

## Report of the Executive Committee for 2009

## 1. Meetings

The IUCr sponsored the following meetings held during 2009:

Second African School and Workshop on X-rays in Materials: Some Established Techniques and Practical Applications, Dakar, Senegal, 19–26 January.

Role of Synchrotron Radiation in the Advancement of Materials, Red Sea, Egypt, 1–5 February.

II Latin-American Symposium on Polymorphism and Crystallization of Drug and Pharmaceutical Products (LAPOLC 2009), Estância de São Pedro, Brazil, 9–11 March.

XII Intensive Course on X-ray Structure Analysis, Durham, UK, 28 March – 6 April.

RapiData 2009, Brookhaven, USA, 19–24 April.

Second International School on Biological Crystallization and International School on Crystallization: Drugs, Foods and Agrochemicals, Granada, Spain, 18–22 and 25–29 May.

High-Pressure Crystallography: From Novel Experimental Approaches to Applications in Cutting-Edge Technologies, Erice, Italy, 4–14 June.

Symposium R on X-ray Techniques for Advanced Materials, Nanostructures and Thin Films – from Laboratory Sources to Synchrotron Radiation, Strasbourg, France, 8–12 June.

2nd School and Workshop on X-ray Micro- and Nanoprobes, Palinuro, Italy, 11–19 June.

ICCOSS XIX (International Conference on the Chemistry of the Organic Solid State), Genoa, Italy, 14–19 June.

Crystallography Online: International School on the Use and Applications of the Bilbao Crystallographic Server, Zarauz, Spain, 21–27 June.

International Conference on Neutron and X-ray Scattering 2009, Kuala Lumpur, Malaysia, 29 June – 1 July.

XX Jubilee International School on Physics and Chemistry of Condensed Matter, Białowieża, Poland, 4–11 July.

Advances in the Characterization of Industrial Materials, Chania, Greece, 10–20 July.

VII International School on Crystallography (Protein Crystallography), Havana, Cuba, 13–17 July.

ACA Annual Meeting, Toronto, Canada, 25–30 July.

XAFS 14 International Conference, Camerino, Italy, 26–31 July.

25th European Crystallographic Meeting (ECM-25) and Satellite Meeting on Mathematical and Theoretical Crystallography ‘Symmetry and Crystallography in Turkish Art and Culture’, 16–21 August.

International Summer School on Fundamentals and Basic Methods of Crystal Growth, Brasov, Romania, 24–29 August.

Advanced Crystallography at High Pressure, Harbin, People’s Republic of China, 27–31 August.

Zürich School of Crystallography, Zürich, Switzerland, 30 August – 12 September.

XIX Brazilian Crystallographic Meeting, Belo Horizonte, Brazil, 9–11 September.

Aperiodic 2009, Liverpool, UK, 13–18 September.

XIV International Conference on Small-Angle Scattering (SAS 2009), Oxford, UK, 13–18 September.

Clay, Clay Minerals and Layered Materials 2009, Moscow, Russia, 21–25 September.

Fourth Crystallographic School ‘Structural Analysis using Single-Crystal X-ray Diffraction Data: Crystallography under Applied Constraints’, Nancy, France, 22–26 September.

Summer Schools on Polycrystalline Structure Determination and Diffraction-Based Structure Analysis, Zakopane, Poland, 25–27 September.

Joint Conference of the Asian Crystallographic Association and the Chinese Crystallography Society (AsCA ’09), Beijing, People’s Republic of China, 22–25 October.

Charge Density Refinement and Analysis, Marrakech, Morocco, 28–30 October.

The Executive Committee met in Toronto, Canada, in July/August. The Finance Committee met in Copenhagen, Denmark, in March, and in Toronto 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 appointments of Co-editors, electronic publishing, archival policy, Special Issues, open access, fraudulent submissions, and other matters concerning the IUCr journals;

- review of contract with Wiley-Blackwell for IUCr journals;

- approval of audited accounts for the previous year;

- revision of Statutes and By-Laws;

- General Fund estimates and level of unit contribution;

- status of membership subscriptions;

- ICSU’s role in science education;

- investment policy;

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

- sponsorship and financial support for meetings, young scientists’ support;

- Journal Grants Fund;

- cooperation with databases, closure of Committee on Crystallographic Databases and 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, consideration of possible new volumes;

- change of publisher from Springer to Wiley for *International Tables*;

- IUCr Newsletter*;

- World Database of Crystallographers*;

- Online Dictionary of Crystallography, appointment of Editor-in-Chief;

- promotional activities;

- redesign of IUCr web pages;

- collection of photographs;

- Laue–Bragg centennial;

- Ewald Prize Selection Committee;

- discussion of arrangements for Madrid Congress.

Other items dealt with in this way were:

- uses 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, support of mmCIF project and CIF handling software;

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

- crystallography in Africa;

- Visiting Professorship scheme;

- review of activities of Commissions;

- review of activities of Regional Associates;

- review of reports of IUCr Representatives on other bodies.

Items concerning the Chester office were:

- staffing requirements in the IUCr office in Chester;

- risk analysis;

- upgrading of office technology, provision of internet services.

## 2. Publications

Volume 65 of *Acta Crystallographica*, Volume 42 of *Journal of Applied Crystallography* and Volume 16 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 2009 was 5440 (*Acta E* alone: 4166), which compares with 4795 in 2008 (*Acta E*: 3556) and 6637 in 2007 (*Acta E*: 5181). The number of pages published was also higher (12 467 compared with 11 295 pages in 2008 and 16 138 pages in 2007). Of the total, 6427 pages were published electronically only.

In 2009, 548 pages were printed for *Acta Crystallographica* Section A (702 in 2008), 790 for Section B (791 in 2008), 1258 for Section C (1197 in 2008) and 1349 for Section D (1294 in 2008). Section E published 5108 electronic only pages (4261 in 2008) and Section F published 1319 electronic only pages (1187 in 2008).

The average lengths of Full Articles in Sections A, B and C increased to 10.3, 9.6 and 3.8 pages, respectively. The average lengths of Full Articles in Sections D, E and F were unchanged from 2008 at 9.1, 1.2 and 4.0 pages, respectively. Average publication times fell for Sections A (5.0 months), B (4.9 months) and E (0.7 months) and increased slightly for Sections C (1.9 months), D (4.5 months) and F (2.8 months). The rejection/withdrawal rates were: Section A 39%, Section B 33%, Section C 52%, Section D 19%, Section E 18% and Section F 9%.

The number of Full Articles published in *Journal of Applied Crystallography* (*JAC*) in 2009 was 131 (120 in 2008). The number of pages increased from 1197 in 2008 to 1212 in 2009. The average review time decreased slightly to 4.3 months and the technical-editing time decreased to 1.0 months; the overall publication time decreased to 5.4 months. The rejection/withdrawal rate was 34%.

The number of Full Articles published in *Journal of Synchrotron Radiation* (*JSR*) in 2009 was 107 (106 in 2008). The number of pages increased to 883 in 2009 (666 in 2008). The average review time increased to 4.4 months and the technical-editing time decreased to 0.9 months; the overall publication time decreased to 5.3 months. The rejection/withdrawal rate was 21%.

IUCr journals were highly ranked amongst crystallographic journals, occupying three of the top six positions in crystallography. *JAC* had the highest impact factor at 3.5. Sections A, B and C, and *JAC* had cited half-lives of >10 years. A total of 2 905 762 downloads of journal articles were made from **Crystallography Journals Online** in 2009. The highest number of downloads was for Section E.

Papers presented at the workshop on New Algorithms in Macromolecular Crystallography and Electron Microscopy, Leiden, The Netherlands, and Proceedings of the CCP4 Study Weekend on Low-Resolution Structure Determination and Validation were published in Section D. Papers presented at the Fifth International Workshop on X-ray Damage to Biological Crystalline Samples were published in *JSR*, which also published a Special Issue on Advances and Synergy of High-Pressure Sciences at Synchrotron Sources. Abstracts communicated at the 25th European Crystallographic Meeting (ECM-25) were published in Section A.

Informal meetings of the Commission on Journals were held in Toronto, Canada, during the ACA meeting, and in Istanbul, Turkey, during ECM-25.

The end of 2009 saw the discovery during routine testing of the checking software of scientific fraud involving papers published in Section E. This problem emphasized the importance of the role of Co-editors and reviewers in making sure that we carefully and thoroughly review all articles that are submitted for publication. Measures have been taken to improve the checking software as a result of experience with the falsified structures, but in the end the quality of our publications relies heavily on the judgements of our Co-editors based on experience and competent advice. Obtaining competent reviews within a reasonable time is getting more and more difficult. The appointment of a review panel (see the report on Section F) may improve the situation, and this deserves further attention.

At the end of the year, more than 160 Section Editors and Co-editors worked on IUCr journals. The work of all these dedicated colleagues and of the competent and equally dedicated staff at Chester is essential to the well being of the journals and highly appreciated.

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

### G. Kostorz, Chair

**4.1.2. *Acta Crystallographica* Section A.** Section A is growing again. In 2009, it published 548 pages in six regular issues and 345 pages of Abstracts for ECM-25 in Istanbul, Turkey. 455 pages were devoted to one Lead Article (tilings and nets), one Feature Article (60 years of IUCr journals), 41 regular Research Papers and five regular Short Communications (excluding Book Reviews and IUCr notices). For comparison, the numbers of pages, without meeting Abstracts, published in the past years are 702 in 2008 (including the 271-page 60-years Celebration Issue), 510 in 2007 and 528 in 2006 (including a 99-page Special Issue). The numbers of pages devoted to submitted Research Papers and Short Communications were 406 in 2008 (five issues), 440 in 2007 and 348 in 2006 (five issues).

The average length of the full papers has gradually increased over the years and is now at 10.3 pages, while the number of full papers per regular issue has decreased to 7.2. The average publication time for

# international union of crystallography

**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
A61	2005	622	74	55	9.2	19	6.1
B61		730	87	84	8.5	3	3.0
C61		1412	439	437	3.2	2	4.0
D61		1681	233	200	7.8	33	3.8
E61		7439	2887	2880	2.6	7	1.1
F61		1102	311	309	3.5	2	3.0
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

*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
38	2005	1045	157	111	7.8	24	4.4	22	2.4
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

*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
12	2005	838	136	115	6.8	5	3.4	16	1.9
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

† 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.

Research Papers decreased from 5.3 to 5.0 months, while the average review time increased from 3.3 to 3.8 months, the same as in 2007. The proportion of withdrawn plus rejected manuscripts has increased from the nearly constant value of 33% of the past years to 39%. There is no backlog in the editorial offices. In general, the statistics look favourable compared to past years'. There are indications of a trend towards fewer and longer publications.

Section A is a high-level journal with a very diverse range of topics. Papers may be classified as methodological, mathematical, of interest to material science or to macromolecular crystallography. Roughly 30% are on methods and theory of structure determination and charge densities, 40% concern symmetry theory, topology, aperiodic structures and crystal chemistry, 30% touch the fields of diffraction physics, diffuse scattering and nanostructures. Two papers concern the history of crystallography. The impact factor for 2008 is 2.051, down from 2.385, but still higher than during the past ten years. The geographical distribution of the authors of the articles is still strongly dominated by Europe 64% (+8), followed by the Americas 21% (-5) and Asia+Australia 15% (-3).

I thank the Co-editors, and in particular the four most solicited ones, for their often difficult work. Thanks are also due to the Chester editorial staff, and in particular to Nicola Ashcroft.

In the pipeline for 2010 are a full and a partial Special Issue (the full Special Issue having appeared in March 2010) and several Lead Articles (one having now been submitted).

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

**4.1.3. *Acta Crystallographica* Section B.** As Editor of the Section I see all the proofs before they go to the authors. Reading those proofs is a pleasure because the papers so often describe in-depth studies of complex and important problems, and because the papers are well written and well illustrated. When I look at the studies that are made now and compare them with what could be done one or several decades ago I am amazed. It must be noted, however, that there is still a place in Section B for careful studies of more limited, but still significant, scope.

The average number of pages per article (9.6) is at an all-time high and would be higher if the supplementary material were not so easily available.

The number of pages printed for Section B was steady between 2008 (790 pages) and 2009 (791 pages) as were the numbers of articles submitted (134 and 138) and published (89 and 91). The reason for most rejections and withdrawals was an inappropriate choice of journal.

The impact factor for 2008 (2.34) is up some from the values of 2.17 and 2.16 in 2006 and 2007. In any event, the strength of Section B is its publishing of articles that are read and cited for many years. The impact factor is not a measure of lasting value.

The time from submission to publication dropped an additional 0.1 month (to 4.9 months) during 2009. Since the time for review went up just slightly, the decrease must be a result of streamlined processing in Chester. The continuing efforts there to upgrade the various types of software related to the publishing process (submission system, error checking, enhanced figures *etc.*) are very much appreciated.

For many years there has been an approximately even balance of papers discussing molecular (organic and metal-organic) structures and inorganic (ionic and network) structures. Examination of the data for the last decade suggests, however, that the proportion of inorganic papers may be rising. The number of papers reporting refinements of modulated structures, which have mostly been inorganic, may be a factor.

During 2009 three Feature Articles were published. Two of them ('Significant Progress in Predicting the Crystal Structures of Small Organic Molecules -- a Report on the Fourth Blind Test' and 'A Non-Mathematical Introduction to the Superspace Description of Modulated Structures') topped the list of *Acta B* articles (1968-) most frequently downloaded in 2009.

There were no changes to the editorial board during 2009.

Section B could not be the success that it is without the generosity of the Co-editors and reviewers, who donate so much time and effort to improving the submitted articles. The skill, dedication, tact and experience of the staff in Chester are also central. They, and especially Jill Bradshaw, improve the language of the papers, make sure that all the supporting data have been submitted, help out authors who are having difficulties, politely prod editors who might have had too many other things to do, and figure out how to lay out the many tables and figures so that the pages look good and are easy to read.

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

**4.1.4. *Acta Crystallographica* Section C.** Section C continues to specialize in the rapid publication of high-quality studies of novel and challenging crystal and molecular structures. In 2009, Section C published 331 papers (31 inorganic, 136 metal-organic, 161 organic and 3 communications) in a total of 1258 pages, compared with 332 papers and 1197 pages produced in 2008 (+5%), but still below 2007 levels. In the same period, the number of submitted papers fell from 751 to 687 (-9%). The proportion of inorganic (10%), metal-organic (41%) and organic papers (49%) remains within the bands of previous years. The citation impact factor was lower than its usual level at 0.56. Average publication times increased slightly to 1.9 months. Approximately 52% of submissions to Section C in the past year were either subsequently withdrawn by the authors or rejected - a significant improvement over the 60% of 2008. The average number of pages per paper continues its upward trend - 3.2 in 2005, 3.6 in 2008 and 3.8 in 2009.

The number of papers published in 2009 remained steady relative to 2008, although there were a couple of months during the year where the number of submitted papers was worryingly low. The statistics concerning submitted papers and the rejection rate may fluctuate considerably from year to year as they can be strongly influenced by the number of attempts by authors to submit *Acta E* style papers to *Acta C* first to see if they have a chance. It is unfortunate that there is not a better way to filter such submissions, because papers that are clearly written for *Acta E* or are very poorly written are a waste of precious Co-editors' and reviewers' time. It appears that some inexperienced authors use multiple resubmission of papers in an iterative process as an attempt to learn how to write papers, but my opinion is that a journal should not be abused excessively in this way by being expected to take the role of teacher for inexperienced people who have no access to learned peers (minor assistance is of course not a problem).

The decrease in impact factor is disappointing. It reflects the sorts of papers we are receiving and the author base. *Acta C* by its name is a journal for crystal structure communications and given the choice of structural journals available to authors, it is hard for *Acta C* to attract key papers. Nonetheless, 2009 saw the publication of several very good papers which addressed interesting structures in depth. The 2009 *Notes for Authors* made it clearer that the journal will consider reports of challenging structure determinations that do not fulfil all validation requirements provided the experiment is properly documented, and we have seen a few papers in this category. Section C now also accepts redeterminations of structures if the original

publication provided little information about the structure itself and the new paper adds considerably to what had been said previously.

The increase in average paper length appears to be mainly a result of an increasing number of figures in papers. At one time (before *Acta E*) we asked for a maximum of two figures per reported structure, but this requirement has been relaxed in recent years. I feel that we need to keep an eye on the number of figures and ensure that their information content is maximized, while retaining clarity, and that low-content figures are removed or combined.

Finding good and thorough referees who respond within a respectable time frame is an increasing problem. The increase in publication times is mainly related to the review time. Sometimes reviewers never respond to any attempt to contact them and this causes considerable waste of time. I think it is probably systemic of the peer review system these days. I have heard reviewers who said they receive six review requests from various journals in a week! Co-editors frequently have to write lengthy critical reports on papers themselves, because some reviewers do a superficial job or do not detect important technical issues.

The validation of structure-factor files introduced during 2008 has been beneficial in the review process, as it has on several occasions revealed 'strange' editing in a CIF. Frequently, it appears that weighting schemes are not updated when a re-refinement is done. I am currently investigating whether this is because of an oversight in a software package. The facility developed in Chester to enable the generation of additional enhanced crystallographic diagrams online either before or at the time of submission is not yet being used very often.

The scandal over fraudulent reports in *Acta E* has heightened our awareness of the need for constant vigilance and I have tried to impress this on the Co-editors. Occasionally, I detect an overlooked incorrect structure at proof stage, but none of these seem to have been fraudulent. We now urge authors to include their refinement instruction files in the CIF, so that things like (usually undocumented) restraints can be assessed and test refinements can be carried out. It may take some time for this practice to become established. While it might seem overkill to ask for such instruction files, test refinements can sometimes be very revealing about unexpected and incorrect refinement strategies and other problems with the structure that might not be immediately apparent from the CIF alone. This is often a consequence of the inexperience of many of our authors.

The outlook for Section C is 'steady as she goes' for the next year. I do not wish to introduce radical changes to the journal at this time, but prefer to offer authors a period of stability in submission requirements.

I wish to thank warmly those Co-editors who have recently retired from the Section C editorial board for their excellent services to the journal and the crystallographic community: Jacques Barbier and Len Barbour. I would also like to take this opportunity to thank all the current Section C Co-editors for their continued outstanding efforts on behalf of Section C. The Chester editorial office staff are magnificent and, in particular, Sean Conway, with whom I have most contact, is tireless in his efforts. He copes admirably with all of my idiosyncratic requests to authors at proof time.

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

**4.1.5. *Acta Crystallographica* Section D.** Section D continues to attract important methodological papers, as well as publishing novel biological structures. In 2009 these two main types of papers were evenly balanced, with nearly 45% of the articles published featuring aspects of methodology and the remainder presenting new structures.

The impact factor of Section D increased to 2.94 during the year. This is likely to be 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. A small number of structural papers were transferred to Section F during 2009, for lack of new insights into biology, chemistry or structure, but we have also noted a general rise in the biological impact of the structural papers published in Section D. The bicentenary of Charles Darwin's birth was also celebrated during 2009 with an essay by Cele Abad-Zapatero. This recognized the importance of evolutionary concepts to the understanding of biological structure.

The CCP4 Special Issue in February 2009 was focused on Low-Resolution Structure Determination and Validation. This area has become more important in recent years as the forefront of structural biology has moved from small proteins and enzymes to large complexes and molecular machines. We thank Randy Read, Gerard Kleywegt and Charles Ballard for their Guest Editorship of this Special Issue. Papers from a workshop on New Algorithms in Macromolecular Crystallography and Electron Microscopy were published in the July 2009 issue of the journal. This workshop brought together experts in computational methods development in macromolecular X-ray crystallography and electron microscopy to discuss algorithms of the future to exploit the latest technology, improve both methods and combine the complementary information from both techniques optimally. We thank Navraj Pannu, Raimond Ravelli and Jan Pieter Abrahams for acting as Guest Editors for these papers.

The number of pages published during 2009 was higher than in 2008, as was the total number of articles: 137 Full Articles and 23 Short Communications were published. The total number of pages was 1349, with the average length of full articles being 9.1 pages. Publication times were similar to 2008, at an average of 4.5 months; the electronic submission system continues to work well.

We welcome one new Co-editor, Professor Rob McKenna, from the University of Florida, to the Section D Board. We thank our reviewers and Co-editors for their work on the journal; we are also extremely grateful to Louise Jones and Simon Glynn in Chester for their superb support and advice.

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

**4.1.6. *Acta Crystallographica* Section E.** The year 2009 has been a difficult one for the journal, its Editors and Co-editors with the realization that in earlier years it had been subjected to significant and systematic scientific fraud. With tremendous assistance from Ton Spek, George Ferguson and a number of editorial staff in the IUCr Chester office more than 100 papers were investigated and shown incontrovertibly to be fraudulent. The articles were retracted and the retractions were accompanied by an Editorial drawing the attention of readers and the wider scientific community to the existence and nature of the fraudulent activities and exposing the corresponding authors and their institutions. The effect was both swift and unexpected with the Editors and the Chester office being bombarded with enquiries from the international media for over a month. The revelations achieved significant exposure with articles commenting on the frauds and their implications in many scientific journals, including *Nature* and leading newspapers such as the *New York Times*. Responses to the legion of media enquiries were kept to a minimum but did give us the opportunity to stress that it was the continuous improvements to our validation systems that first alerted us to the problems and that would in future make such nefarious practices

much easier to detect. The singular benefits of retaining and providing access to .fcf (structure factor) data files, a unique feature of publications in IUCr journals, was also stressed at every opportunity. It is hoped that out of this unhappy episode may come the impetus for other journals reporting crystallographic data to implement similar requirements and to help their reviewers to a better understanding of the information provided by the *checkCIF* process, which is used extensively by a number of other organizations.

Despite these difficulties, contributions to the journal have continued to grow with 4166 papers published in 2009 compared to 3556 in 2008. This steady increase in a stable open-access environment is pleasing and the future of the journal remains secure. Of the published manuscripts, 67% described structures of organic, 31% structures of metal-organic and 2% structures of inorganic compounds. 47% of authors were from the People's Republic of China, 8% each from India and Malaysia, 5% from Pakistan, 4% each from Germany and the USA, 3% from Turkey, 2% from Iran, Japan and Korea and with smaller percentages from other countries. The number of papers withdrawn or rejected for a variety of reasons has increased slightly from 16% to 18%, while the journal's impact factor is 0.4.

We have been fortunate over the past year to increase our pool of Co-editors significantly: David Billing, Olivier Blaque, Parthasarathi Dastidar, Ulrich Flörke, Jerry Jasinski, Gary Nichol, V. R. Pedireddi, Graham Smith and Luc Van Meervelt have joined the ranks of journal Co-editors, which now numbers 57 including the three joint Section Editors. We expect that there will again be some additions to the Co-editorial board in 2010 to accommodate the steady increase in submissions, to spread the load among the Co-editors and to cover for some retirements that may regrettably be imminent. We cannot over-emphasize the excellent work done by our Co-editors or thank them sufficiently. Without their devotion to what can be an extremely taxing job this journal would not exist.

The all-important validation processes, underpinned by *checkCIF* software, continue to evolve and improve thanks to the prodigious efforts of Ton Spek and Mike Hoyland. The checks on submitted structure-factor (.fcf) files are now routine and authors are clearly coming to terms with the fact that they need to check their review documents carefully after submission. For some time now it has been possible for prospective authors to run both the CIF and FCD validation checks together from a link on the main *checkCIF* page. Occasional problems still occur, particularly with twinned crystals, and work to overcome these is currently in progress in consultation with COMCIFS.

Finally, we are especially grateful to the editorial staff in the Chester office for all their help and dedication. In particular, we are indebted to Gillian Holmes and Sean Conway who look after Section E on a daily basis. Our thanks also to Peter Strickland for his sound advice, calm influence and expert management of the fraud investigation process.

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

**4.1.7. Acta Crystallographica Section F.** The fifth year of publication of Section F continued developments to enhance this relatively young journal as a venue for rapid publication of structure and crystallization communications on biological macromolecules. In 2009, 329 original science articles were published in 1319 pages. Importantly, 57 of those articles were structure communications and one was our first example of a new category, the Laboratory Communication. The average time from submission to publication, including peer review, was a rapid 2.8 months.

2009 saw the initiation of several important new developments. The first was an outcome of the streamlining project and the effort to specify those data required for publication. The result is *pubBIO*, a novel set of tools for authors developed by the IUCr to facilitate drafting of crystallographic publications and to speed editorial processing after submission. At its heart is a set of templates for tables for presenting required and recommended data that can be populated by means of a deposition mmCIF or that can be used to create an mmCIF of tabulated data for deposition into databases.

Special thanks go to Gernot Kosterz, Editor-in-Chief, for his steadfast support of these developments and to Peter Strickland, Brian McMahon, Louise Jones and Simon Westrip for the vision and talent to make this happen.

Second, a panel of 30 experienced referees has been assembled to provide reviews at a rate of about one a month, each review returned within a two-week review period. Each Co-editor will be 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 driving down processing times while maintaining high standards of quality. This panel will begin its work early in 2010 simultaneously with the launch of the updated submission system, which has been adapted to manage the interactions and record keeping for the panel.

Third, beginning with the final issue of 2009, we have introduced a special handling option for publication of structural genomics papers. Heretofore, these papers have been submitted and published one at a time just like all the other papers we handle. Structural genomics teams have come to recognize, however, that efficiencies in preparations and impact of their work are enhanced when papers are published in topically related groups. A set of eight papers from the RIKEN-UK collaboration appeared as a group in the most recent December issue. This will be followed in 2010 by an entire Special Issue of approximately 30 papers from the Joint Center for Structural Genomics led by Ian Wilson of the Scripps Research Institute. We anticipate that this will spark demand for similar Special Issues in the future and will serve to shift the balance of papers we publish significantly toward structure communications.

Finally, our impact factor: we received our second impact factor during 2009 and at 0.606 it is slightly, but probably insignificantly, down from the 0.645 we received in 2008. Our current aim is to break the 1.0 barrier – we are confident that we will be there soon.

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

**4.1.8. Journal of Applied Crystallography.** As has always been the case with *JAC*, the spread of topics in 2009 was vast covering everything from powder diffraction through small-angle scattering to certain aspects of biology. *JAC* also continued to be the primary place where crystallographic computer program information is published.

The size of the journal increased slightly in 2009 – the number of Full Articles published was 131 (compared with 120 in 2008) and the number of pages was 1212 (compared with 1197 in 2008). There was also an increase in the number of manuscripts submitted (282 compared with 258 in both 2008 and 2007).

The impact factor remained high at 3.2, making *JAC* the highest ranked IUCr journal; the journal also has a long cited half-life (>10 years). Publication times improved in 2009. The average review time decreased to 4.3 months and the technical-editing time decreased to 1.0 months; the overall publication time decreased to 5.4 months. The average publication time for Short Communications was 3.5 months.

The publication of Special Issues, and Lead and Feature Articles has been under consideration, and work was started in 2009 towards

the publication of a Special Issue on crystallographic education in summer 2010.

My sincere thanks 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 2009, *JSR* published 107 Research Articles and a total of 883 pages in the six issues. This was an increase in both articles and pages as compared with 2008. Two Special Issues were published in 2009; one, which included papers presented at the Fifth International Workshop on X-ray Damage to Biological Crystalline Samples, was published in March (Volume 16, Part 2) with Guest Editors Elspeth Garman and Colin Nave, and the other, entitled Advances and Synergy of High-Pressure Sciences at Synchrotron Sources, was published in December (Volume 16 Part 6) with Haozhe Liu, Tom Duffy, Lars Ehm, Wilson Crichton and Katustoshi Aoki as Guest Editors. We believe that the publication of selected papers from workshops and conferences in such Special Issues is an important service to the synchrotron-radiation community and we plan to continue this policy in the future.

The Facility Information pages continued in 2009. One page per issue is devoted to each of the three third-generation hard X-ray sources (APS, ESRF and SPring-8); these pages provide an opportunity for the facilities to communicate important news and updates to the international community of synchrotron-radiation users.

The average review time for 2009 increased to 4.4 months (3.9 months in 2008) but the technical-editing time was reduced to 0.9 months (2.5 months in 2008) resulting in a lower overall publication time of 5.3 months compared with 2008 (6.4 months).

Efforts to keep *JSR* at the focus of new developing areas of scientific interest saw the addition of the term 'Free-electron lasers' to the list on the journal front cover of topics covered by *JSR*.

The end of 2009 also saw the retirement of Co-editor A. Iida. We would like to take this opportunity to express our thanks for his contribution to *JSR* and to welcome A. Momose as his replacement; we also welcomed a further five new Co-editors in 2009: A. F. Craievich, S. M. Heald, P. A. Pianetta, S. Svensson and J. F. van der Veen, replacing those that retired in the previous year.

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

## 4.2. Commission on *International Tables*

The new Editor of *International Tables for Crystallography* Volume A, Mois Aroyo, has continued to work on the forthcoming Sixth Edition of the volume. This will include important modifications of the content and the arrangement of the text and the tabulated material of the Fifth Edition. The text and data are grouped into three main parts:

Part 1. *Introduction to space-group symmetries.* The aim of the introductory part is to offer a homogeneous text of educational and teaching nature related to the different symmetry items found in the tables of Volume A and Volume A1. An extended version of the introductory chapters of the Sixth Edition will form the essential part of the Sixth Edition of the Brief Teaching Edition. Unfortunately, there has been some delay in the preparation of the texts for the introductory part. For the moment only some of the articles of Part 1 are ready. For different reasons, the authors involved need more time

to prepare their contributions. This delay in the preparation of Part 1 will lead to a delay in the production of the Sixth Editions of Volume A and the Brief Teaching Edition, which had previously been estimated for the end of 2010.

Part 2. *Tables of plane and space groups.* This part starts with guidelines and examples for the use of the tabulated data, followed by the tables of plane and space groups. The new version of the tables of plane and space groups is in a rather advanced state. 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.

Part 3. *Advanced topics in space-group symmetry.* Most of the articles for this part are ready. The corresponding texts and tabulated data have been corrected and updated by the contributing authors. The chapters on crystal lattices and lattice complexes have been substantially revised. The data on normalizers of space and plane groups have been extended to include the chirality-preserving Euclidean normalizers.

The Editors of Volume A1, Hans Wondratschek and Ulrich Müller, finished the preparation of the Second Edition of the volume in 2009. It is expected to be published in 2010. For the Second Edition, all detected errors have been corrected and local 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: one gives instructions on how to relate crystal structures by group-subgroup relations and how to construct trees (Bärnighausen trees) of group-subgroup relations for crystal structures that can be derived from a high-symmetry structure type (aristotype); and the second describes the publicly accessible Bilbao Crystallographic Server, with emphasis on those databases and computer programs that are related to the subjects of this volume.

Part 2 contains the complete listings of the maximal subgroups for each plane group and space group, including their general positions or their generators, their conjugacy relations and the transformations to the conventional settings. 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 parametrized form.

The Editor of Volume B, Uri Shmueli, retired following the publication of the Third Edition in 2008. A successor has yet to be appointed.

Hartmut Fuess, the new Editor of Volume C, met members of the Editorial staff in Chester to discuss plans for the Fourth Edition. Some authors have updated their articles.

The Editor of Volume D, André Authier, reports that there have been no new developments with this volume in 2009.

Vojtech Kopský and Danny Litvin, Editors of Volume E, completed their work on the Second Edition during 2009. Typographical errors have been corrected and additional information has been included in the multi-page, multi-column comparison tables of notations for the seven crystallographic frieze-group types (two-dimensional groups with one-dimensional translations), the 75 crys-

tallographic rod-group types (three-dimensional groups with one-dimensional translations) and the 80 crystallographic layer-group types (three-dimensional groups with two-dimensional translations) to improve ease of use. In the symmetry-operations section for each group table, the Seitz notation of each symmetry operation has been added below the corresponding international notation. The volume will be available early in 2010.

The three Editors of Volume F, Eddy Arnold, Daniel Himmel and Michael Rossmann, report that they are approaching the final stages of preparing the Second Edition. It will include 19 new articles and several articles from the First Edition have been updated. The new articles cover such topics as standard definitions for macromolecular crystallographic statistical indicators, expression of membrane proteins, protein engineering, radiation damage, detection of mero-hedral twinning, determining structures in the presence of mero-hedral twinning, low resolution *ab initio* phasing, robotic crystal loading, whole-cell X-ray diffraction imaging and halogen interactions in biological crystal structures. Articles on software in current use by macromolecular crystallographers and structural biologists, including software for electron microscopy, will also be included. These enhancements should ensure that Volume F continues to be a useful reference for macromolecular crystallographers and structural biologists.

The Editors of Volume G, Syd Hall and Brian McMahon, are following continuing activity within COMCIFS to develop a methods-based dictionary definition language (DDLm) and methods evaluation language (dREL), and will commission chapters to describe these new standards, and CIF data dictionaries based on them, when they have been formally adopted. It is also likely that new dictionaries planned for additional areas of crystallography, and modifications to existing dictionaries, will contribute to the need for a new edition in the relatively near future. The Editors are interested in making best use of the electronic publication medium to provide timely updates of content, and to provide additional services to users.

Plans for a new volume on powder diffraction, EXAFS and XRF were discussed by Hartmut Fuess, Chris Gilmore and IUCr staff in Chester. These plans were welcomed by the Executive Committee and Professor Gilmore was encouraged to develop the proposal further. It was subsequently decided to split this into two new volumes, one covering powder diffraction and a separate volume covering EXAFS and XRF.

The contract between the IUCr and Springer, in which Springer agreed to act as co-publishers of *International Tables*, has ended. From 2010 onwards, *International Tables* will be published in conjunction with John Wiley and Sons.

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

**H. Fuess**, Chair

#### 4.3. Commission on Aperiodic Crystals

The Commission has continued actively to promote aperiodic crystallography in 2009, by organizing meetings and workshops as well as by 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. During 2009, the triennial flagship meeting of the Commission, Aperiodic 2009, took place in Liverpool, UK, 13–18 September. Aperiodic 2009 was chaired by R. McGrath and U.

Grimm, to whom the aperiodic community is indebted for organizing such a stimulating and enjoyable meeting. 110 delegates from 21 different countries attended the conference. There were 13 invited and 40 contributed plenary talks, and more than 40 posters, which were presented at two afternoon/evening poster sessions. The programme started with three tutorial lectures on Sunday afternoon. A public lecture entitled Simple Sets of Shapes that Tile the Plane but Cannot Ever Repeat by Professor Sir Roger Penrose FRS attracted a wide audience.

It was decided at this meeting that Aperiodic 2012 would be held in Australia, and would be organized by Ray Withers.

A related EPSRC-supported workshop on Mathematical Aspects of Aperiodic Order was held in Leicester, UK, in the week preceding the conference, and attracted about 40 participants.

Further to the activities associated with Aperiodic 2009, one Keynote Lecture and a Microsymposium were dedicated to aperiodic crystals at the 25th European Crystallographic Meeting, Istanbul, Turkey, 16–21 August.

The 6th Workshop on Structural Analysis of Incommensurate Crystals took place at the University of Bayreuth, Germany, 5–8 March 2009. This Workshop was organized by S. van Smaalen and the Laboratory of Crystallography of the University of Bayreuth on behalf of Special Interest Group 16: Aperiodic Crystals of the German Crystallographic Association (DGK). The Workshop attracted 31 participants and six lecturers from eight countries.

The most important upcoming meeting for the Commission is ICQ11 to be held in Sapporo, Japan, 13–18 June 2010 (<http://icq11.eng.hokudai.ac.jp/icq11/index.html>). The meeting is chaired by Y. Ishii and T. Ishimasa.

An International School on Aperiodic Crystals will be organized by the Commission, with the support of the Commission on Crystallographic Teaching, Carqueiranne, France, 26 September – 2 October 2010. The school will be chaired by M. de Boissieu, G. Chapuis and S. van Smaalen, (see <http://www-xray.fzu.cz/sgip/isac2010/isac2010.html>).

The Commission maintains internet pages at the web site of the IUCr at <http://www1.iucr.org/comm/capd/index.html>. A web site on all aspects of the crystallography of aperiodic crystals is maintained by the Special Interest Group on Aperiodic Crystals of the European Crystallographic Association, maintained by M. Dusek (Prague, Czech Republic): <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 crystallographic community, particularly through recommending and supporting IUCr proposals to hold meetings, workshops and schools. Numerous meetings of this type will be held in North and South America, Asia and Europe in 2010.

A key activity of the Commission has been to contribute to the design of the upcoming Madrid Congress. The biologically oriented portion of the International Programme Committee has organized an exciting programme with topics ranging across the field of biological and macromolecular structure. 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 2009 included in February: Role of Synchrotron Radiation in the Advancement of Materials (Red Sea, Egypt); in April: XII Intensive School on X-ray Structure Analysis (Durham, UK) and the



RapiData course (Brookhaven, USA); in May: Second International School on Biological Crystallization and International School on Crystallization: Drugs, Foods and Agrochemicals (Granada, Spain); in June: High-Pressure Crystallography: From Novel Experimental Approaches to Applications in Cutting-Edge Technologies (Erice, Italy) and Crystallography Online: International School on the Use and Applications of the Bilbao Crystallographic Server (Zarauz, Spain); in July: VII International School on Crystallography (Protein Crystallography) (Havana, Cuba), the ACA Annual Meeting (Toronto, Canada) and XAFS 14 International Conference (Camerino, Italy); in August: 25th European Crystallographic Meeting (ECM-25) (Istanbul, Turkey), International Summer School on Fundamentals and Basic Methods of Crystal Growth (Brasov, Romania) and Advanced Crystallography at High Pressure (Harbin, People's Republic of China); and in September: Zürich School of Crystallography (Zürich, Switzerland), XIX Brazilian Crystallographic Meeting (Belo Horizonte, Brazil), XIV International Conference on Small-Angle Scattering (SAS 2009) (Oxford, UK) and the Fourth Crystallographic School 'Structural Analysis using Single-Crystal X-ray Diffraction Data: Crystallography under Applied Constraints' (Nancy, France); in October: Joint Conference of the Asian Crystallographic Association and the Chinese Crystallography Society (AsCA '09) (Beijing, People's Republic of China). 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 on Electron Distribution and Chemical Bonding (GRC), 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 (CCSMD) community. In 2009 the main activity was Sagamore XVI, as detailed below, but a great deal of effort for the GRC 2010 and IXS 2010 meetings has also taken place. Last, but not least important, has been the action for promoting and disseminating CCSMD knowledge among new generations and within new geographic areas. As reported below, in 2009 an international workshop on charge density analysis was held in Morocco and one school on a similar subject took place in Spain. Actions for organizing a school about CSMD topics in the form of a satellite of the Madrid Congress, possibly linked to an extra two-day ECDM congress in the same location, also began.

*Sagamore XVI Charge, Spin and Momentum Density Meeting, Santa Fe, New Mexico, USA, 2–7 August 2009.* This meeting was led by Philip Coppens from Buffalo University, assisted by an International Programme and Advisory Committee including many members of this Commission and by a Local Committee headed by Thomas Proffen and Alan Hurd from the Lujan Neutron Scattering Center of the Los Alamos National Laboratory. The meeting attracted 105 scientific participants (plus eight accompanying members) from 16 different countries. It was held under the auspices of this Commission and received IUCr support. Other important sources of support were the Office of Basic Energy Sciences of the US Department of Energy and the National Science Foundation, NSF. The Conference opened with a Keynote Lecture by J. Schneider (DESY, Germany) entitled Science at XUV and Hard X-ray Free Electron Lasers, and was based around eight oral sessions, supplemented by three poster sessions and one session of poster talks. Two

sessions, chaired by Yu Wang and K. H. Schwarz, were dedicated to charge density and included talks on such diverse subjects as relativistic effects on the topology of the charge density (G. Eickerling), the way to push the multipole model to its limits (T. Koritsanszky), non-linear optical properties from wavefunction fitting of X-ray diffraction data (M. Spackman) and the photocrystallographic studies of excited-state structures of photomagnetic complexes (B. B. Iversen and M. Takata). A session on spin density was chaired by B. Gillon and P. Becker, with six talks on topics such as spin densities and excitations (P. Steffens), the site-susceptibilities approach in magnetization density studies (A. Gukasov) and powder diffraction with spin polarized neutrons (E. Lelievre-Berna). The session on momentum density, chaired by M. J. Cooper and A. Bansil, consisted of five talks with the first two Plenary Lectures offering a didactic overview on what can be learnt about intra- and intermolecular structures by inelastic X-ray scattering (K. Hämäläinen) and on which are the latest spin and momentum density studies on hard condensed matter (Y. Sukurai). The morning of the third day was dedicated to a session on the synergy between theory and experiment, chaired by C. Gatti and B. Dittrich and with talks, amongst others, on the post-Hartree–Fock corrections to the wavefunctions of crystalline systems (C. Pisani), the most recent developments in the interacting quantum atom theory (A. M. Pendas) and on charge-density studies of superconducting transition-metal carbides (W. Scherer). In the afternoon attendees could either relax in the Bandelier National Monument Park or visit the Lujan Neutron Scattering Center at Los Alamos, which were both rewarding, though different, experiences. The next two days were dedicated to sessions on time-resolved studies, neutron scattering and nanoparticles, respectively chaired by P. Coppens and D. Miller, A. Hurd and Th. Proffen, and P. Montano and E. Isaacs. The session on time-resolved studies included talks by H. Chapman on prospects for molecular imaging with X-FEL, by J. Spence on the femtosecond crystallography of protein nanocrystals and by D. Miller on the quest for structure–function correlation for biology using femtosecond electron diffraction. The session on neutron scattering exploited the use of such techniques to solve challenging problems in materials science, such as the relationships between crystal structure, magnetism and superconductivity in unconventional superconductors (C. H. Lee, J. Thompson) and the magnetic structure of magnetic nanostructures (J. Schuller). The last session on nanoparticles offered the occasion to listen to talks from very well regarded speakers who do not usually attend Sagamore meetings. Among others, S. Louie gave an overview on the electronic structure of all kinds of grapheme nanostructures, A. W. Castelman introduced cluster-assembled materials as a new frontier in nanoscale science and G. Aeppli gave a talk on nano/quantum magnetism.

Overall, particular thanks go to Philip Coppens for planning and putting together, along with the Programme Committee, a brilliant and cutting-edge programme for this meeting.

The oral presentations were largely from invited internationally renowned speakers but under each topic a number of submitted papers were selected for oral presentation. Poster sessions were extremely well attended, with all posters being available for the whole week.

A closed meeting of the Commission also took place, which *inter alia* discussed proposals of locations for the next Sagamore meeting and planning for the next GRC in 2010, which will be held in the USA (Massachusetts) despite a specific request to move it to Europe. M. Tanaka from SPring-8 (Japan) presented a number of interesting and well suited options and the Commission thus agreed to hold the next Sagamore Conference in Japan (2012). Three alternative charming

and appropriate locations were presented to all attendants by M. Takata during the social dinner.

The Conference venue was very well suited to the conference group size and the internal cosy garden of the venue as well as the picturesque atmosphere of Santa Fe provided a relaxed environment to encourage informal discussion outside the organized sessions.

*European Crystallographic Meeting, ECM-25, Istanbul, Turkey, 16–21 August 2009.* Members of this Commission, C. Gatti, U. Pietsch and Bo Iversen, as respectively Secretary and Chairs of Special Interest Group 2 (SIG#2) on CSMD of the European Crystallographic Association (ECA), took part in the planning of Microsymposia (MS) and Plenary Lectures on topics related to CSMD. This activity is covered by ECA SIG#2 so only very few details are given below.

A Keynote Lecture on Modern Developments in Inelastic X-ray Scattering Under Extreme Conditions of Temperature and Pressure was given by E. Alp and another on High-Pressure Crystallography, Weak Interactions and Electron Density was delivered by A. Katrusiak. Two MS were organized: Accuracy in Experimental Charge Density Determination (chaired by A. A. Pinkerton and S. van Smaalen), and Very-High-Resolution Protein Structures (chaired by C. Jelsch and B. Dittrich). Attendance at these lectures and MS was good.

*International Workshop on the Refinement and Analysis of the Electron Density Obtained from High-Resolution X-ray Diffraction, Marrakech, Morocco, 28–30 October 2009.* This workshop, organized by N. Bouhaida (Marrakech, Morocco) and N. E. Ghermani (Paris, France) in cooperation with an International Scientific Committee (C. Lecomte, C. Gatti and C. Jelsch), had the main aim to disseminate knowledge on electron-density studies from high-resolution X-ray diffraction data within the African/Magreb communities. It was held under the auspices of this Commission and received IUCr sponsorship and young scientist support. Other support came from the ECA, the local University and Nonius–Bruker. The workshop was organized in the form of a three-day school with international teachers on the following topics: Data Collection for Charge Density Studies (S. Dahaoui, Nancy); Electronic Properties from X-ray Diffraction Data (M. Souhassou, Nancy); Multipole Models (M. Souhassou, Nancy); Spin Density from Polarized Neutron Diffraction (B. Gillon, Saclay); Multipole Model Refinement using Multipole Moment Databanks (C. Jelsch, Nancy); Electrostatic Properties from X-ray Diffraction Data (N. Ghermani, Paris); From Charge Density to Density Matrices (P. Becker, Paris); Charge Density Applications to Metallorganic Chemistry (A. Spasojevic, Paris); Electron Density Topology and Chemical Bonding, Quantum Theory of Atoms in Molecules and Crystals (C. Gatti, Milan). The School also included three practical sessions, held by B. Guillot, C. Jelsch and A. Sayd-Tahri on the use of the software *MOPRO*.

A workshop booklet (containing about 100 pages) with extended written lectures from all teachers was distributed among the participants.

The School was attended by about 35 students from four African and four European countries. The level of the School and of the participants was very high and lectures were carefully attended, with many questions posed by students either after the lectures or during the breaks and free time. The school was hosted in an extremely charming venue with exotic gardens and stretches of water. The local organization was very efficient and helpful and everything went smoothly, in a very pleasant atmosphere.

*Charge Density School, Zaragoza, Spain, 31 May – 6 June 2009.* This five-day School, on the basics of charge density research and its applications, was organized by Professor Fernando Lahoz within an

international master on crystallography, sponsored by the University of Zaragoza. The School was attended by international teachers (E. Molins, F. Lahoz, E. Espinosa, S. Pillet, R. Blessing, S. Garcia Granda, L. Farrugia, I. Mata) and was well attended.

**C. Gatti, Chair**

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

The main concern of the Commission (CCGCM) in 2009 was the future of international schools and conferences in the area of crystal growth.

The 17th American Conference on Crystal Growth and Epitaxy in August at Lake Geneva, USA, gave some Commission members and consultants (D. Bliss, H. A. Dabkowska, T. Duffar, K. Kakimoto, K. Tsukamoto and E. Vlieg) the occasion to meet for discussion. The topic was the upcoming International Conference on Crystal Growth (ICCG-16) and the Fourteenth International Summer School on Crystal Growth (ISSCG-14) – both important events for the first time being held in China.

In 2009 the IUCr supported four meetings that were important for the crystal growers:

II Latin-American Symposium on Polymorphism and Crystallization of Drug and Pharmaceutical Products (LAPOLC 2009), Estância de São Pedro, Brazil, March 2009.

The Second International School on Biological Crystallization and International School on Crystallization: Drugs, Foods and Agrochemicals, Granada, Spain, May 2009.

Symposium R on X-ray Techniques for Advanced Materials, Nanostructures and Thin Films – From Laboratory Sources to Synchrotron Radiation, Strasbourg, France, June 2009.

The International Summer School on Fundamentals and Basic Methods of Crystal Growth, Brasov, Romania (<http://rocam.unibuc.ro/intschool/>), August 2009.

Commission members and consultants were involved in both Schools.

In 2009 several requests for writing letters of support for some local and international crystal growth meetings in 2010 were received [applications by M. Caffrey (Ireland), J. M. Garcia-Ruiz (Spain), N. Kulagin (Ukraine), A. Rosales-Riviera (Brazil), J. Wang (China) and A. Zappettini (Italy)]. The Commission's opinion about the relevance for the community was forwarded to the Chair of the Sub-committee on the Union Calendar.

In preparation for the upcoming Madrid Congress the Commission is represented by J. M. Garcia-Ruiz (as a Member of the International Programme Committee). Two excellent Plenary speakers, five Microsymposia and one, very innovative, satellite workshop to be held in Granada were proposed for the Congress.

On another note: It is a pleasure to congratulate P. Rudolph – a former member and consultant to the Commission – who became President of the German Organization for Crystal Growth.

As in previous years many of the Commission members and consultants (H. Dabkowska, T. Duffar, K. Kakimoto, E. Vlieg and J. Wang) were involved in the work of the International Organization for Crystal Growth (<http://www.iocg.org/>).

A list of 2009 and 2010 meetings of interest for the crystal growth community has been published on the new Commission web site (created by H. A. Dabkowska with very much appreciated help from Brian McMahon of the Chester office).

**H. A. Dabkowska, Chair**

## 4.7. Commission on Crystallographic Computing

Following its concentration in the 2008 Kyoto School on the issue of Age Concern, where a significant number of crystallographic software developers are either formally retired or soon to retire, the Commission was very active in 2009 in addressing the topic. Several articles on this theme were published in Commission *Newsletter* No. 10, November 2009 (which appeared jointly as Teaching Commission *Newsletter* No. 3). A leading article by L. M. D. Cranswick and D. Watkin appeared on the IUCr web home page. Arnel Le Bail's Source Code Museum, a collection of early crystallographic programs that are no longer maintained, was transferred in late 2009 to the Commission web site, which resides on the IUCr server, in order to secure its future and to encourage the deposition of additional packages that are not under active maintenance. L. M. D. Cranswick created a gallery of historical portraits of computational crystallographers and uploaded historical group photographs of computing schools and workshops within the IUCr photographic archive, drawing on the collections of A. L. Spek and contributors to recent computing schools.

Preparations for the Computing School to be held in Mieres, Spain, before the Madrid Congress in 2011 are well under way. A preliminary programme and list of invited speakers has been prepared. The meeting web site is live but still under construction (<http://www.iucr.org/resources/commissions/crystallographic-computing/schools/mieres2011>), as many details are still to be finalized.

**H. Powell**, Chair

## 4.8. Commission on Crystallographic Nomenclature

There was not much activity during 2009.

*Nomenclature issues.* The debate concerning the new definitions proposed by Nespolo, Souvignier & Litvin in their paper in *Z. Kristallogr.* (2008), **223**, 605, for the terms 'noncrystallographic symmetry' and 'local symmetry' has continued; the members of the Commission did not, on the whole, support these proposals.

Nomenclature of directions in reciprocal and direct space. The present wording on crystallographic nomenclature in the *Notes for Authors* of *Acta A* was discussed. It was agreed that the present wording is fine; the use of  $\langle 100 \rangle^*$  to represent a direction in reciprocal space is acceptable.

*Online Dictionary of Crystallography.* A new Editor-in-Chief, Gervais Chapuis, was appointed on 3 February 2009. His report for 2009 follows: The Online Dictionary of Crystallography (ODC) is a popular tool, which seems to be much appreciated by the scientific community. A rough estimate shows that some 320 crystallographic definitions are downloaded every day. By the end of 2009, 240 entries were included in the ODC and the last entries concerned definitions centred on aperiodic structures.

The ODC is organized similarly to a WIKI with some exceptions. Not everyone can introduce or modify the definitions. It is the task of the ODC Board of Editors to select specialists who can create or modify definitions. Currently, 46 people have been invited to contribute to the development of the ODC.

The present Board of Editors of the Online Dictionary is: André Authier, Founding Editor; Gervais Chapuis, Editor-in-Chief; Howard Einspahr, Editor for Biocrystallography; Howard Flack, Editor; Brian McMahon, Administrator.

The Online Dictionary may be consulted at the web page: [http://reference.iucr.org/dictionary/Main\\_Page](http://reference.iucr.org/dictionary/Main_Page).

**A. Authier**, Chair

## 4.9. Commission on Crystallographic Teaching

For 2009 the activity of the Commission focused on the organization of the school entitled Crystallography Online: Databases and Programs on the Bilbao Crystallographic Server, in collaboration with the Commission on Mathematical and Theoretical Crystallography. This intensive course was held in Zarauz, Spain, 21–27 June 2009, and was devoted to the use of the virtual possibilities available at the Bilbao Crystallographic Server for teaching and learning crystallography. The course comprised lessons followed by several tutorial sessions and exercises.

In September 2009 the third Zürich Crystallography School – Bring Your Own Crystals (BYOC 2009) was held, as always organized by Dr Anthony Linden and Professor Hans-Beat Bürgi with the help of Professor G. Chapuis. The School was planned in a similar way to the previous schools in the series, trying to improve the organization of the tutorials to make them more fruitful for students. The attendance was limited to about 20 students to make the ratio lecturers/tutors/students very effective.

During 2009 Commission members were involved in the organization of several didactic courses that will be held in 2010, such as the International School of Aperiodic Crystals, or the School of Fundamental Crystallography held in South Africa, and also in the organization of a Microsymposium on Teaching Crystallography, included in the Programme of the European Crystallographic meeting that will be held in Darmstadt in 2010.

Professor Katherine Kantardijeff, after the positive result obtained with sessions on teaching organized for the Osaka Congress in 2008, has collected a series of contributions and is ready to publish these in a Special Issue of *JAC*.

**P. Spadon**, Chair

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

In 2009, the Commission worked on the preparation of a Monograph for the IUCr/OUP Book Series focusing on:

The mathematical theory of symmetry as applied to the study of human artifacts and the different manifestation of the arts;

Applications of crystallographic techniques to the study of artistic artifacts in all its manifestations;

Artistic renderings of crystallographic results.

The Commission on Mathematical and Theoretical Crystallography organized a satellite on Symmetry and Crystallography in Turkish Art and Culture for ECM-25, Istanbul, Turkey, 14–16 August 2009: <http://www.lcm3b.uhp-nancy.fr/mathcryst/istanbul2009.php>.

The Commission contributed to this event by organizing one session:

Izumi Nakai: X-ray Diffraction and Fluorescence Analysis of Archaeological Anatolian Artifacts by Portable Equipments;

Manfred Schreiner: The Monetary History of the Ottoman Empire – The Silver Content of the Akce Coins During the Reigns of Murad III, Mehmed III, and Ahmed I.

At ECM-25 (<http://www.ecm25.org/>), the Microsymposium Crystallography in Art and Archaeology was chaired in partnership with this Commission, with an attractive programme:

Dario P. Benedetti: X-ray Techniques Applied to Art Authentication and Conservation;

Manfred Schreiner: The Hoard of Becin – the Silver Content of the Akce Coins and the Monetary History of the Ottoman Empire;

Lindsay Sawyer: Crystallography and Industrial Design: Past, Present and Future;

David Hradil: Mineralogical and Art-Historic Traits in the Investigation of 'Anonymous' Paintings;

Annegret Haake: The Javanese Colleagues of Karagöz and Their Dress.

In 2009, the Commission was continuously engaged in the promotion of crystallography in such areas as archaeology and art. The Commission strongly encouraged contributions to workshops and meetings on these topics, and has also started to coordinate activities and relationships between crystallographers and artists.

Some relevant upcoming meetings in 2010 are:

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>), including a one-day session entitled Around Rembrandt and his Workshop;

The Microsymposium Crystallography in Art and Archaeology of the 26th European Crystallographic Meeting (ECM-26), Darmstadt, Germany, 29 August – 2 September 2010 (<http://www.ecm26.org/>);

The Hubert Curien International School hosts the 3rd course in Structural and Molecular Archaeology entitled 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)).

The Commission maintains internet pages at <http://www.crystallography.fr/crysac/>.

**E. Doorhyée**, Chair

#### 4.11. Commission on Electron Crystallography

The year 2009 was a slightly quieter one, with much of the focus of members being towards (i) the International Microscopy Congress (IMC-17) to be held in Brazil in 2010, with seven members of the Commission involved as session Chairs, (ii) organizing the 43rd Erice Crystallographic Course, 2–12 June 2011, chaired by Professors A. Avilov, U. Kolb and L. Meshi, and (iii) the next triennial meeting.

A summer school on precession electron diffraction was held in Lille, France, 5–10 July 2009, with more than 40 participants, with a large participation by members of the Commission.

*Sub-committee on International Tables.* It was brought to our attention that Volume B of *International Tables* had been updated in 2008, but that Volume C would be completely renewed. Therefore all attention was focused on Volume C. For this, the Commission successfully functioned in 2009 as an advisory board to provide input on the sections that need to be updated, as well as providing names for potential authors to contact who are experts in the various areas. The further handling is now in the hands of the Commission on International Tables. The role of the Commission on Electron Crystallography is currently to be available for further advice, in case the suggested authors are not available for a contribution or in case the sections to be updated should be further discussed.

*Sub-committee on Software for Electron-Based CIF entries.* The Sub-committee has prepared a list of CIF entries for electrons and contacted COMCIFS. A contact person, David Brown, was appointed by COMCIFS and he will help us to build up the CIF dictionaries for electrons.

On a related topic, an invited perspective by the Chair of the Commission [*Surface Science* (2010), **604**, 878–881] has raised the issue of fully reporting atomic positions for surface structures, both those determined from DFT calculations as well as from other techniques such as LEED. The journal *Surface Science* has now changed its policy and is requiring atomic positions to be reported. Discussions are continuing both within the surface-science community as well as with other parts of the IUCr on how best to accommodate surface structural data within CIF and related formats.

*Sub-committee on the Gjøannes Medal.* The Sub-committee has received several extremely strong nominations. Based upon their recommendations, the next Gjøannes Medal will be awarded to Professors A. Howie and M. J. 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 Sub-committees on (i) Dynamical Diffraction, (ii) Software for Electron Imaging, Diffraction and Crystallography and (iii) Aberration Definitions have nothing to report.

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

Crystallography at high pressure continues to expand its presence at national and international research facilities serving the condensed-matter-science community. Most notably, 2009 saw the construction of a beamline dedicated to high-pressure research at the new synchrotron facility PETRA-III in Hamburg, Germany.

The aim of the Commission is to create the means for educating the current and future communities of high-pressure scientists in crystallographic techniques, and to provide a platform for discussion and dissemination of novel ideas and scientific achievements in this field. The main tool for achieving this goal is regular workshops in each of the two years between the triennial IUCr Congresses.

*2009 Commission workshop.* The 2009 Commission workshop, entitled Advanced Crystallography at High Pressure, was held at the Harbin Institute of Technology (HIT) in Harbin, People's Republic of China, 19–22 July 2009. The meeting assembled more than 80 scientists from 13 countries. The Local Organizing Committee was chaired by Commission member Haozhe Liu (HIT, People's Republic of China). The topics of this workshop covered the whole range of activities of the Commission and included crystal structures and phase transitions, new materials, earth and planetary science, soft and biological matter, physical and chemical properties, theory and computations, and developments in techniques for high-pressure studies at synchrotron, neutron and laboratory-based facilities. The meeting organizers paid special attention to arrange dedicated slots for talented young scientists and students. All current and immediate past members of the Commission were actively involved in the organization of the work of the meeting, and several chaired sessions during the meeting. Six oral and six poster presentations were selected to be documented in a Special Issue of *High Pressure Research*. The meeting was financially supported by the IUCr and HIT. The meeting web site can be found at [http://shp.hit.edu.cn/Meetings/2009IUCr\\_HP/Home.htm](http://shp.hit.edu.cn/Meetings/2009IUCr_HP/Home.htm).

*2009 Erice School.* From 4–14 June 2009, a total of 122 participants convened at the Ettore Majorana Centre for Scientific Culture in Erice, Italy, for the 41st Course of the International School of Crystallography, co-directed by Commission members E. Boldyreva (Novosibirsk, Russia) and P. Dera (Chicago, USA). This was the second course dedicated to high-pressure research, which followed the very successful first course, organized in 2003 by A. Katrusiak and P. McMillan. The intensive programme of the School spanned ten days and covered a variety of topics including elements of physics, chemistry, materials science, engineering, implications for geology, planetary sciences, biology and pharmaceuticals. 56 lectures were given by 46 speakers. The lectures have been grouped into several

thematic blocks: experimental techniques, phenomena, phase transitions, structures and properties, materials of technological importance, and materials and systems of biological importance, including pharmaceuticals. Five workshops were an integral part of the School and provided hands-on experience for the student participants and a chance to assimilate and test their new knowledge and skills. The School also featured a round-table discussion on the improvement of data collection and processing in high-pressure single-crystal diffraction experiments. For the 2009 Erice School, the tradition of providing live transmission of video feed over the internet has been continued thanks to the efforts of J. Irwin (USA), and K. Dziubek and A. Budzianowski (Poland). A detailed report of the 2009 School has been published in the *IUCr Newsletter* and is also available at the School web site. Proceedings of the School are being published in *NATO Science for Peace and Security Series B: Physical Science*. The School was sponsored by NATO, IUCr, ICDD, NSF, COMPRES, ECA, Kappa-psi, as well as several industrial sponsors.

*Planning for the 2010 Commission workshop.* The Commission selected Gatlinburg, Tennessee, USA, and the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL), the new national facility for neutron science in the USA, as the site of the 2010 workshop. Dr C. Tulk from ORNL will chair the Local Organizing Committee. The meeting web site can be found at <http://neutrons.ornl.gov/conf/IUCr2010/>.

*Planning for the Madrid Congress.* Dr F. Fabbiani is the Commission representative on the International Programme Committee of the Madrid Congress. The Commission proposed seven Microsymposia for the Congress, three of which are joint applications with other Commissions.

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

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

Lively discussions amongst the members and consultants of the Commission (CIMS) were mainly performed *via* email, but those members and consultants who attended the European Crystallographic Meeting held at Istanbul met in person at the occasion of the meeting of SIG-5 of the ECA. 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/>).

SIG-5 and CIMS agreed to strengthen their links. Following the suggestion given to CIMS and the Commission on Structural Chemistry (CSC) by the Executive Committee of the IUCr in Osaka to create some kind of stable link between these Commissions with distinct but related interests, both Commissions decided to exchange consultants. A. Beatty has become the representative of the CSC in CIMS, replacing L. B. McCusker who wished to resign as consultant to CIMS. The representative of CIMS in CSC is P. Mercier.

P. Mercier has become the liaison officer of CIMS for the *IUCr Newsletter*.

CIMS was involved in the following meetings, held in 2009:

International Conference on Neutron and X-ray Scattering 2009 (ICNX 2009), Kuala Lumpur, Malaysia, 29 June – 1 July 2009 (<http://online.nuclearmalaysia.gov.my/sems/icnx2009/>).

European Mineralogical Union (EMU) – School on Advances in the Characterization of Industrial Minerals, Chania, Greece, 14–18 July 2009 ([http://www.univie.ac.at/Mineralogie/EMU\\_School\\_2009/welcome.htm](http://www.univie.ac.at/Mineralogie/EMU_School_2009/welcome.htm)). CIMS consultant G. Ferraris was a speaker. CIMS member H. Effenberger is Secretary of the EMU. It is intended to further the cooperation between EMU and CIMS.

Symposium on Crystallography of Inorganic Materials at High Pressure at AIRAPT 2009, the International Conference on High Pressure Science and Technology, Odaiba, Tokyo, Japan, 26–31 July 2009 (<http://www.airapt.org/>). The Symposium was proposed by Commission member T. Nagai, who was also convener of the Symposium. CIMS consultant J. B. Parise was an invited speaker.

ICCOSS XIX – International Conference on the Chemistry of the Organic Solid State, Sestri Levante, Italy, 14–19 June 2009. Despite its name the conference was considered to provide sufficient overlap with the genuine interests of CIMS to justify support.

Conference on Clays, Clay Minerals and Layered Materials, Zvenigorod, Moscow, Russia, 21–25 September 2009 (<http://www.cmlm2009.ru>). W. Depmeier was a member of the Scientific Committee and also a speaker.

CIMS has supported the application for financial support by the IUCr for the following meeting planned to be held in 2010:

NACC-1, the 1st North African Crystallography Conference, Casablanca, Morocco, 23–26 November 2010 ([www.nacc1.univ.ma](http://www.nacc1.univ.ma)). A. Thalal and W. Depmeier are members of the Scientific Committee.

Members of CIMS were actively involved in the 25th European Crystallographic Meeting, ECM-25, Istanbul, Turkey, 16–21 August 2009 (<http://www.ecm25.org/>):

Two poster prizes related to the mission of CIMS were granted, *viz* the *Zeitschrift für Kristallographie* Prize (E. Mugaioli and colleagues, one of whom was W. Depmeier) and the EMU Poster Prize. The selection panel for both prizes consisted of H. Effenberger and G. Ferraris. A. Thalal was a member of both the Organizing and the Programme Committees. G. Ferraris and W. Depmeier chaired Keynote Lectures. O. Yakubovich and M. Nespolo chaired Microsymposia. Oral presentations were given by H. Effenberger, G. Ferraris and W. Depmeier.

CIMS suggested that after the retirement of H. Fuess as an officer of the Executive Committee of the ECA its Focus Area 2 (Materials and Minerals) was under-represented. W. Depmeier was proposed by six councillors as a candidate for one of the open positions, and finally elected during the council meeting. His special task in the Committee is, amongst others, the relationship with the IUCr, its Regional Associates and national organizations.

Some additional personal achievements:

O. Yakubovich has given an invited lecture at the XXVIII Memorial Workshop dedicated to Academician N. V. Belov (Moscow, 18 December 2009): Defects' Ordering as a Parameter of Crystal Structure Stability (Illustrated by the Silicate Minerals).

Following his presentation at ECM-25, W. Depmeier was invited to give three lectures in Austria covering the same topic, *viz* Minerals as Advanced Materials.

G. Ferraris edited a special themed issue of *Zeitschrift für Kristallographie* entitled Layered Materials: Structure and Properties, with contributions by J. Rocha and colleagues, and by W. Depmeier (<http://www.atypon-link.com/OLD/toc/zkri/224/5-6>). The front-cover picture was by W. Depmeier and one of the back-cover pictures was by J. Rocha and his colleagues. G. Ferraris has been appointed Series Editor of the EMU *Notes in Mineralogy*; the series includes volumes related to the EMU Schools.

W. Depmeier was elected a member of the International Programme Committee of the Madrid Congress.

D. Pushcharovsky continued to act as Assistant Editor of the *European Journal of Mineralogy*, *Zapiski RMO (Proceedings of the Russian Mineralogical Society)* and *Crystallography Reports*.

**W. Depmeier**, Chair

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

*Scientific activity in 2009.* During 2009 the Commission (MaTh-Cryst) organized two main activities:

Crystallography Online: International School on the Use and Application of the Bilbao Crystallographic Server was held at the Hotel Aisia Emperatriz Zita in Lekeitio, a small fishing town on the coast of the Basque Country, about 60 km west from Bilbao, 21–27 June 2009. The School was supported by the Spanish National Committee for Crystallography, the IUCr Commission on Crystallographic Teaching and ECA Special Interest Group No. 5: Mineral and Inorganic Crystallography. Participants were lodged at the same venue and could profit from evening sessions (that lasted until 11 p.m.) for additional exercises and question-and-answer sessions with the lecturers. The School was attended by 56 participants from 15 countries. Topics of the School were Symmetry Databases for Point and Space Groups, Applications of Group–Subgroup Relations Between Space Groups, Crystal Structure Transformations and Alternative Descriptions, Solid-State Physics and Chemistry Applications of Group Theory, Selection Rules in Spectroscopy: Phonon Selection Rules, Structural Pseudosymmetry, Symmetry-Mode Analysis of Ferroic Structures, Domain-Structure Analysis, Structural Phase Transitions, and Symmetry in *Ab Initio* Calculations. Didactic material from the School is available from the web site of the Bilbao Crystallographic Server (<http://www.cryst.ehu.es>).

A satellite conference of the 25th European Crystallographic Meeting (ECM-25), Istanbul, Turkey, 14–16 August 2009, devoted to Symmetry and Crystallography in Turkish Art and Culture, organized in cooperation with the Commission on Crystallography in Art and Cultural Heritage. The conference was attended by 34 participants from 17 countries. The first day was devoted to the analysis of symmetry, patterns and meaning in Anatolian monuments and crafts; the second day concerned experimental studies of Anatolian art and coins and was completed by a ‘Do it yourself’ workshop. On the third day the participants could enjoy a guided excursion to Turkish mosques, the Turkish and Islamic Arts Museum and The Sokollu Mehmet Pahsa Camii. Collected Abstracts and didactic material from the presentations are available from the conference web site (<http://www.crystallography.fr/mathcryst/istanbul2009.php>).

*Scientific Activities in 2010 and later.* Planned activities include, at present:

A School on Fundamental Crystallography, Bloemfontein, South Africa, 12–16 April 2010 (see <http://www.crystallography.fr/mathcryst/SouthAfrica2010.php>).

Two Summer Schools on (i) Topological Crystal Chemistry: Theory and Practice and (ii) Irreducible Representations of Space Groups, in Nancy, France, 21 June – 2 July 2010 (see <http://www.crystallography.fr/mathcryst/nancy2010.php>).

A satellite conference of ECM-26, Darmstadt, Germany, 27–29 August 2010 (see <http://www.crystallography.fr/mathcryst/darmstadt2010.php>).

A School on Fundamental Crystallography, Montevideo, Uruguay, 29 November – 4 December 2010 (see <http://www.crystallography.fr/mathcryst/montevideo2010.php>).

Several other activities have been proposed and are currently under discussion:

A school in Tunisia, probably in January 2011, with Professor Mongi Debbabi as local organizer.

A workshop on crystallographic software and its mathematical crystallographic background, Tokyo University, Japan, May 2011, with local organizers S. Ito and K. Fujimoto, details to be confirmed.

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

A workshop on colour symmetry and crystalline networks in Manila, the Philippines, organized by Commission member R. Felix.

A contribution to an American meeting for which W. L. Duax has promised to help 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 three first 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 the participants at 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 on Geometric Algebra in Crystallography, currently under consideration in the IUCr/OUP Book Series Monographs in Crystallography.

*Web-related activities.* Didactic pages directly hosted on our server are so far limited to twinning and OD structures and we regret the lack of activity and contribution from members and consultants to expand the existing pages and to create new ones.

**M. Nespolo**, Chair

#### 4.15. Commission on Neutron Scattering

The main event for the neutron community in 2009 was the Ninth International Conference on Neutron Scattering (ICNS), Knoxville, Tennessee, USA, 3–7 May 2009. This Conference, organized by the Neutron Scattering Society of America, served as a privileged discussion forum between neutron users and specialists in neutron techniques from all over the world. The Committee reviewed over 650 Abstracts submitted for and integrated over 240 talks, including plenary and invited talks, into ten topical areas and 41 sessions. Over 650 registrants from six continents and 29 countries attended the Conference. The principal accomplishments of neutron scattering in the past three years were highlighted, and a consensual final message was the importance to reach the broader scientific community and the major role of neutron scattering in future challenges in energy, climate, health and beyond.

In 2009 the landscape of neutron sources attained a widespread distribution and unprecedented performances, offering particularly attractive opportunities for the neutron science community.

Remarkable upgrades have taken place at many facilities. The ILL (France) has completed the first phase of its Millennium Programme, and the second phase is well underway and has already delivered upgraded instruments, giving an improvement factor of 20 in the average detection rate across the instrument suite since the Programme started. After five years of construction, the ISIS (UK) Second Target Station has opened its doors for the first scheduled experiments. The recently refurbished High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL, USA) operated for its second full year at full power (85 MW). Simultaneously, major infrastructure projects are being commissioned. The Spallation Neutron Source (SNS), also at ORNL, broke the 1 MW barrier for the first time. At J-Parc (Japan) several instruments of the Materials and Life Science Experimental Facility started on-beam commis-

sioning to be ready to open their user programme in the near future. The scheduled stage of the modernization of Reactor IBR-2 (JINR, Dubna, Russia) was finished in 2009 and the start up of the reactor IBR-2M is planned at the end of 2010. In Australia, ANSTO obtained Federal Government funds for the addition of three neutron spectrometers at the OPAL research reactor, with completion planned for 2013.

In 2009 there was also clear progress in future projects such as the site decision for the future 5 MW long-pulse European Spallation Source (ESS) to be built in Lund, Sweden.

To promote access in view of the optimization of this impressive range of cutting-edge techniques, it is necessary to reach and attract the widest possible scientific community and a great effort continues to be undertaken to train new neutron users with significant participation of members of this Commission. No less than 15 dedicated schools and education initiatives were held in 2009. Additionally, several meetings were organized that frequently conjugate techniques that might be considered as competitors yet are complementary, like synchrotron X-rays. Some of these are: the workshop Neutrons and X-rays meet Biology, Berlin, Germany; the XIV International Conference on Small-Angle Scattering (SAS 2009), Oxford, UK; Polarized Neutrons and Synchrotron X-rays for Magnetism 2009, Bonn, Germany; or the II Higher Education Courses for CIS countries (former USSR Republics) Synchrotron Radiation and Neutron Research of Nanosystems in Dubna and Moscow, Russia. The second Asia–Oceania Neutron Scattering Association neutron school, which focused on applications in nanoscience, was hosted by ANSTO in August 2009.

The International Conference on Neutron and X-ray Scattering 2009 (ICNX 2009), Kuala Lumpur, Malaysia, was supported by this Commission and sponsored by the IUCr. An International Conference on Neutrons in Biology, organized by Commission member P. Langan, was held in Santa Fe, USA, October 2009, to review recent progress and to celebrate B. Schoenborn's many contributions to neutron protein crystallography. The Proceedings will be published in *Acta Crystallographica*. In October 2009 the former Chair of this Commission, M. Steiner, was elected as the new Chair of the European Neutron Association.

In 2008, the Commission sadly felt the absence of one of its members. Professor Robert Bau died on 28 December 2008. He was a distinguished researcher in the field of X-ray and neutron diffraction crystallography and an active member of this Commission. He will be missed by the Commission and the whole neutron community.

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

#### 4.16. Commission on Powder Diffraction

A member of the ECA EPDIC Committee is currently also a member of the CPD, but the Chair believes that better communication with some of the smaller communities is a worthwhile endeavour. To this end the CPD Chair contacted the Co-Chairs of the Australian X-ray Analytical Association (AXXA) as a first step and subsequently wrote an article on the history and activities of the CPD for the December 2009 issue of the *AXAA Newsletter*. The CPD information poster produced in late 2008 was exhibited at a number of meetings in 2009, including the ICDD Spring Meeting, the ACA meeting in Toronto and the Denver X-ray Conference. Thanks are due to L. M. D. Cranswick for printing the posters and looking after the display at the ACA meeting (amongst many other things).

The 2009 CPD meeting was held as planned during the ACA meeting in Toronto, Canada. Attendance was fairly low but a number of issues were discussed. These included the proposed new volume on

powder diffraction of *International Tables*. The 2010 meeting of the CPD is scheduled to be held during the EPDIC meeting in Darmstadt, Germany. It is likely that the European location should result in an improved attendance. During 2009 the CPD received six applications for Commission support towards IUCr sponsorship for meetings and workshops, of which five were supported after consultation with the Commission membership. It is notable that the number of applications was very heavily weighted towards European meetings with the only exception being a meeting in South America. This geographical bias is a concern and obviously much remains to be done in educating meeting organizers about possible IUCr support.

The CPD web site was moved from servers at the Rutherford Appleton Laboratory to what hopefully will be a permanent home at the IUCr in Chester (<http://www.iucr.org/resources/commissions/powder-diffraction>). The Chair would like to thank Brian McMahon (IUCr, Chester) for his considerable assistance in setting up the new web site and transferring the existing content. In this process some pages on the Quantitative Phase Analysis Round Robin were retrieved from archives and are now available again, including all the files (and there are lots of them) for download. Some new content was added in the form of suggested hands-on 'self-test' materials for organic structure solution from powder diffraction data. Two of the three materials (aspirin and sucrose) should be found in most households so availability and cost will not be a problem. The third (caffeine) is readily sourced from regular chemical suppliers at minimal cost. The CPD Chair had some discussions with representatives from the Cambridge Structural Database at the Toronto ACA about criteria for assessing the quality of structures determined from powder data. There were discussions within the CPD membership about holding a meeting on validation of structures from powder diffraction data, possibly as a satellite to the Madrid Congress. However, the close proximity of a major powder diffraction meeting in Erice was seen as a major impediment to attendance at a satellite meeting as well as the main IUCr Congress. There is a consensus that a meeting on structure validation would be valuable, and possible dates and venues will be revisited later, possibly for some time in 2012.

**P. Whitfield**, Chair

#### 4.17. Commission on Small-Angle Scattering

*Commission meetings and communication.* Commission members communicated by e-mail or during personal meetings at national and international conferences. Most Commission members were present at the International Conference on Small-Angle Scattering in Oxford (SAS 2009), and the Commission held a closed meeting during the conference. During the meeting several topics were discussed, including the possible development of glassy carbon as a SAXS and SANS intensity calibration reference standard, and the use of data format standards. During the year, routine communications were accomplished by e-mail.

*Activities.* The most prominent event of 2009 was SAS 2009. Most of the Commission members served on the International Advisory Committee. The Conference was attended by 434 participants from 32 countries. There were 452 contributed presentations of which 144 were oral presentations and 308 were poster presentations.

The scientific programme of the Conference contained ten Plenary Lectures from various scientific fields and 29 sessions. The sessions covered polymers, various aspects of instrumentation, biological systems, colloids, membranes and bilayers, ceramics, glasses and porous systems, magnetic systems, metallic systems, theory and

modelling, fibre diffraction and hierarchical systems, liquid crystals and rheo-SAS, surfaces and interfaces, environmental science, imaging, dynamical techniques, and time-resolved techniques.

In coordination with the organizers of SAS 2009, the Commission made a call to the SAS community to prepare applications from scientific institutions willing to host the next SAS Conference in 2012. Together with the SAS organizers, the Commission formed a Committee with the task of evaluating the bids. The members of the Committee were representatives of the SAS community, previous and current SAS Conference organizers, and members of the Commission. The Evaluation Committee suggested that the sites and organizers for the next two Conferences should be decided in Oxford to allow longer-term planning and ensuring continuity of the Conference series. The Evaluation Committee also provided feedback on the bids. Applications from Sydney, Berlin and Knoxville were received and presented at SAS 2009 in a specially devoted session. The suggestion of selecting Conference sites and organizers for the Conferences in 2012 and 2015 was well received by the Conference participants. After a ballot by the participants, Sydney, Australia, was selected as the venue of SAS 2012, and Berlin, Germany, was selected as the venue for SAS 2015.

In the period up to the SAS 2009 Conference, the Commission was consulted on various matters by the Conference organizers and provided advice. The Commission members were also very active during the Conference and were members of the Award Committees. The Prize for Lifetime Achievement in SAS (the 'Andre Guinier Award') was awarded to Professor Dr Vittorio Luzzati, Emeritus Research Scientist, Centre de Génétique Moléculaire du CNRS, Gif-sur-Yvette, France, for his long and distinguished career in X-ray scattering.

As a consultant of the Commission, D. Svergun was involved in a discussion on the principle of the publication of Proceedings of SAS Conferences, initiated by the organizers of the SAS 2012 meeting in Sydney. The Commission has also already provided consultancy on a number of additional matters to the organizers of the SAS 2012 meeting.

Professor J. Trehwella is a member of the International Programme Committee of the Madrid Congress.

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

N. Yagi conducted a beamline practice on SAXS during 10–12 July at the SPring-8 summer school. Y. Amemiya presented a lecture on small-angle scattering and N. Yagi conducted a beamline practice on SAXS at the Asia–Oceania Forum for Synchrotron Radiation Research (AOFSSR) Cheiron school. This school was organized by the AOFSSR and held at SPring-8, 29 September – 8 October.

R. Serimaa gave a lecture course entitled Synchrotron Radiation in Materials Research at the Department of Physics, University of Helsinki, January–May 2009 with 2 × 2 lectures per week. R. Serimaa also contributed with a lecture entitled Studies on Nano- and Microstructures using X-rays at the international PhD course Biosynthesis, Composition and Degradation of Plant Cell Walls, Helsinki University, 26 August 2009.

V. V. Volkov and colleagues from the Laboratory of Small-Angle Scattering of the Russian Academy of Sciences gave a 32-hour lecture course entitled Methods for Small-Angle Scattering in Investigation of Nanostructured Media during the spring semester of 2009 for students of the Physical Department of Moscow State University. They also conducted a six-hour training course (Practicum) for the students. The topic of the Practicum was Determination of Shape of Nanoparticles from Small-Angle Scattering Data. During the

training, the students obtained knowledge about the possibilities and limitations of the SAS method, performed numerical experiments in data treatment and interpretation, and learnt to solve ill-posed inverse problems in physics. In total, 23 students were involved in 2009.

D. Svergun gave the following lectures: ATASAS Overview and Tutorial at the SAXS Workshop, SSRL, Stanford, USA, April 2009; *Ab initio* and Rigid Body Methods, and SAXS Remote Data Collection at the Biological SAXS Course and Workshop, Singapore, May 2009; Biological Small-Angle Scattering from Solutions: What Does it Yield? at the Practical Workshop on Characterization of Protein Complexes in Structural Biology, Hamburg, Germany, July 2009; Basics of SAXS and *Ab Initio* Methods at the Biological SAXS Course, SLS/Villigen, Switzerland, December 2009.

In connection with the Sixth Nordic Workshop on Scattering from Soft Matter, January 2009, J. S. Pedersen organized a Tutorial School on Scattering Methods Applied to Soft Matter, with more than 40 participants. He also contributed with lectures and a tutorial on small-angle scattering at five different courses at Aarhus University. He is also 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.

*Community-building activities.* The members of the Commission continued to contribute to the widening of the community of SAS users in their laboratories and large-scale facilities. They also took part in conferences, workshops and meetings devoted to the future development of SAS.

D. Svergun worked as a deputy Chair of Working Group V (Complementary Methods) of the European INSTRUMENT initiative. J. S. Pedersen has acted as a consultant of the Working Group.

Y. Amemiya acted as the President of the Japanese Society for Synchrotron Radiation Research from January to September 2009.

A. Allen is involved in several initiatives at NIST. Following the NIST-hosted canSAS V workshop in 2007, progress has continued in 2009 on development of standardized portable 1D data formats (both IUCr SAS CIF and SAS NeXus), priorities for developing candidate standards for SAXS and SANS, as well as more general standardization issues. A very successful session on this subject was held at the SAS 2009 conference. NIST continues to pursue development of a small-angle X-ray diffraction wavelength standard reference material (SRM). Also, an international round robin exploring the potential of glassy carbon as a SAXS (and possibly SANS) intensity standard reference material was completed in 2009. A publication on glassy carbon standards for SAXS publication has been prepared and the work on NIST Reference Materials for nanoparticle size continues.

P. Thiyagarajan is Programme Manager of Neutron Scattering at the Office of Basic Energy Sciences, US Department of Energy, and in his work he promotes the application of SAS techniques in relevant research areas and thus contributes to enlarging the scientific community employing the techniques.

G. Kostorz gives occasional invited talks on small-angle scattering.

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

The small-angle scattering technique has been promoted in several lectures by D. Svergun:

Introduction to SAXS and Overview of SAXIER presented at the Workshop on New Applications of SAXS, Liverpool, UK, 16 February 2009.



Small-Angle Solution Scattering as a Complementary Method to Macromolecular Crystallography presented at the American Crystallographic Association Meeting, Toronto, Canada, 27 July 2009.

Small-Angle Scattering from Biomacromolecular Solutions: Automation, Interpretation, Applications presented at the International Small-Angle Scattering Conference, Oxford, UK, 15 September 2009.

Small-Angle Solution Scattering as a Tool for Systems Biology presented at the International Conference on Structural Systems Biology, Hamburg, Germany, 24 September 2009.

Recent Advances in Biological Small-Angle X-ray Scattering from Solutions presented at the Pittsburg Diffraction Society Conference, Athens, GA, USA, 29 October 2009.

Biological Small-Angle X-ray Scattering, a Rapid Method to Study Overall Structure and Conformational Changes presented at Protein Structure Determination for Industry, Basel, Switzerland, 10 November 2009.

Structure Analysis of Biomacromolecular Solutions by Small-Angle X-ray Scattering presented at the GRASP Conference, Montreal, Canada, 23 November 2009.

In addition to these lectures, Commission members have presented a large number of lectures at international conferences and meetings. At the International Conference on Small-Angle Scattering in Oxford, J. Trehwella gave the Plenary Lecture Protein Complexes in Biomolecular Signalling: the View from Small Angles and J. S. Pedersen gave the Plenary Lecture Analysis of Small-Angle Scattering Data from Complex Structures using Monte Carlo Integration Schemes: Protein Decorated Micelles and Perforated Membranes.

*Consultant activities.* D. Svergun and J. S. Pedersen served as members of the Scientific Committee at Geesthacht Neutron Scattering Facility (GeNF) at GKSS Research Centre, Geesthacht, Germany. D. Svergun is also a member of the Scientific Advisory Committee of Diamond, UK.

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

Y. Amemiya and N. Yagi acted as technical advisors for the new undulator SAXS beamline at SPring-8 (BL03XU), which was built by a consortium of 19 chemical/polymer companies.

V. V. Volkov and the SAS Laboratory at the Institute of Crystallography provided consultancy specialists for about ten scientific institutes in Russia, in part, from the Institute of Molecular Biology, the Institute of Physical Chemistry, the Institute of Elemento-Organic Compounds, the Institute of Inorganic Chemistry *etc.* In total, about 400 samples were investigated with, for example, self-organized polymers, organic media with metal nanoparticles, liquid crystals, magnetic fluids, clusters of DNA complexes, and proteins in solution (M1 protein from flu virus, complexes of cytochrome with different ligands, shaperonin).

*Organizational activities.* N. Yagi acted as a Chair of the Organizing Committee of the SPring-8 Summer School. Y. Amemiya was a council member of the AOFSTR and N. Yagi was a member of the Local Organizing Committee of the Cheiron school. In addition, N. Yagi was an organizer of the SAS session in AsCA '09 (Joint Conference of the Asian Crystallographic Association and Chinese Crystallography Society) held in Beijing, People's Republic of China, 22–25 October.

R. Serimaa was a member of the 2009 EMBL Priority Committee (Synchrotron Radiation Research of Biological Systems, Hamburg Outstation), and is a board member of the Finnish Synchrotron Radiation User's Organization (FSRUO). FSRUO was founded in 2009 and its main purpose is to promote and represent inter-

disciplinary basic and applied scientific research using synchrotron radiation and free electron lasers in Finland.

The group of D. Svergun co-organized several courses on small-angle scattering around the globe, including: BioSAXS course, SLS/Villigen, Switzerland, December 2009; the SAXS part of the Protein Complexes Course, Hamburg, Germany, June 2009; BioSAXS course, Singapore, May 2009; and BioSAXS course, SSRL/Stanford, USA, April 2009. D. Svergun and members of his group gave lectures and tutorials at these courses.

J. S. Pedersen organized the Sixth Nordic Workshop on Scattering from Soft Matter that took place in Aarhus, Denmark, in January 2009 with 80 participants. He is also a member of the Organizing Committee of the 10th European Summer School entitled Scattering Applied to Soft Condensed Matter, Bombannes, Gironde, France, June 2010.

*Technical activities.* A. Allen and G. Kostorz have continued to serve as Co-editors for the *Journal of Applied Crystallography*. In addition, G. Kostorz is Editor-in-Chief of IUCr journals.

N. Yagi designed a small-angle camera for BL03XU at SPring-8.

V. V. Volkov and the staff of their SAS laboratory have participated in the designing of the new universal SAS station in the Kurchatov Institute of Synchrotron Radiation in Moscow, which is planned to be built at the synchrotron source.

A. Allen has continued his involvement in the development of Reference Materials. Following the successful issue in 2008 of three nanoparticle Reference Materials: NIST RMs 8011, 8012 and 8013 (for, respectively, 10 nm, 30 nm and 60 nm gold nanoparticles in aqueous suspension – for use primarily in biological research applications), NIST has continued to work on developing TiO<sub>2</sub> and (possibly) Ag nanoparticle Reference Materials (both for biomedical and for environmental health and safety applications). As with the Au nanoparticle Reference Materials, SAXS/USAXS measurements are likely to be involved. A research paper on glassy carbon as a potential SAXS intensity standard was accepted for publication in *Metallurgical and Materials Transactions*. A. Allen contributed to the drafting of a possible ISO TC24/SC4 (particle size committee) SAXS particle size standard. Activities are ongoing.

D. Svergun's group implemented an automated pipeline for a biological solution SAXS experiment and data analysis at the EMBL synchrotron SAXS beamline (DESY, Hamburg, Germany). This opened the way for full automation of the SAXS experiment and even for remote access to the beamline. At 12:00 CET on 26 May 2009, EMBL Hamburg linked up to the Nanyang Technological University's (NTU) School of Biological Science (SBS) in Singapore to conduct the world's first remote synchrotron small-angle X-ray scattering experiment. Members of the SAXS group from EMBL Hamburg travelled to Singapore to give a course on biological SAXS to students from the SBS. The first remote SAXS experiment was scheduled as part of the course and was watched by about 60 students, professors and local dignitaries.

**J. S. Pedersen, Chair**

#### 4.18. Commission on Structural Chemistry

The activities of the Commission (CSC) in 2009 were opened with a wide and vivid discussion, carried out by e-mail exchanges, that followed the comments made during the CSC meeting at the Osaka Congress. The Commission had been stimulated to consider how to relate with other Commissions that could express a potential partial overlap of interests, such as the Commission on Inorganic and Mineral Structures (CIMS) and the Commission on Crystallographic Teaching (CCT). After recognizing the great importance of inter-

disciplinary connections between Commissions, expressed also by the proposal for several joint Microsymposia involving CSC in the Osaka Scientific Programme, the CSC suggested the building of permanent links between related Commissions by exchanging consultants. Consequently, CSC member A. Beatty was appointed as consultant for CIMS, and conversely CIMS member P. Mercier was appointed as consultant for the CSC. The CSC consultant P. Mueller was also added to the consultants for the CCT. This arrangement has proved very effective, since in many instances information was passed smoothly between Commissions, for instance in redirecting requests of support for scientific and educational events.

The Commission has also been involved in the preparation of the proposals for the Scientific Programme for the Madrid Congress. Three members of the International Programme Committee are related to the interests of CSC: R. Kuroda, L. Nassimbeni and T. N. Guru Row. The CSC has submitted to them a wide list of titles for Microsymposia that are of relevant interest in the CSC field, together with potential names for Chairs and keynote speakers.

During 2009 two scientific events strongly related to structural chemistry have been supported by the CSC:

Indaba 6, Berg-en-Dal, Kruger National Park, South Africa, 30 August – 4 September 2009, whose organization was discussed among CSC members.

ICCOSS XIX (International Conference on the Chemistry of the Organic Solid State), Sestri Levante, Genoa, Italy, 14–19 June 2009.

The CSC has also approved the endorsement of other events that will take place in 2010:

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 Chemical Crystallography Workshop, Canada Analytical X-ray (MAX) Diffraction Facility, McMaster University, Hamilton, Ontario, 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 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 (X-FELs) and energy recovery linacs (ERLs). The Commission is very pleased to note the enormous progress made by several XFEL projects including the European XFEL and FLASH in Hamburg, Germany, LCLS in Stanford, USA, and SCSS in Harima, Japan, as well as ERL R&D projects in Cornell, USA, and Tsukuba, Japan. Detector developments were also accelerated in preparation for these next-generation light sources.

Louis Delbaere, who was a member of the Commission until he joined the IUCr Executive Committee in 2008, stayed as a liaison between the Commission and the Executive Committee until October 2009 when he passed away, which deeply saddened all the Commission members.

The Commission members usually communicate *via* e-mails, but throughout the year subsets of the Commission members met at international conferences to discuss relevant and current issues of the Commission. For example, in September 2009 in Melbourne, Australia, we met during SRI 2009 to discuss possible collaboration with the Commission on XAFS to co-organize a workshop on XAFS

standardization of experimental protocols and data analysis. The workshop has been proposed for 2010 but is currently pending until appropriate financial support from various sources is secured. It is anticipated that this will held in early 2011.

The Commission continued to support the RapiData course on automated data collection at NSLS, Brookhaven National Laboratory, USA, 11–16 April 2010. In particular it supported the participation of Latin-American students.

The fourth AOFSSR (Asia–Oceania Forum for Synchrotron Radiation Research) workshop was held in Shanghai, People's Republic of China, 31 November – 1 December 2009. Special issues focused on AOFSSR were published in *Synchrotron Radiation News* with articles featuring developments in Asia and Oceania. The third Cheiron School was held at SPring-8, Japan, 2–11 November 2009, and was attended by 55 young scientists and engineers from nine countries: Australia, People's Republic of China, India, South Korea, New Zealand, Singapore, Taiwan, Thailand and Japan. Members of the Commission were involved in the programme preparation and lecturing on both occasions.

Members of the Commission were involved in the triennial international Synchrotron Radiation Instrumentation meeting in Melbourne, Australia, September 2009. In particular, R. Garrett served as the Chair of the Technical Programme Committee of which H. Graafsma was also a member. G. Kulipanov and S. Wakatsuki were members of the SRI 2009 International Advisory Committee. The meeting attracted 681 delegates drawn from 28 countries, and highlights included the remarkable progress in the FEL sources. Half a year later, 15–18 February 2010, the Biology and Synchrotron Radiation (BSR), another triennial international meeting, will be held in Melbourne, Australia, and again members were involved in the planning of the meeting during 2009. In particular, S. Wakatsuki, as a member of the International Advisory Committee, arranged a timely invitation for Professor Ada Yonath to the meeting as a plenary speaker of BSR and Medical Application of Synchrotron Radiation (MASR), a concurrent international workshop, shortly after the announcement of the Nobel Prize in Chemistry 2009 for her work on ribosome structures.

C. Nave played an active role in the preparation of the 6th Radiation Damage Conference, Stanford, CA, USA, March 2010. This is a biannual international meeting to discuss the fundamental processes of radiation damage in biological samples, implications for structure interpretation and exploitation of radiation damage in structural determination. A Special Issue in *Journal of Synchrotron Radiation* is being prepared from the talks in the workshop.

The Commission recommended S. Pascarelli of the ESRF as a member of the International Programme Committee of the Madrid Congress to promote synchrotron-related topics and speakers with particular emphasis on LINAC-based light sources, detectors and instrumentation, coherence, inelastic X-ray scattering, materials under extreme conditions, surfaces and interfaces, combined methods, structural biology, cultural heritage *etc.* The Commission also discussed joint sessions with the Commission on XAFS.

In response to Professor Larsen's concern on how to improve the recognition of beamline scientists of macromolecular protein crystallography beamlines, the Commission started discussions on the role of staff scientists and how best their work could be acknowledged and credited by the community. These discussions were carried out *via* e-mail exchanges as well as face-to-face meetings at SRI and BSR/MASR. At the latter conference, in particular, some of the Commission members attended a meeting organized by Professor Larsen to discuss the issue with protein crystallography beamline scientists worldwide. The Commission considers that it is indeed a

serious issue not only in structural biology but also in the other areas of synchrotron science and there is a strong need to introduce some effective measures to ameliorate the situation. The discussion is continuing with some new developments such as a possible new form of short publication to disseminate information on beamline characteristics.

**S. Wakatsuki**, Chair

#### 4.20. Commission on XAFS

*Commission organization.* In order to further increase its efficiency, the Commission (CXAFS) defined an internal organization in line with the general statement of principles regarding IUCr Commissions. A Steering Committee has been formed by I. Ascone (Chair), C. T. Chantler (Secretary) and B. Hedman. Two CXAFS consultants (S. S. Hasnain and A. M. Molenbroek) have been assigned to the Steering Committee for the preliminary formulation of plans.

Moreover, CXAFS has created a Working Group on XAFS Nomenclature in order to propose contributions to the IUCr Online Dictionary. Participants have been selected taking into account their high profile, their field of activity and their regional location. To ensure a clear connection between CXAFS and IXAS (International X-ray Absorption Society), many members come from both communities.

P. Glatzel (CXAFS and IXAS) was nominated to coordinate this Working Group. Other members are: C. T. Chantler (CXAFS), M. Newville (IXAS), J. Rehr (Theory), Tsun-Kong Sham (IXAS and Theory), R. Strange (Biology) and A. M. Molenbroek (CXAFS).

*Commission meetings and communication.* A Commission meeting was held in the Palazzo Ducale, Camerino, Italy, 27 July 2009, during the International XAFS Conference, XAFS 14. Moreover, several discussions took place among the following Commission members during this Conference: I. Ascone, K. Asakura, G. Azavedo, F. Boscherini, C. T. Chantler, P. Glatzel, B. Hedman and F. Jalilvand. A detailed report has been sent to the IUCr Executive Committee.

The ISRP-11 International Symposium in Melbourne, Australia, was also an opportunity to develop Commission activity (participants I. Ascone, C. T. Chantler and P. Glatzel).

Many meetings and discussions among members of the Working Group on XAFS Nomenclature were also organized by P. Glatzel in July (during XAFS 14 in Italy) and September (during the ISRP-11 Symposium, in Melbourne, Australia). In Italy the participants were P. Glatzel, C. T. Chantler, M. Newville, J. Rehr, Tsun-Kong Sham and R. Strange; in Melbourne, the participants were P. Glatzel, C. T. Chantler, J. Rehr and Tsun-Kong Sham.

Moreover, Commission members communicated by e-mail or during personal meetings at other national and international conferences.

*Organization of congresses and workshops.* CXAFS members contributed to the increase of interaction among XAFS researchers and other groups in the IUCr, through the organization of three congresses/meetings. F. Boscherini co-organized the meeting on X-ray Techniques for Advanced Materials, Nanostructures and Thin Films: from Laboratory Sources to Synchrotron Radiation. This meeting was held in the framework of the European Materials Research Society Spring Meeting, Strasbourg, France, 8–12 June 2009, and was endorsed/supported by CXAFS and three other IUCr Commissions (SAS, Synchrotron Radiation, and Crystal Growth and Characterization of Materials).

CXAFS organized Symposium S3 of XAFS 14 on the Complementarity of XAS and Diffraction Techniques. This was held on 29

July 2009 in the morning, allowing a high attendance. Lectures were given by well known experts in the field, including S. Billinge, D. Bowron, H. Renevier, R. Strange and V. Streltsov. This was the first joint symposium organized by CXAFS and IXAS during an XAFS Conference. Moreover, during the plenary section, at the end of XAFS 14, I. Ascone presented the Commission's activity to about 500 delegates of the XAFS community.

IUCr sponsorship of XAFS 14 is acknowledged with sincere thanks. During the July meeting, CXAFS decided that similar initiatives should continue and that contacts should be maintained with the organizers of XAFS 15.

Endorsed activities also included the Eleventh International Symposium on Radiation Physics (ISRP-11), Melbourne, Australia, 21–25 September 2009 and the related International Workshop, Melbourne, 26–27 September 2009, linked to both ISRP-11 and to the SRI conference.

These two events, organized by C. T. Chantler, were also extremely useful for exchanges between members. The Symposium presented new fundamental experiments and applications across biomedical, chemical and engineering fields and in border protection, geothermal and many other areas. Subjects that were once regarded as fundamental research in experimental and theoretical atomic and molecular physics now make vital contributions to developing new materials, forensic sciences, pharmaceuticals and metrology standards. Emerging fields included intense X-ray sources, imaging techniques, instrumentation and synchrotron beamlines. Numerous bursaries were provided for young scientists to attend from first-world, regional and third-world countries. Over 305 Abstracts, 200 participants and 38 countries were represented; this was the second largest of the series. A robust and vigorous Workshop on Advances in Analytical Techniques with sub-themes Geology, Conservation Science, Forensic Science, Border Technology and Environmental Science held sessions on XRF and XRD, XAFS, Raman, IR, SEM and imaging. ISRP-11 was coordinated by the International Radiation Physics Society and the School of Physics, University of Melbourne, supported by DEST, Australia, and the Australian Synchrotron. The Opening Address was attended by the Victorian Cabinet Secretary, Mr Tony Lupton; the Vice-Chancellor, University of Melbourne, Professor Glyn Davis; and Professor Dudley Creagh, University of Canberra and President of the IRPS.

The Commission has planned to endorse and support the organization, in 2010, of the following meetings:

BioXAS Study Weekend, satellite meeting of Biology and Synchrotron Radiation Conference, Melbourne, Australia, 14–15 February 2010.

The symposium Synchrotron Radiation: Emerging Techniques and Applications, co-organized by K. Asakura during PACIFICHEM 2010 (Pan Pacific Chemical Society Meeting), Hawaii, 15–20 December 2010.

The Commission has also decided to organize a workshop in 2010 on Improving the Data Quality and Quantity for XAFS Experiments, in cooperation with the Commission on Synchrotron Radiation. This interaction is considered very important, particularly in view of the organization of the Madrid Congress. Several actions have been undertaken to make progress on this project: (a) two meetings in September between the Chairs of the two Commissions were held in Melbourne to define jointly the aims of the workshops; (b) definition of the programme, including suggestions from both Commissions; (c) a detailed budget; (d) contacts with possible hosting laboratories (ESRF and DESY). The preparation of this workshop will continue in 2010.

*Web site.* For many years, F. Boscherini has been in charge of the Commission's web site, hosted by the University of Bologna, Italy. The part concerning the compendium of XAFS beamlines has been updated. In 2009, F. Boscherini, with the agreement of the IUCr and CXAFS, has transferred the site to the centralized IUCr site. The advantages of this are multiple: the web site is officially maintained, the procedure for modification is easier, and finally this should encourage the involvement of other Commission members to contribute to its development.

*BioXAS data deposition at JSR: data interchange format.* The Commission has been requested to develop the project concerning XAFS data deposition. Members should define relevant information on data (format, file size and total number of files) and the XAFS community should be consulted, involving the International XAFS Society. Technical aspects have been examined and different solutions proposed. However, some concerns have been expressed on the procedure used for data deposition. Given the complexity of this item, which involves many scientific communities, the discussions will continue by e-mail and during the coming meetings.

*Contribution of CXAFS to IUCr Online Dictionary.* The Working Group on XAFS Nomenclature, appointed in order to contribute to the IUCr Online Dictionary, has been highly efficient. The objective was to propose a list of items relative to XAFS terminology with their definitions, selecting the most frequently used XAFS terms and standard definitions used currently in the XAFS community.

The working methods have been defined. Meetings and exchanges, through a number of web tools for communication across the internet, allowed an easy exchange of ideas. As required, members initially compiled a list of terms to be defined and then proceeded to the appropriate tasks relating to the definition of these. At the end of 2009, 15 items had been proposed; they will be evaluated during 2010 by an Independent Advisory Panel, which reports to the Chair of the Commission. In the case of any controversy, more than one definition will be introduced in the IUCr Dictionary. Finally, entries should be approved by the whole Commission.

**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 2009 the Executive Committee approved sponsorship of various schools and meetings, mostly with financial support. Those held in 2009 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 2010, but approved in 2009, are listed below.

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

Powder Diffraction and Rietveld Refinement School, Durham, UK, 18–22 April 2010.

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

Third Annual School on Advanced Neutron Diffraction Data Treatment using the FullProf Suite, Tenerife, Spain, 2–8 May 2010.

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

Diffraction at the Nanoscale: Nanocrystals, Defective and Amorphous Materials, Villigen, Switzerland, 24–30 May 2010.

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

Second Chemical Crystallography Workshop, Hamilton, Ontario, Canada, 25–29 May 2010.

Structure and Function from Macromolecular Crystallography: Organization in Space and Time, Erice, Italy, 3–13 June 2010.

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

Summer Schools on Mathematical and Theoretical Crystallography, Nancy, France, 21 June – 2 July 2010.

ACA Annual Meeting, Chicago, USA, 24–29 July 2010.

Fourteenth International Summer School on Crystal Growth (ISSCG-14), Dalian, People's Republic of China, 1–7 August 2010.

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 2010.

Sixteenth International Conference on Crystal Growth in conjunction with the Fourteenth International Conference on Vapor Growth and Epitaxy, 8–13 August 2010.

Tenth Conference of the Asian Crystallographic Association, Busan, Korea, 31 October – 3 November 2010.

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 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 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 charged with maintaining and developing the Crystallographic Information Framework (CIF), which includes syntax and dictionary language standards as well as a number of dictionaries

written according to these standards. In the second half of 2009, COMCIFS formed a working group to thrash out remaining issues with the new dictionary language ('DDLm') framework. As the year was drawing to a close, the final touches were being put on to one component of this framework, an updated CIF syntax specification, dubbed 'CIF2'. This has been distributed to the community for comment prior to final adoption by COMCIFS. The working group's attention has now moved on to discussion of DDLm itself.

Work is ongoing on a number of draft dictionaries. A draft small-angle-scattering dictionary (sasCIF) is at an advanced stage, and an updated symmetry dictionary is in development. A draft dictionary for expressing restraints and constraints in single-crystal refinements is currently under review by the core dictionary maintenance group.

Recognizing that the procedure for adding definitions to CIF dictionaries can be both impenetrable and discouraging for non-CIF experts, COMCIFS has developed and tested a streamlined fast-track procedure for adding single definitions to a dictionary. Under this procedure, the relevant dictionary working group has six weeks to comment and develop the definition, following which COMCIFS has a further six weeks to discuss and accept the proposal. An announcement of a web portal for submission of such fast-track proposals should be expected in the near future.

**J. Hester**, Chair

## 8. Committee on Crystallographic Databases

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

## 9. IUCr Newsletter

Four issues of the IUCr Newsletter were prepared in 2009 (Volume 17-1 to 17-4) with 17-4 being mailed in January 2010. This report will cover all of Volume 17. All of the issues were 24 pages in length. As in previous years, the content covered activities of the IUCr and its Regional Associates and its Commissions, Letters to the Editor, news concerning crystallographers and crystallography in general, awards, elections, resources, obituaries, meeting reports, book reviews, future meeting announcements, and a general meeting calendar.

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 two pages to brief summaries of selected articles recently published in IUCr journals. Issues 1 and 3 contained a report on Crystallography in Great Britain and Ireland and issue 4 contained the first half of a report on Crystallography in Canada.

Additional meeting and workshop reports were published covering activities in Switzerland, Germany, Egypt and India.

The mailing list remained about the same in 2009 with an average distribution of 18 364. Twenty-one 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. Kvik, France; A. Nangia and Executive Secretary, India; Ismunandar, Indonesia; P. Spadon, Italy; A. Satomi, Japan; A. Hamid Othman, Malaysia; R. Rendle, New Zealand; J. Lipkowski, Poland; M. Costa, Portugal; W. Klooster, Singapore; L. Nassimbeni, South Africa; J. Schefer, Switzerland; Yu Wang, Taiwan; K. Haller, Thailand; H. Kooijman, The

Netherlands; G. Diaz De Delgado, Venezuela.) Individual distributions were sent to 84 additional countries.

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

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

In 2009, the cooperation between Oxford University Press (OUP) and the IUCr/OUP Book Series Selection Committee continued to be good.

Two new volumes in the series IUCr Monographs on Crystallography were published: No. 22, *Structural Crystallography of Inorganic Oxysalts*, by S. V. Krivovichev (publication date 22 January 2009); and No. 23, *The Nature of the Hydrogen Bond*, by G. Gilli and P. Gilli (publication date 25 June 2009).

Two new volumes in the series IUCr Texts on Crystallography were published: No. 12, *The Basics of Crystallography and Diffraction*, Third Edition, by C. Hammond (publication date 7 May 2009); and No. 13, *Crystal Structure Analysis – Principles and Practice*, Second Edition, by A. J. Blake, W. Clegg, J. M. Cole, J. S. O. Evans, P. Main, S. Parsons and D. J. Watkin (publication date 18 June 2009).

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). (The membership of the Committee and the recommended procedure for submitting a proposal may be found *via* the web page at <http://www.iucr.org/iucr/index.html/advisory-committees/book.html>.) 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)

The ACA Council met three times in 2009 – a spring meeting on 4 April near O'Hare airport, Chicago, a summer meeting on 24 July in Toronto, Canada, and a fall meeting on 3 October in Buffalo. R. Von Dreele was the 2009 ACA President, J. Kelly ACA Vice-President, M. L. Hackert Past-President, B. Santarsiero Treasurer and C. Wilmot Secretary. J. Britten was the Canadian Representative on the ACA Council and L. T. J. Delbaere served as IUCr representative.

*Highlights from the ACA Annual Meeting, Toronto, Ontario, Canada, 25 – 30 July 2009.* The 2009 ACA Annual Meeting was a great success. The Programme Chair was J. Britten and the Local Chair was D. Rose. There were over 900 participants (the fourth highest attendance) and about 275 lectures and 360 posters.

There were two workshops on 24/25 July:

JANA – Incommensurate Crystal Structures, with Chairs J. A. Kaduk and O. Gourdon;

Handling Twinning in Macromolecular Crystallography, with G. M. Sheldrick, G. Murshudov and P. Zwart, presiding.

The Transactions Symposium was Phase Transitions organized by R. J. Angel and I. Swainson.

The following awards were presented:

Warren Award to Shih-Lin Chang of National Tsing Hua University, Taiwan; his lecture on Coherent Dynamical Interaction in X-ray

Multiple Diffraction and Crystal Cavity Resonance was published in the spring 2010 issue of *Reflexions*;

Buerger Award to M. James;

Etter Early Career Award to S. Bobev.

Several prizes were awarded to the best poster presentations in various areas of crystallography, including an IUCr poster award.

The Plenary Lectures were:

E. N. Baker on Celebrating Crystallography;

P. Coppens on New Developments in X-ray Photocrystallography.

A total of 74 students were provided with travel grants, many international students receiving funds from the IUCr travel grant.

*ACA Business Meeting.* The following items were considered:

2010 membership dues – regular membership remains essentially unchanged (regular USD 100), postdocs can remain at the postdoc rate (USD 40) until ten years after PhD (increase from five years), country membership is USD 200 per year;

The Council approved a vote by membership of an ACA Fellows Programme;

Abstracts were only offered on CD at Toronto – it was suggested that some hard copies of the Abstracts should be available at the registration desks for those who did not have a laptop;

Hotel rates: members felt the hotel rate was too high and would like WiFi to be available;

Coffee breaks/lunches – having lunch concessions available would be good for keeping registrants together and therefore mixing; the IUCr managed to have cheap lunchtime concession stands, why could the ACA not do the same?

Upcoming Annual Meetings: 2010 – Chicago (Programme Chair R. J. Angel, Local Chair B. Santarsiero) – the Awards to be given at this meeting will be the Fankuchen, Trueblood and Etter Early Career; 2011 – New Orleans (Programme Chair C. Cahill) – the Awards to be given at this meeting will be the Patterson and the Etter Early Career; 2012 – Boston.

Governance of IUCr: concern was expressed about representation on IUCr matters.

A crystallography school was held at McMaster University in Hamilton, Ontario, Canada, prior to the ACA 2009 Annual Meeting, with a focus on teaching of crystallography;

A Small Molecule Crystallography Summer School run by C. Lake has ACA support through 2010; there will be no Macromolecular Crystallography Summer School in 2010.

*Elections and Other Council Actions.* The following were elected: ACA Vice-President T. F. Koetzle; ACA Council Treasurer B. Santarsiero. Also elected were 12 SIG chairs plus members of three standing committees.

The Council decided to go forward with an early ACA meeting in 2014 – the year that the IUCr Congress will be held in Montreal. A site near the west coast would be the preferred location to minimize the impact on the attendance at the IUCr Congress.

We were all deeply saddened to hear that Louis Delbaere passed away suddenly on 5 October 2009 while returning from the fall ACA Council meeting in Buffalo. Louis will be remembered for his winning and ever-present smile and his enthusiastic passion for his chosen science – X-ray crystallography. Louis was a member of the IUCr Executive Committee.

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

## 11.2. Asian Crystallographic Association (AsCA)

AsCA continues to play a leading role in the nurturing of collective crystallographic activities in the Asia-Pacific region. The present

office bearers are J. M. Guss (President, Australia), Se Won Suh (Vice-President, Korea) and K. Haller (Secretary/Treasurer, Thailand). The major activity in 2009 was the joint meeting of AsCA and the Chinese Crystallographic Society in Beijing, People's Republic of China, 22–25 October 2009. This meeting was a great success with the largest ever attendance (~200) for an AsCA meeting. In addition to the exciting science, the 'rising-stars' session, which is a first for an AsCA meeting or a meeting of any of the Regional Associates, provided the opportunity for six early-career researchers selected from the submitted Abstracts to present their work to a Plenary Session on the final day of the meeting. The presentations in this final Plenary Session were of a very high standard.

It is necessary to mention some of AsCA's major initiatives and some of the problems it faces. The first initiative, originally proposed by Y. Ohashi as IUCr President, was the formation of a regional grouping of Asian nations who are recognized as a joint member of the IUCr. Together they have a single vote at IUCr General Assemblies but individuals from the countries may attend. The annual dues of CHF 1000 are currently shared by the Society for Crystallographers in Australia and New Zealand (SCANZ) and the Crystallographic Society of Japan.

The second major initiative is to utilize interest from the accumulated reserves of AsCA, currently about AUD 120 000, to support attendance at AsCA meetings by students and early-career scientists from the region. AsCA offered five such scholarships for the 2009 meeting, each valued at USD 1000. It is the intention of the AsCA Executive that a similar level of support will be provided for the forthcoming meeting in Busan, Korea, in 2010. It was noted that additional sources of funding to increase the total AsCA investment portfolio are required to sustain these initiatives in the long term.

The third initiative by Y. Ohashi supported by the AsCA President is an agreement from the President of the IUCr, S. Larsen, to provide direct financial support from the IUCr for attendance by two members of the AsCA Council who would not otherwise be able to attend Council meetings. This initiative recognizes the special circumstances faced by a number of member countries of AsCA, but at its meetings in 2010 the IUCr Executive Committee will be discussing a permanent arrangement for Council meetings of all the Regional Associates.

Preparations are underway for the full AsCA meeting to be held in Busan, Korea, 31 October – 3 November 2010. The Programme format will be the same as that for the Beijing meeting, including a rising-stars session. Registration fees will also be similar.

A proposal that Adelaide in Australia should host a joint AsCA/SCANZ conference and Bragg centenary celebration in November 2012 (centenary of the presentation of Lawrence Bragg's paper to the Cambridge Philosophical Society, which detailed the first crystal structure and Bragg's equation) received strong support from the AsCA Council and the Committee was requested to bring forward a definite proposal including dates, costs, details of accommodation *etc.* to the next AsCA Council meeting.

Interest was expressed by representatives of Bangladesh, China, India, Thailand and Vietnam to hold the 2013 AsCA conference in their respective countries. The Committee was pleased to see so much interest in hosting the meeting; this is recognition that AsCA conferences are highly regarded. Proposals were requested to be brought forward to the next AsCA Council meeting.

AsCA will continue to seek support of its programs from the IUCr. Some of the problems of the Asian crystallographic community are different to those elsewhere. The various countries are geographically far flung and there needs to be more in the way of systematic bilateral and multilateral initiatives among the countries of the region so that

the scientific communities in these countries get to know each other better. Travel and research support for students and young workers is also very limited, and there is a need for more funding in these areas. Economic growth in the Asian region should also be paralleled by scientific and infrastructural growth. The IUCr should ensure that crystallographic research in some of the more disadvantaged regions of Asia is put on a firmer footing. A greater representation of younger crystallographers from the Asia-Pacific region in the activities of the IUCr is strongly desirable. The IUCr could also become more involved in mentoring activities, even as some of the Asian countries are rapidly trying to become integrated with the international scientific mainstream.

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

### 11.3. European Crystallographic Association (ECA)

The present membership of the ECA Executive Committee is: President: S. Garcia-Granda (Spain); Past-President: J. R. Helliwell (UK); Vice-President: A. Roodt (South Africa); Secretary: P. Bombicz (Hungary); Treasurer: R. Kuzel (Czech Republic); Members: L. Van Meervelt (Belgium), W. Depmeier (Germany) and A. Bacchi (Italy); Education Coordinator and ECA Webmaster: M. Nespolo (France).

The ECA supported the following meetings in 2009:

(1) Crystallography Online: International School on the Use and Applications of the Bilbao Crystallographic Server, Lekeitio, Spain, 21–27 June 2009 (EUR 1250).

(2) The Role of Symmetry in Condensed Matter, Giens Peninsula, France, 11–18 May 2009 (EUR 750).

(3) High-Pressure Crystallography: From Novel Experimental Approaches to Cutting-Edge Technologies, Erice, Italy, 4–14 June 2009 (EUR 1500).

(4) 4th Crystallographic School on Structural Analysis using Single-Crystal X-ray Diffraction, Nancy, France, 22–26 September 2009 (EUR 750) (dedicated to Magreb region).

(5) ECM-25 Istanbul, Turkey, 16–21 August 2009 (EUR 2000).

(6) EuroXX International School on Physics and Chemistry of Condensed Matter, Białowieża, Poland, 4–11 July 2009 (EUR 1000).

Future ECA meetings will be held as follows:

(1) ECM-26: Darmstadt, Germany, August/September 2010.

(2) ECM-27: Bergen, Norway, August 2012.

(3) ECM-28: Warwick, UK, August 2013.

At ECM-26 a special feature will be the joint meeting with EPDIC; this promises to be a relatively larger meeting and exhibition. ECM-27, being held in 2012, will highlight the centennial of the Friedrich, Knipping and von Laue experiment. The year 2013, the year of ECM-28, is the centenary of the first crystal structure being solved by the Braggs in the UK.

The ECA Perutz and Bertaut Prize Committees work independently from the ECA Executive Committee and are chaired by A. Roodt. The 4th Max Perutz ECA Prize was awarded but not accepted, therefore there was no prize in 2009. The 2010 Prizes are to be awarded during ECM-26 in Darmstadt. Donations to these prize funds are possible *via* the ECM-26 web site.

The establishment of a General Interest Group (GIG) – Network of Young Chemists in the ECA region is in progress, conducted by A. Bacchi. The ECA is pleased to support the activities of the younger generation of crystallographers – such as their organization of scientific meetings, sessions and exchanges of information. By request, the parallel establishment of a General Interest Group for Senior Scientists is also proceeding. This GIG comes together to preserve the history of crystallography, the archive of materials, to

play an important part in teaching, consider special requirements of senior scientists *etc.*

There is also an increasing emphasis on the education of future generations of crystallographers at postgraduate, graduate and schools' levels. In the establishment of a European Graduate School of Crystallography (Masters and PhD) M. Nespolo has submitted a proposal for an Erasmus Mundus Master Course in a collaboration of several Universities, most importantly: Université Henri Poincaré, Nancy, France; Charles University, Prague, Czech Republic; and Univerisità degli studi di Padova, Italy, with contributions from the Universities of Antwerp, Liège, Belgium; Pais Vasco, Aveiro and Oviedo, Spain; and the European Synchrotron Radiation Facility, Grenoble, France.

A. Bacchi is monitoring the performance of the SIGs. The aim is that all SIGs should have a web site before the end of 2010. The number of ECA individual members registered with each SIG does not reflect the total number of researchers involved in the work of the respective SIG. It is the task of the SIGs to convince as many researchers as possible to become ECA individual members and express their explicit interest for the SIG's activities. There are several SIGs that coordinate or sponsor prizes or organize schools and workshops. Performance of the SIGs is also measured by the participation in the work of the Programme Committee of the ECMs, with an organizational effort focused on Keynote Lectures and Microsymposia. The reinvention of the five Focus Areas works well. To strengthen the contact with the SIGs, the ECA Executive Committee will continue its personal meetings with the SIG officers on the day of the Opening Ceremony of the ECMs, as started last year in Istanbul. Some SIGs have a well established connection with the corresponding IUCr Commissions; a well functioning link with all the relevant IUCr Commissions is desirable.

The ECA leaflet that was prepared first in 2008 by R. Kuzel has been updated. The number of Corporate Affiliate Members (CAMs) of the ECA is now over 30. The goal is to encourage the new CAMs to continue membership for several years. It is highly important to enlarge the number of the individual members of the ECA. In the ECA region the focal points are encouraging the activity of the Baltic countries, how to involve more countries in Africa and the integration of new candidate countries into the Association.

The ECA is grateful to the IUCr for providing column space on a regular basis in its *Newsletter* in which the ECA Officers write on topics of policy and community interest within the ECA, and thereby encourage wider debate within the IUCr as a whole.

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

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

No formal meeting of the IOCG (<http://www.iocg.org/>) was planned or organized in 2009. A few members of the Executive Committee of the IOCG met during the American Conference on Crystal Growth in Lake Geneva, USA, discussing the future changes in the organization.

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/>) will be held in Beijing, People's Republic of China, 8–13 August 2010. Members and consultants of the IUCr Commission on Crystal Growth and Characterization of Materials (S. Baldochi, H. A. Dabkowska, T. Duffar and K. Kakimoto) are strongly involved in the work of the Programme and Advisory Committees of both meetings. Commission member J. Wang serves as a General Secretary for this venue.

The 14th International School on Crystal Growth (Chair Mu Wang) will be 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 are lecturing at the School, which is supported by the IUCr.

Detailed information about both the Conference and the School is posted at the IOCG web site.

The IOCG President for 2007–2010 is A. A. Chernov (USA) and the President-Elect is R. Fornari (Germany). The new Executive Committee was elected and will be confirmed during the next General Assembly of the IOCG, which will take place in Beijing during ICCG-16 in August 2010.

National Associations for Crystal Growth were 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. With this in mind the Executive Committee of the IOCG is organizing a meeting of European Chairs, Secretaries and Representatives of National Groups and Institutions for Crystal Growth. This meeting is devoted to consolidation of crystal growth activities in Europe and it will be held at the Institute for Crystal Growth, Berlin, Germany, 20–21 April 2010. There will be a motion to strengthen the European network, increase the impact of projects devoted to crystal growth in the European Union and possibly create a European Association for Crystal Growth (the Asian Association for Crystal Growth already exists). H. A. Dabkowska is attending this meeting as the IUCr representative to IOCG. She will also chair the first session.

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

### 11.5. International Centre for Diffraction Data

The IUCr Representative attended the 2009 ICDD Spring Meeting in March to represent the Commission on Powder Diffraction (CPD) and the IUCr. Discussions included the proposed joint Denver X-ray Conference (DXC)/ACA meeting in 2013 (now defunct) and better communicating the roles of the CPD and the ICDD given the mutual representation each has (there is an ICDD representative on the CPD and the CPD Chair is the IUCr Representative to the ICDD).

**P. Whitfield**, IUCr Representative

## 12. Representatives on Other Bodies

### 12.1. IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

The definition of the mole was updated at the August 2009 meeting of the ICTNS in Glasgow, UK, to read:

The mole, unit of amount of substance of a specified elementary entity, which may be an atom, molecule, ion, electron, any other particle or a specified group of such particles, is such that the Avogadro constant is equal to exactly  $6.022\,141\,79 \times 10^{23}$  per mole.

Thus we have the exact relation  $N_A = 6.022\,141\,79 \times 10^{23} \text{ mol}^{-1}$ . The effect of this definition is that the mole is the amount of substance of a system that contains  $6.022\,141\,79 \times 10^{23}$  specified elementary entities.

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:

(1) *Towards Defining Materials Chemistry*; (2) *Evaluation of Measurement Data – The role of measurement uncertainty in conformity assessment*.

**A. Authier**, IUCr Representative

### 12.2. International Council for Scientific and Technical Information (ICSTI)

The ICSTI web site (<http://www.icsti.org>) carries a new mission statement accompanying the organization's 2008–2010 Strategic Plan: '[ICSTI] fosters cooperation among all stakeholders engaged in the scientific communication process with the aim of improving the effectiveness of scientific research. It fully exploits its unique position at the intersection of scientific and technical knowledge creation, organization, dissemination and use, to identify and act upon key challenges, without politicized or commercially driven agenda. ICSTI is a broad-based, international, not-for-profit membership organization.'

During 2009, there were significant efforts to attract new members to ICSTI, and to increase cooperation with other stakeholders. These efforts included a summit meeting between the Executive Boards of ICSTI and CODATA at ICSU Headquarters in Paris in March 2009, at which were discussed common approaches to the ICSU Priority Area Assessment (PAA) on scientific data and information. B. McMahon, the IUCr's CODATA Representative, represented the IUCr at this meeting and throughout 2009 on the ICSTI Executive Board as alternate for J. R. Helliwell who was busily involved with duties and activities in his role as President of the European Crystallographic Association.

ICSTI nominee H. Gruttemeier (France) was appointed to the ICSU *Ad Hoc* Strategic Coordination Committee on Information and Data (SCCID), which is intended to establish and assert a visible and effective strategic leadership role in the worldwide policies, management and stewardship of scientific data and information.

The ICSTI Summer Conference took place in the Library and Archives Canada building, in Ottawa, held in June, with the theme Managing Data for Science. The 16 speakers provided a helpful overview of the challenges for the publishing and library communities arising from the increasing availability of research data. They showed that many of these challenges and difficulties – identified, for example, in successive CODATA conferences – are becoming more generally recognized, and that progress is being made in addressing them in some scientific fields, and in the formulation of science policy at national levels. The compelling message of the conference was the need to develop a coherent plan for managing data as an essential component of any research project. Significantly, due recognition was given to the differing needs of different communities; individual disciplines need to assess their own requirements for management and long-term preservation. Further, preservation strategies needed to analyze critically what exactly did need to be preserved and for how long. An account of the conference can be found at <http://www.iucr.org/resources/data/meeting-reports/icsti-2009>.

The ICSTI Technical Activities Coordinating Committee (TACC) project on Numeric Data: Citation Techniques and Integration with Text culminated in a workshop establishing a consortium of major scientific libraries to act as registration agencies for unique identifiers for data sets. This consortium, led by the German National Library of Science and Technology, subsequently adopted the name DataCite (<http://www.datacite.org>). Another TACC project of interest, entitled Multimedia Search and Retrieval, continued through 2009 to collect



multimedia materials for indexing full-spoken content in audio or video files through voice-recognition technology.

The IUCr took the lead in a new TACC project, entitled 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 was planned for exploring this topic at the 2010 ICSTI Winter Meeting.

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

## 12.3. International Council for Science (ICSU)

Since the triennial General Assembly was held in Maputo, Mozambique, October 2008 (see the 2008 Report) and the Meeting of Scientific Unions will be held in Paris in April 2010, there were no important decisions and meetings in 2009. Most important meetings will be held in 2010. The ICSU Regional Office for Africa reported four science plans and has established functioning networks of experts and students. The four plans are as follows: sustainable energy, global environmental change, health and human well being, and hazards and disasters. The details are shown at <http://www.icsu-africa.org>.

**Y. Ohashi**, IUCr Representative

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

*Collaboration with the International Council for Science, ICSU.* CODATA continued its close collaboration with ICSU in 2009. Two CODATA nominees, M. Zgurovsky (Ukraine) and P. Cilliers (South Africa), were appointed to the newly formed World Data System Scientific Committee (WDS-SC). CODATA nominee R. Chen (USA) was appointed to the new ICSU *Ad Hoc* Strategic Coordination Committee on Information and Data (SCCID), one of the goals of which is to establish and assert a visible and effective strategic leadership role, on behalf of the global scientific community, in relation to the policies, management and stewardship of scientific data and information.

Efforts to increase collaboration with the International Council for Scientific and Technical Information (ICSTI) included guest attendance at the ICSTI Winter Meeting Workshop on Primary Data for Libraries and Information and a summit meeting between the CODATA and ICSTI Executive Boards at ICSU Headquarters in Paris in March 2009 (which the undersigned attended in the role of alternate IUCr delegate to ICSTI).

*Collaboration with GEO, the Group on Earth Observations.* A Symposium on Data Sharing Plans for GEOSS and the Benefits of Data Sharing for Science took place in Washington DC, USA, in conjunction with the GEO-VI Plenary in November 2009. The Symposium was organized by the US National Committee for CODATA, together with the National Committee for DIVERSITAS and the US National Committee on Geodesy and Geophysics.

CODATA continued its work and close collaboration with GEO on the development of implementation guidelines for the GEOSS Data Sharing Principles. CODATA Secretary-General R. Chen and P. Uhler were appointed as Co-Chairs of the GEO Data Sharing Task Force (DSTF). The DSTF was established in spring 2009, and is working on an Action Plan to develop working procedures for data sharing within GEOSS and to articulate additional steps needed to implement the GEOSS Data Sharing Principles.

In support of these activities, CODATA prepared two important publications: *Toward Implementation of the Global Earth Observa-*

*tion System of Systems Data Sharing Principles*, jointly published by the CODATA *Data Science Journal* and the *Journal of Space Law*; and a Special Issue of the CODATA *Newsletter* containing an interview with the Executive Director of GEO, on Data Sharing within GEOSS.

*Building European activities with the support of the European Commission.* CODATA's Task Group on Global Information Commons for Science – EU-GICSI Activities co-led the organization of the Second COMMUNIA Conference on Global Science and Economics of Knowledge-Sharing Institutions under the EU-funded thematic network on the Public Domain in the Digital Age. The Conference drew more than 100 participants to Turin, Italy, 28–30 June 2009, to discuss the rationale, policy support and practical feasibility of arrangements designed to emulate key public domain conditions for collaborative research. A summary report of the Conference is available online at <http://www.communia-project.eu/node/283>.

*The Polar Information Commons.* This project, launched in March 2009 with support from ICSU, aims to establish a sustainable long-term framework for the preservation of and access to polar data, building on recent 'commons' approaches developed in other scientific fields and bringing new stakeholders and participants into polar data management. The core project team has developed the concept of a Polar Information Commons (PIC) which will serve as an open, virtual repository for polar scientific data and information and provide a shared, community-based cyberinfrastructure for research, education, planning and management in the polar regions. Presentations about the PIC concept have been given or are planned at a number of relevant meetings. Details are available on the PIC web site at <http://www.polarcommons.org/>.

I acknowledge the most useful 2009 *Highlights* document posted on the CODATA web site at <http://www.codata.org> in compiling this report.

**B. McMahon**, IUCr Representative

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

The main objective of COSPAR (<http://cosparhq.cnes.fr/>) is 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 the creation of national and international organizations and specialist working groups.

In July 2008 the 37th COSPAR Scientific Assembly was held in Montreal, Canada. As COSPAR acts mainly as a body responsible for organizing biennial Scientific Assemblies, the year 2009 was devoted to organizing the next meeting, the 38th COSPAR Assembly, to be held in Bremen, Germany, 18–25 July 2010.

The majority of COSPAR activities deal with space topics (such as astrobiology, atmosphere studies or investigation of natural and artificial ecosystems). The most interesting COSPAR division for the IUCr is the Scientific Commission on Materials Science in Space (MSS), chaired by V. Shevtsova (Belgium) and co-chaired by S. Amiroudine (France), W.-R. Hu (People's Republic of China) and S. Yoda (Japan). The Commission reviews fundamental – theoretical and experimental – experiments in materials and fluid sciences performed in space, utilizing reduced gravity for their objectives. This approach helps to understand emerging fields by recommending promising avenues for future research. It also coordinates exchanges of information on relevant scientific subjects.

Different experiments on growth of crystals in microgravity were at some point a part of these programs. In 2009 the COSPAR

**Table 2**

Income and Expenditure Account (in Swiss Francs) for the year ended 31 December 2009.

	2009		2008	
<b>Income</b>				
Membership subscriptions		158 046		159 353
Sales				
Journals, back numbers and single issues	4 428 868		4 334 082	
Books	120 359		268 897	
Open Access Grant	31 728	4 580 955	46 284	4 649 263
Investment income				
Income from investments	89 373		102 284	
Bank interest	2 064		32 996	
(Loss)/Profit on sale of investments	—	91 437	(22 993)	112 287
Other income				
Royalties and copyright fees	8 533		13 744	
Advertising income	193 711		227 689	
STAR/CIF income	12 709	214 953	7 793	249 226
<b>Total income</b>		<u>5 045 391</u>		<u>5 170 129</u>
<b>Expenditure</b>				
Journals				
Publication costs	606 104		641 289	
Editorial expenses	322 575		249 213	
Technical editing	1 470 547		1 624 148	
Subscription administration	109 885	2 509 111	122 410	2 637 060
Books				
Publication costs	96 605		33 566	
Editorial expenses	32 340		72 304	
Technical editing	103 122	232 067	228 159	334 029
Newsletter				
Publication costs	112 630		105 873	
Editorial expenses	123 384	236 014	121 678	227 551
President's Fund and other Grants and Young Scientists' support		165 977		93 642
General Assembly and Congress costs		40 614		114 660
Committee meetings and expenses		71 129		119 870
Publications and journals development				
General	587 946		673 563	
Editors' meetings	2 079		4 466	
STAR/CIF	21 302		42 686	
Promotion	162 268	773 595	245 389	966 104
Subscriptions paid		11 167		12 237
Visiting Professorship Programme		4 862		8 994
Administration expenses:				
General Secretary and Treasurer: Honorarium to Treasurer	10 537		13 302	
Audit and accountancy charges	66 097		61 756	
Legal and professional fees	7 649		12 032	
Travelling expenses	18 051		4 795	
Bank charges	2 112	104 446	2 514	94 399
Executive Secretary's office:				
Salaries and expenses	300 892		341 547	
Travel expenses of IUCr Representatives on other bodies	14 656		14 279	
Sponsorship of meetings	11 611		6 621	
IUCr/FIZ agreement	(18 745)		(17 131)	
Bad debts	5 638	314 052	—	345 316
Depreciation		41 570		45 921
<b>Total expenditure</b>		<u>4 504 604</u>		<u>4 999 783</u>

**Table 2 (continued)**

	2009	2008
<i>Surplus of income over expenditure (before realized exchange losses)</i>	540 787	<i>170 346</i>
Realized fluctuations in rates of exchange		
Exchange movement on trading activities	122 575	<i>(349 133)</i>
Surplus/(deficit) of income over expenditure (after realized exchange losses)	663 362	<i>(178 787)</i>
Movement in market value of investments in year	639 751	<i>(972 646)</i>
Unrealized fluctuation in rates of exchange		
Exchange movement on trading activities	(22 019)	<i>(28 347)</i>
Investment activities	74 401	<i>(872 743)</i>
Total recognized gains/(losses) relating to the year	1 355 495	<i>(1 995 829)</i>
<b>Opening fund accounts at 1 January 2009</b>	3 023 501	<i>5 019 330</i>
<b>Closing fund accounts at 31 December 2009</b>	4 378 996	<i>3 023 501</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.

President was R.-M. Bonnet (France) and the Vice-Presidents were W. Hermsen (The Netherlands) and E. C. Stone (USA). The members of the Bureau are: M.-H. Jiang (People's Republic of China), M. E. Machado (Argentina), G. G. Shepherd (Canada), R. Sridharan (India), L. Zelenyi (Russia) and J. B. Zielinski (Poland).

COSPAR co-sponsored the following meetings or events in 2009:

International Year of Astronomy (IYA), Interantional Astronomical Union, 2009.

Titan Planetary Protection Workshop, Pasadena, CA, USA, 9–10 December 2009.

6th European Space Weather Week (ESWW6), Bruges, Belgium, 16–20 November 2009.

URSI/COSPAR International Reference Ionosphere Workshop, Kagoshima, Japan, 2–7 November 2009.

11th International Association of Geomagnetism and Aeronomy (IAGA) Scientific Assembly, Sopron, Hungary, 23–30 August 2009.

27th International Symposium on Space Technology and Science (27th ISTS), Tsukuba City, Japan, 5–12 July 2009.

Workshop on Planetary Protection, Outer Planet Satellites and Small Bodies, COSPAR, Vienna, Austria, 15–17 April 2009.

Frontiers of Space Astrophysics: Neutron Stars and Gamma Ray Bursts, Alexandria, Egypt, 30 March – 4 April 2009.

1st Panda Symposium on Products of Astrophysical Outflows, Lijian, Yunnan, People's Republic of China, 30 March – 3 April 2009.

5th European Conference on Space Debris, Darmstadt, Germany, 30 March – 2 April 2009.

**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

<sup>1</sup> The full audited accounts are available from the IUCr electronic archives (Reference ES0381). Services for accessing these data are described at the back of the journal.

Accounts, are given in Tables 2, 3 and 4, respectively.<sup>1</sup> For comparison, the figures for 2008 are provided in italics. The accounts are presented in CHF.

The UNESCO rates of exchange, as issued by the ICSU Secretariat, 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 2009 have been translated into CHF in the balance sheet at the rate operative at that date. For the income and expenditure accounts, transactions have been translated into CHF by applying the rates appropriate to the individual dates of these transactions. As a consequence of the fluctuation in exchange rates, overall an apparent gain has arisen on the assets of the Union, in terms of CHF, amounting to CHF 174 957. In the accounts this gain has been assigned as 'Realized' (CHF 122 575) and 'Unrealized' (CHF 52 382). The gain attributable to investment activities has been assigned to the General Fund and the gain attributable to trading activities has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 2009. It should be noted that this overall gain in CHF is not a real gain of money, but rather a gain on paper resulting from the accounts being expressed in CHF.

Investments are noted in the balance sheet at their market value at 31 December 2009.

The balance sheet shows that the assets of the Union, including the gain resulting from fluctuations in rates of exchange, have increased during the year, from CHF 3 023 501 to CHF 4 378 996. The movement in market value of the investments was CHF 639 751 in 2009 (CHF –972 646 in 2008). The significant gain in value of the investments in 2009 is a result of the well known market situation (following significant losses in 2008).

The following transfers were made from the Journals Fund: CHF 120 000 to the Publications and Journals Development Fund; CHF 160 000 to the Research and Education Fund; CHF 200 000 to the General Assembly and Congress Fund; CHF 50 000 to the *Newsletter* Fund; CHF 25 000 to the President's Fund; and CHF 25 000 to the Ewald Fund.

The following comments refer to figures in the full accounts.

**Table 3**

Balance sheet (in Swiss Francs) as at 31 December 2009.

	2009	2008
<b>Fixed assets</b>		
Tangible fixed assets	45 880	43 124
Investments at market value	2 509 238	1 797 102
	<u>2 555 118</u>	<u>1 840 226</u>
<b>Current assets</b>		
Stock	119 120	182 162
Cash at bank and in hand		
Current accounts	54 872	49 463
Deposit and savings accounts	946 052	601 391
Cash with Union officials	7 706	17 108
	<u>1 008 630</u>	<u>667 962</u>
Debtors, accrued income and payments in advance	1 162 842	674 538
Subscriptions due from Adhering Bodies	6 000	13 000
	<u>1 168 842</u>	<u>687 538</u>
<b>Total current assets</b>	2 296 592	1 537 662
<i>Creditors: amounts falling due within one year</i>	(472 714)	(354 387)
<b>Net current assets</b>	1 823 878	1 183 275
<b>Total funds</b>	4 378 996	3 023 501

**Table 4**

Summary of Fund Accounts (in Swiss Francs) as at 31 December 2009.

	As at 1 January 2009	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 2009
					Trading	Investments	
					—	—	
<b>Fund accounts</b>							
General Fund	(1 863 590)	—	(289 896)	639 751	(36 206)	74 401	(1 475 540)
President's Fund	96 241	25 000	(17 196)	—	2 489	—	106 534
Journals Fund	2 592 932	(580 000)	1 346 877	—	80 362	—	3 440 171
<i>International Tables</i>	(304 387)	—	(150 498)	—	(10 880)	—	(465 765)
Publications and Journals Development Fund	847 102	120 000	(64 913)	—	21 579	—	923 768
Research and Education Fund	955 618	160 000	(163 517)	—	22 773	—	974 874
Ewald Fund	490 972	25 000	—	—	12 341	—	528 313
<i>Newsletter</i> Fund	89 309	50 000	(89 331)	—	1 195	—	51 173
General Assembly and Congress	119 304	200 000	(30 739)	—	6 903	—	295 468
	<u>3 023 501</u>	<u>—</u>	<u>540 787</u>	<u>639 751</u>	<u>100 556</u>	<u>74 401</u>	<u>4 378 996</u>

The General Fund account shows a deficit of CHF 289 896, as compared with a deficit in 2008 of CHF 347 375. The administrative expenses were CHF 408 057 in 2009 as compared with CHF 440 098 in 2008. Of this amount, CHF 179 520 was charged to the publications of the Union.

The expenses of the Union Representatives on other bodies were CHF 14 656. The cost of the Finance Committee meetings held in 2009 was CHF 14 155, while the Executive Committee meeting cost CHF 56 974. The income from the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 18 745. The subscriptions from Adhering Bodies were CHF 158 046. Interest on bank accounts and investments credited to the General Fund was CHF 91 437.

Grants totalling CHF 17 196 were paid from the President's Fund in 2009.

The Journals Fund account for 2009 shows a surplus of CHF 1 346 877 before the transfer of CHF 580 000 to the other fund accounts, as compared with a surplus of CHF 1 068 593 in 2008 before the transfer of CHF 620 000 to the other fund accounts.

The subscription rates were increased for 2009. In 2009, the number of paid subscriptions were as follows: *Acta Crystallographica*: Section A 557 (607) including 42 (49) personal subscriptions (values for 2008 are given in parentheses); Section B 548 (600) including 33 (41) personal subscriptions; Section C 524 (573) including 27 (32) personal subscriptions; Section D 529 (571) including 56 (72) personal subscriptions; *Journal of Applied Crystallography*: 483 (526) including 49 (60) personal subscriptions; *Journal of Synchrotron Radiation*: 183 (189) including 35 (40) personal subscriptions. The income from consortial sales is a significant additional income, comparable to that from standard subscriptions.

The cost of the technical-editing office has been divided between the Journals Fund and the *International Tables* Fund in percentages based on the staff time spent on each publication. The technical-editing costs for the Journals Fund were CHF 1 401 448 [for 12 017 published pages (5440 papers)] as compared with CHF 1 510 701 in 2008 [11 295 published pages (4795 papers)]. Submissions to the open-access-only *Acta E* increased to 4166 in 2009 from 3556 in 2008. The Journals Fund has also been charged with admin-

istration expenses as in previous years as shown in the General Fund.

The *International Tables* account shows a deficit of CHF 150 498, as compared with a deficit of CHF 127 969 in 2008. The net sales income was CHF 89 026 in 2009 as compared with CHF 198 829 in 2008. From January 2010 the publisher will change from Springer to Wiley.

The *Newsletter* Fund account received a transfer of CHF 50 000 from the Journals Fund in 2009. The cost to the Union of producing the *Newsletter* in 2009 was CHF 89 331.

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 2009, CHF 30 390 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 146 902 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 2009 this Fund incurred expenses totalling CHF 30 739 and received a transfer of CHF 200 000 from the Journals Fund.