included in the final document.

The revised document has been submitted to each member of the AC by the Commission Chair.

*Volume of International Tables for Crystallography dedicated to XAFS.* This project would be a great opportunity for the XAFS community and several exchanges/contacts have been dedicated to this item.

During the meeting of the International Programme Committee for the Madrid Congress, discussions started between C. J. Gilmore and I. Ascone concerning the opportunity to include XAFS-related items in the new volume of *International Tables for Crystallography* planned to cover mainly powder-diffraction techniques.

Following the IUCr decision to consider the dedication of a specific volume to the XAFS technique, a detailed document with suggestions for the content of the volume was submitted to the IUCr Editorial Office at the beginning of December 2010.

*Development of XAFS standards and criteria.* The Commission (CXAFS) has promoted the development and acceptance of standards and criteria in XAFS measurements and analysis.

The preparation of the Workshop on Improving the Data Quality and Quantity for XAFS Experiments, in cooperation with the Commission on Synchrotron Radiation, continued in 2010. Several meetings and exchanges took place with the ESRF, which had agreed to host this event. Unfortunately, CXAFS met difficulties in completing the budget and S. Wakatsuki proposed the Photon Factory as the hosting laboratory, involving in the organization

eminent Japanese colleagues from KEK and the Japanese XAFS Society. CXAFS also collaborated with H. Oyanagi, IXAS Chair, on the organization of this event. The workshop will be held in December 2011.

*Congresses, workshops, symposia, Summer School in 2010.* CXAFS members contributed to the increase of interactions among XAFS researchers and other groups in the IUCr through the organization of congresses, meetings, symposia and workshops. The Commission endorsed/supported the following meetings:

(1) BioXAS study weekend, a satellite meeting of the Biology and Synchrotron Radiation Conference, Melbourne, 14–15 February 2010. This has been the fourth meeting of a series dedicated to the biological applications of XAFS. As for previous meetings, CXAFS supported its organization and three CXAFS members (I. Ascone, S. S. Hasnain and B. Hedman) participated in the steering committee.

(2) 7th International Conference on Inelastic X-ray Scattering (IXS 2010), World Trade Center, Grenoble, France, 11–14 October 2010. This conference, co-organized by P. Glatzel, covered electronic resonant and non-resonant scattering (in the soft and hard X-ray regime), emission spectroscopy, meV-resolved atomic dynamics, nuclear inelastic scattering, Compton scattering, and thermal diffuse scattering (<http://www.esrf.eu/events/conferences/ixs2010/>).

(3) Symposium on Synchrotron Radiation: Emerging Techniques and Applications, co-organized by K. Asakura during Pacificchem 2010 (Pan Pacific Chemical Society Meeting), Hawaii, USA, 15–20 December 2010.

(4) A Summer School on Structural Molecular Biology Low-Z XAS has been promoted by B. Hedman at SSRL/SLAC Stanford, USA, 20–23 July 2010. The goal of this Summer School was to disseminate information about the scientific opportunities in low-energy XAS applications and train participants on the theoretical aspects and practical data analysis of different experimental techniques (<http://www-conf.slac.stanford.edu/smbxas-ss/2010/>).

*Organization of events in 2011: Madrid Congress.* (1) The Commission was represented on the International Programme Committee by I. Ascone. The Commission promoted five Microsymposia for the Madrid Congress, four of these in association with other Commissions. One Keynote Lecture will be presented by S. S. Hasnain on XAFS Contribution to Protein Structure–Function Investigations, and B. Hedman will chair this session. (2) CXAFS has supported the XAFS Tutorial for Crystallographers and Beginners (Workshop 1 of the Congress) organized by I. Ascone and J. García Ruiz, in cooperation with the Local Organizing Committee and International X-ray Absorption Society. As for the Tutorial organized on the occasion of Osaka Congress by K. Asakura, the purpose is to give a general introduction and analytical methods for crystallographers and beginners in the field of XAFS. In order to increase the interactions with crystallographers, this time the Tutorial is to be held on 22 August in the same building as the Congress.

**I. Ascone**, Chair, and **C. T. Chantler**, Secretary

## 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 2010 the Executive Committee approved sponsorship of various schools and meetings, mostly with financial support. Those held in 2010 are listed at the beginning of this

Report of the Executive Committee. Those scheduled for 2011, but approved in 2010, are listed below.

XIII Intensive School on X-ray Structure Analysis, Durham, UK, 26 March – 3 April 2011.

RapiData 2011, Brookhaven, USA, 3–8 April 2011.

Improving the Data Quality and Quantity for XAFS Experiments, Tsukuba, Japan, 12–13 April 2011 [postponed].

School on Fundamental Crystallography, Mahdia, Tunisia, 25–29 April 2011 [postponed].

X-ray Techniques for Materials Research – from Laboratory Sources to Free Electron Lasers Symposium at the European Materials Research Society Spring Meeting, Nice, France, 9–13 May 2011.

Workshop on Crystallographic Software, Tokyo, Japan, 22–26 May 2011 [postponed].

Third International School on Biological Crystallization, Granada, Spain, 22–27 May 2011.

SMARTER 2 Structure Elucidation by Combining Magnetic Resonance, Computation Modelling and Diffraction, Aveiro, Portugal, 23–27 May 2011.

ACA Annual Meeting, New Orleans, USA, 28 May – 2 June 2011.

Electron Crystallography – New Methods to Explore Structure and Properties of the Nanoworld, Erice, Italy, 2–12 June 2011.

The Power of Powder Diffraction, Erice, Italy, 2–12 June 2011.

International School on Resonant Elastic X-ray Scattering in Condensed Matter (REXS 2011), Aussois, France, 13–17 June 2011.

Zürich School of Crystallography – Bring Your Own Crystals, Zürich, Switzerland, 13–26 June 2011.

XVII International Conference on Crystal Chemistry, X-ray Diffraction and Spectroscopy of Minerals, St Petersburg, Russia, 20–24 June 2011.

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. The present Chair is Professor J. M. Perez-Mato. For up-to-date contact information, application procedures and rules, see <http://www.iucr.org/iucr/sponsorship/meetings.html>.

Applications for sponsorship of satellite meetings require the approval of the Chair of the Organizing Committee of the main meeting. Meetings (other than satellite meetings) scheduled to be held within two months 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 two and three 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. Meetings (other than satellite meetings) scheduled to be held, in the respective region, within 15 days before or after a meeting of a Regional Associate (American Crystallographic Association, Asian Crystallographic Association, European Crystallographic Association) will not be considered for sponsorship. For any meetings scheduled to be held between 15 days and one month before or after a meeting of a Regional Associate, the application for sponsorship requires the approval of the Chair of the Regional Associate Programme Committee.

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

## 6. Sub-committee on Electronic Publishing, Dissemination and Storage of Information (CEP)

The Executive Committee closed this advisory committee at its meeting in Toronto in 2009.

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

COMCIFS is tasked with maintaining and developing the Crystallographic Information Framework, which includes syntax and dictionary language standards and dictionaries written according to those standards. Last year's report described work on a new syntax standard, dubbed 'CIF2', as being almost complete. Unfortunately, a few remaining issues took the bulk of 2010 to resolve. As the year drew to a close, COMCIFS had just voted to accept the new standard, although the standard currently remains in draft form in order to address an issue raised by a dissenting voter.

The significant effort put in to the syntax discussion by COMCIFS members has not hindered developments in the area of CIF dictionaries. After several years of development, the CIF Restraints and Constraints dictionary has been approved. The new 'fast-track' process for adding single items to current dictionaries has produced several updates to the core dictionary. A working group was formed in 2010 to develop a twinning dictionary. Other ongoing dictionary development projects include an updated symmetry dictionary and modulated structures dictionary.

Adoption of imgCIF as a preferred format for raw image data took another step forward in 2010 with the announcement that the Dectris Pilatus-6m detector used on many macromolecular beamlines was now capable of producing fully imgCIF compliant data files. A number of other detector image formats are easily transformed into imgCIF/CBF using tools provided by the CBFlib project, which provides software tools for working with imgCIF and imgCBF. This project has seen an order of magnitude increase in downloads over the last two years, a strong indicator of increased uptake of imgCIF and imgCBF.

**J. Hester**, Chair

## 8. Committee on Crystallographic Databases

The Executive Committee closed this advisory committee at its meeting in Toronto in 2009. It has been replaced by a Working Group of Database Users.

## 9. IUCr Newsletter

2010 was the first year that production of the *IUCr Newsletter* was carried out remotely in Alaska and all issues were completed and at the printer before the end of the year. All issues were 24 pages in length. As in previous years, the content covered topics such as activities of the IUCr, its Regional Associates and Commissions, Letters to the Editor, news concerning crystallographers and crystallography in general, awards, election results, resources, meeting reports, book reviews, future meeting announcements, and a general meeting calendar. Sadly, each issue of 2010 carried multiple obituaries as the crystallographic community lost a number of long-time practitioners.

Each issue carried a President's column written by S. Larsen. Editorial responsibilities were shared by W. L. Duax and J. Flippen-Anderson. P. Potter was responsible for layout and all phases of production and distribution.

Each issue devoted at least two pages to brief summaries of selected articles recently published in IUCr journals. Issue 1 highlighted the 2009 annual meetings of two of the three Regional Associates (ACA and ECA). Issue 2 completed the report on Crystallography in Canada. The articles on the history of Crystallography in Spain were split across Issues 3 and 4. Issue 2 contained a preview article for the Madrid Congress and the call for papers was included in Issue 4.

Additional meeting and workshop reports were published covering activities in Italy, Poland, the USA, France, the Czech Republic, Croatia, Japan, Belgium and Hungary.

The mailing list remained about the same in 2010 with an average distribution of 18 250. Twenty countries assist in the effective and economic distribution of the *Newsletter*. (Distributors: H. Fodil: Algeria; P. Jensen: Australia; J. Valderrama: Colombia; B. Kojic-Prodic: Croatia; J. Hasek: Czech Republic; A. Nangia and Executive Secretary: India; Ismunandar: Indonesia; P. Spadon: Italy; CrSJ: Japan; A. Hamid Othman: Malaysia; J. Lipkowski: Poland; M. Costa: Portugal; W. Klooster: Singapore; L. R. Nassimbeni: South Africa; J. Schefer: Switzerland; Yu Wang: Taiwan; K. Haller: Thailand; H. Kooijman: The Netherlands; G. Diaz De Delgado: Venezuela.) Individual distribution was sent to 84 additional countries.

**W. L. Duax** and **J. L. Flippen-Anderson**, Editors

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

In 2010, the cooperation between Oxford University Press (OUP) and the IUCr/OUP Book Series Selection Committee was quite productive.

Two new volumes have been published in the Monographs on Crystallography series:

No. 25: *Neutron Protein Crystallography – Hydrogen, Protons, and Hydration in Bio-macromolecules*, by N. Niimura and A. Podjarny (publication date 17 February 2011).

No. 16: *Diffuse X-ray Scattering and Models of Disorder*, by T. R. Welberry (publication date 14 January 2010).

Two new volumes have been published in the Texts on Crystallography series:

No. 15: *Fundamentals of Crystallography*, third edition, by C. Giacovazzo, H. L. Monaco, G. Artioli, D. Viterbo, M. Milanesio, G. Ferraris, G. Gilli, P. Gilli, G. Zanotti and M. Catti (publication date 10 February 2011).

No. 14: *Crystal Structure Analysis – A Primer*, third edition, by J. P. Glusker and K. N. Trueblood (publication date 27 May 2010).

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 Committee

## 11. Regional Associates and Scientific Associates

### 11.1. American Crystallographic Association (ACA)

During 2010, J. Kelly served as ACA President, T. Koetzle as ACA Vice-President, R. Von Dreele as Past-President, B. Santarsiero as Treasurer, and C. Wilmot as Secretary. J. Britten was the Canadian representative and M. L. Hackert served as IUCr representative on the ACA Council. The ACA Council met three times in 2010, a spring meeting near O'Hare Airport in Chicago on 10 April, a summer meeting at the Sheraton in Chicago on 23 July, and a fall meeting on 9 October in Boston where the ACA will hold its 2012 conference. The paid membership of the ACA was about 1850 by fall of 2010.

The highlight of the year was the ACA Annual Meeting held in Chicago, 24–29 July 2010. The Programme Chair for this meeting was R. Angel and the Local Chair was B. Santarsiero. The meeting was a success with over 620 abstracts and 963 attendees. The meeting featured five workshops: Global Phasing Software Suite for Macromolecular Crystallography (G. Bricogne); *PLATON* (L. Daniels); Sulfur-SAD Data Collection and Phasing (B. C. Wang, J. Rose and others); Getting the Most out of the *CCP4* Suite With Particular Emphasis on Low Resolution Refinement and Model Building (C. Ballard); and an unusual outreach/professional development workshop organized by C. Lind entitled Crystallography: World of Wonders for high-school teachers in the Chicago area.

The meeting also featured a number of excellent Plenary Lectures and Transaction Symposia. The operation of the ribosome was presented from three different perspectives by those who shared the 2009 Nobel Prize in Chemistry – T. Steitz, V. Ramakrishnan and A. Yonath. J. A. Ibers gave a Plenary Lecture in the Transactions Symposium entitled The First Element, organized in memory of R. Bau, and a special symposium New Tools – New Lights was organized in memory of L. T. J. Delbaere. Symposia were also organized in honour of A. L. Spek (Trueblood Award) for his outstanding contributions to chemical crystallography and crystallographic computing, and R. Triebel (Etter Early Career Award) for his achievements in elucidating the substrate specificity and catalytic mechanism of histone methyltransferases. D. J. Watkin was selected as the Fankuken Awardee for his stewardship of the crystallographic software package *CRYSTALS*. His lecture was postponed and will be presented in New Orleans in 2011. Several poster prizes were awarded to the best poster presentations in various areas of crystallography, including an IUCr poster award.

In New Orleans in 2011, the triennial Patterson Award will be presented to K. Moffat (University of Chicago) and the annual Etter Early Career Award to Y. Mozharivskij (McMaster University).

The ACA Council heard a report from the IUCr President, S. Larsen, reminding us of plans for the Madrid Congress and General Assembly, where again all three 2009 Nobel Laureates in Chemistry will be featured. She also described efforts by the IUCr to lead an effort to make 2013, the 100th anniversary of the famous Bragg experiment, officially designated by UNESCO and the United Nations as the International Year of Crystallography (IYCr).

ACA Business Meeting Items: The ACA received ~100 applications for travel awards. A total of about USD 35 400 was awarded in travel awards, including a number of international student travel awards funded by a grant from the IUCr.

A new award (Robert Bau Award in Neutron Diffraction) was created by Margaret Churchill, Robert Bau's widow. The ACA Council also announced plans for the new ACA Fellows Programme with plans to announce the first group of ACA Fellows in New Orleans in 2011.

The only 2010 Summer School was the Small Molecule Crystallography Summer School run by C. Lake. There was no Macromolecular Crystallography Summer School in 2010. However, a Second Chemical Crystallography Workshop (CCW) was held at McMaster University, 25–29 May 2010, as a satellite to the Chemical Society of Canada meeting in Toronto. Also, the 8th Canadian Powder Diffraction Workshop took place at Pavillon Ringuet, Université du Québec à Trois-Rivières, Québec, Canada, 21–23 June 2010.

On a sad note, we lost a number of outstanding members of our ACA family in 2010, including L. M. D. Cranswick, a member of the Canadian National Committee for Crystallography, Chair of the IUCr's Commission on Crystallographic Computing, and a member of the 2014 Montreal IUCr Congress planning committee. In honour of Lachlan, The Mineralogical Society has named a new Argentinian mineral Cranswickite.

Upcoming ACA Annual Meetings include 2011 in New Orleans with Programme Chair C. Cahill and Local Chairs E. and C. Stevens. The 2012 ACA meeting will be in Boston, and Hawaii is being considered for 2013. The ACA Council decided to move to a four-day Annual Meeting in 2013, and to investigate the possibility of also doing this in 2012.

The fall 2010 elections resulted in G. Phillips being elected as the 2011 ACA Vice-President, D. Rose as the new Canadian Representative, S. Ginell (Communications Committee), J. Krause (Continuing Education Committee) and J. Reibenspies (Data, Standards and Computing Committee), plus new Chairs elected to head the 12 SIGs.

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

### 11.2. Asian Crystallographic Association (AsCA)

The 10th Conference of AsCA (AsCA 2010) was held at BEXCO, Busan, Korea, 31 October – 3 November 2010. There were 415 presentations (83 oral and 332 posters). The distribution of presentations was: 155 biological, 156 non-biological, 90 technology, and 7 others. Attendance was the highest yet for an AsCA meeting, with 626 registrations, of which 229 were Korean and 235 were students. Exhibitors took 31 booths. Nine of 58 applications for travel support were honoured. Eight of 38 rising-star applications were awarded, and five poster prizes were awarded (two IUCr, two AsCA, one RCSB PDB). J. Martin served as the Chair of the International Programme Committee and Se Won Suh was the Chair of the Local Organizing Committee. The AsCA Council Meeting was held in Busan, Korea, 2 November 2010. New Executive Officers for the 2010–2013 term were elected as follows: President, Se Won Suh (Korea); Vice-President, P. Chakrabarti (India); Secretary-Treasurer, A. Vrielink (Australia).

*Current activities.* The current activities of AsCA include planning for the meetings in Adelaide, Australia, in December 2012, jointly with the Society for Crystallographers in Australia and New Zealand (SCANZ) and in November/December 2013 at a location to be decided. R. Withers is the Chair of the International Programme Committee and J. Carver is the Chair of the Local Organizing Committee for the 2012 Adelaide meeting. AsCA plans to use some of its accumulated reserves to fund access to these meetings by young scientists in the region. The IUCr is also expected to provide support.

*Future Scientific Meetings of AsCA.* In the past the major (triennial) AsCA meetings have been held in a country without a large domestic crystallographic community with a view to fostering the development of crystallography throughout in the Asian region. The

full AsCA calendar therefore runs as follows: IUCr Congress – Joint AsCA/local meeting – Full AsCA meeting.

AsCA 2012: The AsCA council in 2009 approved the proposal to host a joint AsCA meeting in Adelaide, Australia, in 2012. W. L. Bragg was born in Adelaide and received his first degree from the University of Adelaide. The joint AsCA/SCANZ conference and Bragg centenary celebration will be held in the Adelaide Convention Centre, Adelaide, Australia, 2–6 December 2012. November 2012 will mark the centenary of the presentation of Lawrence Bragg's paper to the Cambridge Philosophical Society defining Bragg's equation. The Bragg symposium will be a public forum with speakers including descendants of Lawrence Bragg, his former students and high-profile scientists.

The Scientific Advisory Committee of AsCA 2012 is as follows: G. R. Desiraju, Indian Institute of Science, Bangalore, India; Zhi-Jie Liu, AsCA 2009 Organizer, People's Republic of China; Se Won Suh, Seoul National University, Korea; M. Takata, SPring-8, Japan; S. Wakatsuki, Photon Factory, Japan; B. J. Kennedy, University of Sydney, Australia; A. Vrielink, University of Western Australia, Australia; B. Kobe, University of Queensland, Australia; D. Goossens, Australian National University, Australia; R. Withers, Australian National University, Australia; S. Batten, Monash University, Australia; E. N. Baker, University of Auckland, New Zealand; S. Wilkins, CSIRO, Australia; J. Varghese, CSIRO, Australia.

AsCA 2013: Crystallographers in both Bangladesh and Vietnam are eager to host the 12th Conference of AsCA (AsCA 2013) in November/December 2013. The venue for AsCA 2013 will be finalized by the AsCA Council Meeting to be held in Madrid in August 2011.

*Financial Report.* The trustees of AsCA are M. A. Spackman, A. Vrielink and C. Bond at the University of Western Australia. All the funds are currently held as cash deposits in Australian dollars. The total funds as of 25 May 2011 are AUD 164 021.27.

**G. R. Desiraju**, IUCr Representative

### 11.3. European Crystallographic Association (ECA)

The present membership of the ECA Executive Committee is: S. Garcia-Granda, President; J. R. Helliwell, Past President; A. Roodt, Vice-President; P. Bombicz, Secretary; R. Kuzel, Treasurer; A. Bacchi, Officer; L. Van Meervelt, Officer; W. Depmeier, Officer; and M. Nespolo, Education Coordinator. P. Scardi attends executive meetings as EPDIC Chair.

*Meetings.* The 2010 ECA meeting was held in Darmstadt, Germany, 29 August – 2 September, and was a great success with 1047 delegates attending. It was timed to run back-to-back with the 2010 EPDIC meeting.

Future ECA meetings will be held as follows: 2012 Bergen, Norway, 6–11 August; 2013 Warwick, UK, 25–29 August.

Bids for 2015 will be reviewed at the Madrid Congress.

*Overview of supported meetings in 2011.* The ECA will support the following meetings in 2011:

EMU School 2011: Layered Mineral Structures and their Application in Advanced Technologies, Rome, Italy (EUR 750);

School on Fundamental Crystallography, Mahdia, Tunisia (EUR 750);

Electron Crystallography: New Methods to Explore Structure and Properties of the Nanoworld, Erice, Italy (EUR 1250);

Heart of Europe Biocrystallography Meeting HEC, Zagan, Poland (EUR 1000);

The Power of Powder Diffraction, Erice, Italy (EUR 1250);

The Zürich School of Crystallography, Zürich, Switzerland (EUR 1000);

5th European Conference on Neutron Scattering, Prague, Czech Republic (EUR 1000).

The ECA provided EUR 3000 to ECM-26 to waive the registration fees of senior researchers from less developed countries. A limit of two from any country was imposed.

*Prizes.* In 2011 the Max Perutz Prize will be awarded to C. Lecomte, Nancy Université and CNRS, France, and the Felix Bertaut Prize will be awarded to T. Fennel, Institut Laue-Langevin, Grenoble, France.

*Membership issues.* The Adhering Body Chemists and Technologists of Macedonia has been a new National Member of the ECA since 2010; contact has been re-established with Russia and Serbia. The Union of the Regional Committee of Crystallographers from Algeria, Latvia, Morocco, Tunisia, Turkey and Ukraine was established in 2008. The Adhering Bodies of these countries are ECA National Members. The ECA pays one group IUCr membership fee for these countries for a period of two terms.

A new system of networking groups is being introduced. These are named General Interest Groups (GIGs) and follow the same rules as the SIGs. They will start to operate after a change in ECA Statutes in Madrid 2011. The GIG Young Crystallographers is already established and has operated enthusiastically *ad interim* since 2010. The GIGs for Senior Crystallographers and for Teaching may be established in the future.

The ECA has Corporate Affiliation Members; these are now represented on ECA Council.

An application for the new Erasmus Mundus call in 2011 was submitted in order to establish a European Educational Programme in Crystallography.

The ECA is keen to participate in the International Year of Crystallography and would welcome discussions with the IUCr.

**C. J. Gilmore**, IUCr Representative

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

2010 for the crystal growth community was the year of two of the most important triennial meetings. These were the 16th International Conference on Crystal Growth (ICCG-16) and the 14th International School on Crystal Growth (ISSCG-14), both very professionally organized in the People's Republic of China.

The Sixteenth International Conference on Crystal Growth (ICCG-16), together with the Fourteenth International Conference on Vapor Growth and Epitaxy (ICVGE-14) (<http://iccg16.tipc.cn/>) were held in Beijing, People's Republic of China, 8–13 August 2010. Commission on Crystal Growth and Characterization of Materials (CCGCM) members and consultants (S. Baldochi, K. Byrappa, H. A. Dabkowska, T. Duffar, K. Kakimoto and K. Tsukamoto) were strongly involved in the work of the Programme and Advisory Committees of both meetings. Commission member J. Y. Wang served as an excellent General Secretary for this venue. The purpose of the meeting was to provide a forum for presentations and discussions of recent developments and achievements in all aspects of crystal growth through the various sessions integrating fundamental, experimental and industrial growth processes, characterization, and applications. Such discussions help to stimulate the review of foundational theory and current practices and to exchange new ideas during many informal social activities.

Award lectures were presented by M. E. Glicksman (recipient of Frank Prize, Fundamental Issues Associated with Dendritic Growth Kinetics), J. J. DeYoreo (Laudise Prize, Technology and Scientific

Basis of Rapid Growth of Perfect Crystals from Solutions) and V. Maltsev (Schieber prize, Single Crystal Growth of Novel Rare-Earth-Doped Orthoborates for a New Generation of Bulk and Waveguide Near-Infrared Lasers).

The Conference received 1464 abstracts. It was a truly international event, with abstracts from around the world: 630 from the People's Republic of China, 242 from Japan, 126 from India, 114 from Russia, 79 from the USA, 55 from Germany, 31 from France, 26 from the Ukraine, 19 from the UK, 14 each from South Korea and Spain, the rest from Algeria, Armenia, Australia, Austria, Canada, Czech Republic, Denmark, Italy, Iran, Mexico, The Netherlands, Poland, Romania, Thailand, Belgium, Norway, Israel, Turkey, Hungary, Sweden, Bangladesh, The United Arab Emirates, Ireland, Brazil, Slovenia, The Philippines, Singapore, Sweden and Switzerland. The registered number of attendants was 1100, among them 521 from People's Republic of China and 579 from the rest of the world. In terms of numbers of both abstracts and attendants, this conference held records for any ICCG conference so far.

The new Executive Committee of the IOCG was elected and it was confirmed during the General Assembly of the IOCG in Beijing. The new President is R. Fornari (Germany), Co-Vice-Presidents are T. F. Kuech (USA) and E. Vlieg (The Netherlands), the Secretary is K. Kakimoto (Japan), and the Treasurer is V. Fratello (USA). The members of the EC are: H. A. Dabkowska (Canada), J. Derby (USA), T. Duffar (France), J. M. Garcia-Ruiz (Spain), Y. Mori (Japan), K. Roberts (UK), P. Rudolph (Germany), A. Voloshin (Russia), Past President: A. A. Chernov (USA) and Honorary Principal Founder: M. Schieber (Israel). The *ex officio* members of the Executive Committee are the Chair of ICCG-17: S. Krukowski (Poland), and the Co-Chairs of ICCG-16: M. Jiang (People's Republic of China) and C. Chen (People's Republic of China).

According to the new IOCG President, R. Fornari, the Agenda for the Triennium 2010–2013 is as follows: coordination and promotion of meetings on crystal growth (including the bilateral or trilateral meetings between neighbouring nations), increasing the number of national organizations, promotion of the crystal growth schools 'located where the prospective students are', and promotion and support of more basic initiatives such as Master courses (an example is a Master Programme, initiated by J. M. Garcia-Ruiz, that takes place annually in Spain) as well as re-starting the European Conference on Crystal Growth. Lobbying the various governments in favour of crystal growth discipline will also be seriously considered. The 14th International School on Crystal Growth (ISSCG-14, Chair Mu Wang) was held in Dalian, People's Republic of China, 1–7 August 2010 (<http://www.isscg14.org.cn/>). Commission members K. Kakimoto, K. Tsukamoto and E. Vlieg lectured at the School. Altogether there were 20 lectures, supported by a very highly prized, innovative, experimental hands-on experimental part. The level of the School was intended for young researchers interested in gaining a fundamental knowledge of crystal growth and epitaxy. The proceedings may be found at <http://scitation.aip.org/proceedings/confproceed/1270.jsp>.

The Conference and School were both supported by the IUCr, enabling 18 young scientists to attend. Altogether both meetings were hailed as very innovative and successful, owing to the hard work and great organization skills of our Chinese colleagues. Detailed information about the IOCG, ICCG-16 and ICCG-15 meetings and other related information are posted at the IOCG web site (<http://iocg.org/>).

The next international meetings ICCG-17 and ISSCG-16 (Chair W. Sadowski) will be held in Poland, respectively in Warsaw and Gdansk, in 2013, and the 2016 meetings will take place in Japan.

In October 2010 the Executive Committee of the IOCG organized a meeting of European Chairs, Secretaries and Representatives of national groups and institutions involved in crystal growth. This venue was devoted to consolidation of crystal growth activities in Europe and it was held in the Institute for Crystal Growth in Berlin. The National Associations for Crystal Growth are active in promoting crystal growth science in their own countries as well as in collaborating in the organization of international events related to crystal growth. Unfortunately it was noticed in the community that the loss of expertise and reduction of activities in the general area of crystal growth ultimately slows down the development of innovative products for energy production and storage, telecommunications, health, homeland security, traffic and mobility, sensors and safety, detectors as well as electronics and optics. This negative aspect is further accompanied by an impoverishment of research in the area of solid-state physics, nuclear physics, biology and biophysics. The purpose of the two-day venue in Berlin was to strengthen the European crystal growing network, increase the impact of projects devoted to crystal growth in the European Union and possibly create the European Association for Crystal Growth. H. A. Dabkowska attended this meeting, invited as the IUCr representative to the IOCG. After this meeting the Irish National Association of Crystal Growth was created and enthusiastically accepted as a new Member of the IOCG in November 2010.

Other meetings important for the crystal growth community held in 2010 were:

Adsorption, Absorption and Crystal Growth, Gargnano, Italy, 18–23 April 2010;

IX International Conference of The Polish Society for Crystal Growth, ICPSCG-9, Gdansk, May 2010;

Second International School of Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials, Granada, Spain, 24–28 May 2010;

Gordon Research Conference in Crystal Engineering, Waterville Valley Resort, New Hampshire, USA, 6–11 June 2010;

BIMR Summer School on Crystal Growth, Hamilton, Canada, 23–25 June 2010;

2010 Annual Conference of the British Association for Crystal Growth (BACG 2010), Manchester, UK, 5–7 September 2010;

MSANDT 2010 in Solidification and Crystal Growth Technology for Industrial Applications: Developments in the Past Century, Houston, USA, 17–21 October 2010.

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

## 11.5. 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.i-x-s.org/>).

**P. Whitfield**, IUCr Representative

## 12. Representatives on Other Bodies

### 12.1. 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.



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

- Definitions of Terms Relating to Crystalline Polymers;
- Definition of The Hydrogen Bond.

**A. Authier**, IUCr Representative

## 12.2. 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.

The IUCr took the lead in a new ICSTI Technical Activities Coordinating Committee (TACC) project on Interactive Journal Articles, intended to survey existing examples in fields such as optical sciences, crystallography, chemistry, structural biology and chemistry, mathematics, astronomy and statistics. A workshop organized by B. McMahon was held at the 2010 ICSTI Winter Meeting in Paris, France, at a venue graciously provided by Y. Epelboin, former member of the IUCr Committee on Electronic Publishing, Dissemination and Storage of Information. A number of open-access publications arising from the Workshop appeared in a Special Issue of the journal *Information Services and Use*, including The Record of Experimental Science: Archiving Data with Literature [Helliwell, J. R. & McMahon, B. (2010). *Information Services and Use*, **30**, 31–37] and Interactive Publications and the Record of Science, a full account of the Workshop [McMahon, B. (2010). *Information Services and Use*, **30**, 1–16]. Video recordings of the Workshop are available at [http://www.congres.upmc.fr/ICSTI\\_2010/index.html](http://www.congres.upmc.fr/ICSTI_2010/index.html).

The summer ICSTI Congress for 2010 was held in Helsinki, Finland, and was organized by the Society of Finnish Information Specialists and was entitled From Information to Innovation. The finale of the Conference was the launch of the World Wide Science Alliance project, which includes extensive use of the Microsoft language translation tools. The proceedings may be found at <http://www.vtt.fi/inf/pdf/symposiums/2010/S267.pdf>.

The Helsinki Conference was accompanied by a very interesting commercial exhibition of mainly Finnish companies but also from other countries as well as multinationals. The Conference was preceded by the ICSTI business meetings. An interesting project report presented at the TACC was the South Korean technical development project for accessing scientific journal literature from the iPhone.

Preparations were made to attend the winter ICSTI Conference in February 2011 to be held in Redmond, Washington, USA, at the Headquarters of the Microsoft Corporation on the topic Multimedia and Visualization Innovations for Science. The science areas are to be covered in 12 talks to include crystallography and structural science in a talk by R. Hanson (see <http://prezi.com/khaylnfjmbbs/jmol-icsti/>).

J. R. Helliwell acknowledges with gratitude the close collaboration with the IUCr Managing Editor, Peter Strickland, and with IUCr's Representative to CODATA, B. McMahon.

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

## 12.3. International Council for Science (ICSU)

An ICSU meeting for Union Representatives was held in Paris, France, 7–8 April 2010. Representatives of 27 of the 30 member Unions attended the meeting. From the Executive Board, the

President, Past President, President-Elect, two Vice-Presidents, Treasurer, Secretary-General and seven out of eight board members attended.

On the first day, implementation of the ICSU Strategic Plan 2006–2011 was discussed. After the discussion several reports on International Years and trans-Union activities were delivered. The representative of IUPAC reported the preparation of IYC2011. Since he asked IUCr to support IYC2011, I answered that the IUCr would support IYC2011 but IUCr also expects IUPAC support for IYCr2013. Then the item on Development of the ICSU Strategic Plan 2012–2017 was discussed. In the evening, the French Academy of Sciences invited us to an evening reception. On the second day, three important items, ICSU finances, weighted voting and the grants programme, were discussed. Then the activities of the ICSU Regional Offices (Africa, Asia and Pacific, Latin America and Caribbean) were reported. In the afternoon, the item Science for Policy, ICSU's Role in Sustainable Development, was discussed, including the relation with the United Nations, the Intergovernmental Platform on Biodiversity and Ecosystem Services, and other Union interactions.

In the Summary of the second day, I asked all the ICSU Scientific Union representatives to support our proposal for IYCr2013. (After the Meeting, the President of the IUCr met officers of UNESCO and the organizer of IYC2011 and received some important information concerning submission of the proposal for IYCr to UNESCO and the UN.)

The most important and urgent item was the weighted voting system. The dues structure was changed at the General Assembly in 2008. The annual membership fees for most members, especially for national members of large countries, were markedly raised. But the fee for the IUCr, to our surprise, was decreased. Although the national members whose membership fees were raised had accepted the decision at the previous General Assembly, they strongly demanded to change the equal voting system to a weighted voting system. This problem will be decided at the next General Assembly to be held in Rome, Italy, in 2011.

All the activities of ICSU are strongly inclined to environmental problems, such as the new Global Initiative on Earth System Research for Global Sustainability. Most of the Scientific Unions, Mathematics, Physics, Chemistry, Biology and Geology, have shown great contributions to ICSU activities. I expect that IYCr2013 will contribute to the activities of ICSU such as International Education, Data and Information, and Universality of Science.

**Y. Ohashi**, IUCr Representative

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

The major event for CODATA during 2010 was the biennial conference and General Assembly held in Stellenbosch, South Africa, 24–27 October 2010.

*CODATA Conference.* The theme of the 22nd International CODATA Conference was Scientific Information for Society: Scientific Data and Sustainable Development. This first CODATA meeting in Africa was described by President K. Lal as the fulfilment of a dream, and concentrated heavily on aspects of the CODATA Strategic Plan that were most relevant to the developing world: a commitment to work vigorously against the digital divide, and to foster education and maximum access to scientific data for the benefit of society. The meeting included high-level strategic addresses from the South African Minister for Science, from the Head of the Science Policy Division of UNESCO, and from the ICSU Vice-President for Scientific Planning and Review.

Sessions of particular relevance to the IUCr covered the related topics of validating published research against its underlying data; and making the underlying data available as a published work in its own right. A presentation of the data flow from experiment to publication in crystallography, including the IUCr journals' emphasis on validation through *checkCIF*, was well received and was subsequently referenced in early meetings of the newly constituted ICSU World Data System. A session on Data at Risk was also of interest, from the viewpoint especially of preserving early crystallographic software packages.

A full meeting report is available at <http://www.iucr.org/resources/data/meeting-reports/codata-2010>.

**General Assembly.** The General Assembly reviewed activities relating to its Strategic Plan 2006–2012. Work towards a global information commons had involved collaboration with Science Commons and the Global Biodiversity Information Facility (GBIF) in developing the CC0 protocol; active partnership in the European COMMUNIA conference; and close involvement in the launch of the Polar Information Commons. The Sharing Data Across the Digital Divide activities included the organization of the CODATA 2010 Conference in South Africa; involvement with the GEO Data Sharing Task Force; authorship of a data sharing implementation White Paper; and engagement with follow-up activities to the World Summit on the Information Society. The General Assembly voted for a formal review of progress, and the establishment of a working party to prepare a Strategic Plan for the next 5–6 years, to be informed by the ICSU Plan anticipated in 2012.

A proposal to create an International Data Academy was presented. Such an institution would secure the services of experts in scientific and technical data management, typically those who had served CODATA in various time-limited roles as Officers or members of Task Groups; and also provide some training and possible career development for younger scientists.

The Officers of CODATA (terms of office in parentheses) are: President: Huadong Guo (People's Republic of China; 2010–2014); Vice-Presidents: T. Gojbori (Japan; 2010–2014), F. Kuznetsov (Russia; 2010–2014); Secretary General: R. Chen (USA; 2008–2012); Treasurer: M. Sabourin (Canada; 2008–2012). Ordinary Members of the Executive Board are listed on the CODATA web site at <http://www.codata.org>.

The 2010 CODATA Prize was awarded to P. Uhlir of The National Academies in Washington, DC, for extensive work in the areas of scientific and technical data management and policy. Uhlir has worked on the relationship of intellectual property law for digital content to research and development policy; and has been active within CODATA in initiatives such as Global Information Commons for Science (GICSI).

**Other activities.** CODATA launched the Polar Information Commons, to help preserve and make available the scientific data generated under the International Polar Year, in Oslo, Norway, June 2010. The launch was attended by approximately 100 people and the Polar Information Commons (PIC) booth was visited by dignitaries including Crown Prince Haakon of Norway and Prince Albert II of Monaco.

CODATA continued its collaboration with ICSU through participation on the *ad hoc* ICSU Coordinating Committee on Information and Data, with meetings of the Committee in Paris in February and September.

CODATA, a Co-Chair of the GEOSS Data Sharing Task Force (DSTF), continued its collaboration with GEO (Group on Earth Observations) leading to the VII GEO Plenary and Ministerial meeting in Beijing in November 2010. The meeting approved a Data

Sharing Action Plan, presented to delegates by the DSTF, and adopted the Beijing Declaration: 'Noting with particular satisfaction, the GEOSS Data Sharing Implementation Guidelines and Action Plan and the establishment of the operational GEOSS Common Infrastructure (GCI), which significantly improves access to global Earth observation data and resources'.

**B. McMahon**, IUCr Representative

## 12.5. ICSU Committee on Space Research (COSPAR)

The 38th Assembly of the Committee on Space Research (COSPAR) was held in the Hanseatic city of Bremen, Germany, 18–25 July 2010.

COSPAR (<http://cosparhq.cnes.fr/>) was established in 1958 by the International Council of Scientific Unions (now the International Council for Science), with the main objective to promote international collaboration on various levels 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 cooperation of national and international organizations and specialist working groups.

The main COSPAR activities are devoted to space topics (such as astronomy, space travel and exploration or climate research). The most interesting division of COSPAR for the IUCr, the Scientific Commission on Materials Science in Space (MSS, Commission G), deals with scientific experiments on materials performed in a reduced gravity environment. Different experiments on growth of crystals and dendrites in microgravity were, at some point, part of these programmes, now the stress is more on combustion and biotechnology. The MSS Commission reviews fundamental theoretical and experimental approaches, helping to understand emerging fields, and recommends promising avenues for future research. It also coordinates exchange of information on scientific subjects. The MSS Commission is chaired by V. Shevtsova (Belgium), with Vice-Chairs S. Amiroudine (France) and S. Yoda (Japan). For the Bremen meeting the Commission received twice as many abstracts (40) as for the meeting in Montreal. The presentations dealt mostly with microgravity experiments conducted in drop towers, parabolic flights, photon satellites and on the International Space Station. Four half-day symposia reported on the effects of gravity on physio-chemical processes.

The financial situation of COSPAR is satisfactory and recommendations were made to initiate new activities such as holding a multidisciplinary General Symposium – every other year, starting in July 2013. The Symposium will focus on training and education with special activities dedicated to teachers, students, young professionals and the general public.

*Advances in Space Research (ASR)*, an official journal of COSPAR, 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. The journal home page is <http://ees.elsevier.com/asr>.

The COSPAR President for the period 2010–2014 is G. Bignami (Italy) and the Vice-Presidents are R. Lin (USA) and 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).

In total there are 13 International Scientific Union Members with representatives to COSPAR.

The Local Organizing Committee of the 38th Assembly, headed by H. J. Rath, did an excellent job. There were 4836 delegates (including

**Table 2**  
Income and Expenditure Account (in Swiss Francs) for the year ended 31 December 2010.

	2010		2009	
<b>Income</b>				
Membership subscriptions		153 000		158 046
Sales				
Journals, back numbers and single issues	4 125 605		4 428 868	
Books	277 625		120 359	
Open Access Grant	4 883	4 408 113	31 728	4 580 955
Investment income				
Income from investments	88 162		89 373	
Bank interest	971		2 064	
(Loss)/Profit on sale of investments	—	89 133	—	91 437
Other income				
Royalties and copyright fees	13 719		8 533	
Advertising income	189 731		193 711	
STAR/CIF income	13 113	216 563	12 709	214 953
<b>Total income</b>		<b>4 866 809</b>		<b>5 045 391</b>
<b>Expenditure</b>				
Journals				
Publication costs	612 887		606 104	
Editorial expenses	333 134		322 575	
Technical editing	1 371 567		1 470 547	
Subscription administration	108 200	2 425 788	109 885	2 509 111
Books				
Publication costs	54 802		96 605	
Editorial expenses	68 842		32 340	
Technical editing	79 378	203 022	103 122	232 067
Newsletter				
Publication costs	113 779		112 630	
Editorial expenses	113 157	226 936	123 384	236 014
President's Fund and other Grants and Young Scientists' support				
		137 421		165 977
General Assembly and Congress costs				
		30 058		40 614
Committee meetings and expenses				
		125 750		71 129
Publications and journals development				
General	538 906		587 946	
Editors' meetings	—		2 079	
STAR/CIF	8 667		21 302	
Promotion	165 831	713 404	162 268	773 595
Subscriptions paid				
		11 400		11 167
Visiting Professorship Programme				
		5 048		4 862
Administration expenses:				
General Secretary and Treasurer: Honorarium to Treasurer	9 544		10 537	
Audit and accountancy charges	59 186		66 097	
Legal and professional fees	16 450		7 649	
Travelling expenses	5 279		18 051	
Bank charges	2 569	93 028	2 112	104 446
Executive Secretary's office:				
Salaries and expenses	305 507		300 892	
Travel expenses of IUCr Representatives on other bodies	16 922		14 656	
Commission (income)/expenses	(8 908)		—	
Sponsorship of meetings	4 479		11 611	
IUCr/FIZ agreement	(18 862)		(18 745)	
Bad debts	(3 170)	295 968	5 638	314 052
Depreciation				
		41 481		41 570
<b>Total expenditure</b>		<b>4 309 304</b>		<b>4 504 604</b>

**Table 2 (continued)**

	2010	2009
<i>Surplus of income over expenditure (before realized exchange losses)</i>	557 505	<i>540 787</i>
Realized fluctuations in rates of exchange		
Exchange movement on trading activities	(161 625)	<i>122 575</i>
Surplus/(deficit) of income over expenditure (after realized exchange losses)	395 880	<i>663 362</i>
Movement in market value of investments in year	198 698	<i>639 751</i>
Unrealized fluctuation in rates of exchange		
Exchange movement on trading activities	(68 593)	<i>(22 019)</i>
Investment activities	(246 259)	<i>74 401</i>
Total recognized gains/(losses) relating to the year	279 726	<i>1 355 495</i>
<b>Opening fund accounts at 1 January 2010</b>	4 378 996	<i>3 023 501</i>
<b>Closing fund accounts at 31 December 2010</b>	4 658 722	<i>4 378 996</i>

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.

2417 regular participants and 586 students) from 64 nations. 4503 abstracts were submitted.

The next COSPAR Assembly will be held in Mysore, India, 14–24 July 2012, whereas the following one (2014) is planned in Moscow, Russia.

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

### 13. Finances

Extracts from the full financial statements, namely the Income and Expenditure account, Balance Sheet and Summary of Fund Accounts, are given in Tables 2, 3 and 4, respectively.<sup>1</sup> For comparison, the figures for 2009 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 2010 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 476 477. In the accounts this loss has been assigned as ‘Realized’ (CHF 161 625) and ‘Unrealized’ (CHF 314 852). The loss attributable to investment activities has been assigned to the General Fund and the loss attributable to trading activities has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 2010. 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.

<sup>1</sup> The full audited accounts are available from the IUCr electronic archives (Reference ES0388). Services for accessing these data are described at the back of the journal.

Investments are noted in the balance sheet at their market value at 31 December 2010.

The balance sheet shows that the assets of the Union, including the loss resulting from fluctuations in rates of exchange, have increased during the year, from CHF 4 378 996 to CHF 4 658 722. The movement in market value of the investments was CHF 198 698 in 2010 (CHF 639 751 in 2009). The significant gain in value of the investments in 2009 was a result of the well known market situation (following significant losses in 2008).

The following transfers were made from the Journals Fund: CHF 75 000 to the Publications and Journals Development Fund; CHF 160 000 to the Research and Education Fund; CHF 100 000 to the General Assembly and Congress Fund; CHF 50 000 to the *Newsletter* Fund; and CHF 25 000 to the President’s Fund.

The following comments refer to figures in the full accounts.

The General Fund account shows a deficit of CHF 303 856, as compared with a deficit in 2009 of CHF 289 896. The administrative expenses were CHF 391 282 in 2010 as compared with CHF 408 057 in 2009. Of this amount, CHF 181 818 was charged to the publications of the Union.

The expenses of the Union Representatives on other bodies were CHF 16 922. The cost of the Finance Committee meetings held in 2010 was CHF 14 864, while the Executive Committee meetings cost CHF 63 030. The income from the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 18 862. The subscriptions from Adhering Bodies were CHF 153 000. Interest on bank accounts and investments credited to the General Fund was CHF 89 133.

Grants totalling CHF 16 738 were paid from the President’s Fund in 2009.

The Journals Fund account for 2010 shows a surplus of CHF 1 132 016 before the transfer of CHF 410 000 to the other fund accounts, as compared with a surplus of CHF 1 346 877 in 2009 before the transfer of CHF 580 000 to the other fund accounts.

The cost of the technical-editing office has been divided between the Journals Fund and the *International Tables* Fund in percentages based on the staff time spent on each publication. The

**Table 3**  
Balance sheet (in Swiss Francs) as at 31 December 2010.

	2010	2009
<b>Fixed assets</b>		
Tangible fixed assets	52 746	45 880
Investments at market value	2 458 959	2 509 238
	2 511 705	2 555 118
<b>Current assets</b>		
Stock	93 829	119 120
Cash at bank and in hand		
Current accounts	46 360	54 872
Deposit and savings accounts	1 327 174	946 052
Cash with Union officials	9 347	7 706
	1 382 881	1 008 630
Debtors, accrued income and payments in advance	1 070 171	1 162 842
Subscriptions due from Adhering Bodies	5 500	6 000
	2 552 381	2 296 592
<b>Total current assets</b>		
	2 552 381	2 296 592
<i>Creditors: amounts falling due within one year</i>	(405 364)	(472 714)
<b>Net current assets</b>	2 147 017	1 823 878
<b>Total funds</b>	4 658 722	4 378 996

**Table 4**  
Summary of Fund Accounts (in Swiss Francs) as at 31 December 2010.

	As at 1 January 2010	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 2010
					Trading	Investments	
<b>Fund accounts</b>							
General Fund	(1 475 540)	—	(303 856)	198 698	70 866	(246 259)	(1 756 091)
President's Fund	106 534	25 000	(16 738)	—	(5 146)	—	109 650
Journals Fund	3 440 171	(410 000)	1 132 016	—	(186 597)	—	3 975 590
<i>International Tables</i>	(465 765)	—	25 261	—	19 748	—	(420 756)
Publications and Journals Development Fund	923 768	75 000	15 776	—	(45 484)	—	969 060
Research and Education Fund	974 874	160 000	(142 468)	—	(44 491)	—	947 915
Ewald Fund	528 313	—	—	—	(23 685)	—	504 628
<i>Newsletter</i> Fund	51 173	50 000	(91 310)	—	(442)	—	9 421
General Assembly and Congress	295 468	100 000	(61 176)	—	(14 987)	—	319 305
	4 378 996	—	557 505	198 698	(230 218)	(246 259)	4 658 722

technical-editing costs for the Journals Fund were CHF 1 325 614 [for 13 156 published pages (5431 papers)] as compared with CHF 1 401 448 in 2009 [12 467 published pages (5440 papers)]. Submissions to the open-access-only *Acta E* decreased to 4113 in 2010 from 4166 in 2009. 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 surplus of CHF 25 261, as compared with a deficit of CHF 150 498 in 2009. The net sales income was CHF 208 783 in 2010 as compared with CHF 89 026 in 2009. From January 2010 the publisher changed from Springer to Wiley.

The *Newsletter* Fund account received a transfer of CHF 50 000 from the Journals Fund in 2010. The cost to the Union of producing the *Newsletter* in 2010 was CHF 91 310.

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. From 2000, costs associated with the Crystallographic NeXus Project to provide CD-ROMs (containing crystallographic software and web material) free of charge to developing countries have been charged to this Fund. In 2010, CHF 4397 was provided from this Fund as journal subsidies in connection with the Journal Grants Fund, which was set up to assist institutions that have difficulties in meeting the full subscription price. CHF 126 513 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.

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 2010 this Fund incurred expenses totalling CHF 61 175 and received a transfer of CHF 100 000 from the Journals Fund.