

Report of the Executive Committee for 2008

1. Twenty-First General Assembly and International Congress of Crystallography

The Twenty-First General Assembly and International Congress of Crystallography were held at the Osaka International Convention Centre, Osaka, Japan, 23–31 August 2008, by invitation of the Science Council of Japan and the Japanese National Committee for Crystallography. A report, including a detailed report of the General Assembly, has been published [*Acta Cryst.* (2009), A65, 390–442]. The General Assembly and Congress were attended by 2477 scientists, 140 accompanying members and 58 exhibitors from 66 countries and territories. The Eighth Ewald Medal and Prize were accepted by Dr D. Sayre at the Opening Ceremony. The first Gjønnes Medal in Electron Crystallography was awarded to J. Gjønnes. There were 36 Keynote Lectures, 98 Microsymposia and Open Commission Meetings. The abstracts in the published book of Collected Abstracts were prepared from electronic submissions and were also provided on a CD-ROM. A commercial exhibition comprising 58 companies and booksellers was organized. The General Assembly met on the evenings of Sunday 24 August, Monday 25 August and Thursday 28 August. Applications for membership from the Regional Committee of Crystallographers from Algeria, Latvia, Morocco, Tunisia, Turkey and Ukraine (Category I) and from the Regional Committee of Crystallographers from Bangladesh, Malaysia, Singapore, Thailand and Vietnam (Category I) were accepted. The withdrawal of the Adhering Body for Venezuela was confirmed. The change in the name of the Adhering Body for Korea was accepted. The change in Category of Adherence of the Adhering Body for India (from Category II to Category III) was accepted. The Minutes of the Twentieth General Assembly in 2005 were approved. Amendments to the Statutes and By-Laws were considered but not approved. The General Assembly received the triennial financial report and the reports of the Executive Committee, the Commissions, the Scientific Associates and Regional Associates and the Union Representatives on Other Bodies since the Twentieth General Assembly in 2005. New officers of the Union, Chairs and members of Commissions and Union Representatives were elected; the full list of these people is given as an Appendix to the report of the Twenty-First General Assembly and Congress. The formation of a new Commission on Crystallography in Art and Cultural Heritage was approved. Reports of the Chair of the Sub-committee on the Union Calendar, of the Chair of the Committee for the Maintenance of the CIF Standard, of the Chair of the Committee on Crystallographic Databases and of the Editors of the *IUCr Newsletter* were received. The good progress of the IUCr/Oxford University Press Book Series was noted. The General Assembly approved the recommendation that the unit contribution should remain unchanged at CHF 1000 for the years 2009–2011 inclusive. It reaffirmed its decision to hold the Twenty-Second General Assembly and Congress in Madrid, Spain, in 2011. It also provisionally accepted an invitation from the National Research Council for Canada to hold the Twenty-Third General Assembly and Congress in Montreal, Canada, in 2014. The Executive Committee met for several days before and most days during the Congress, mainly to deal with matters directly related to the business of the General Assembly and the work of the Commissions.

2. Other meetings

The IUCr sponsored the following meetings held during 2008:

II International Workshop on Layered Materials: ‘Structure and Properties’, Vercelli, Italy, 28–29 March.

Rietveld Refinement Training School, Durham, UK, 30 March – 3 April.

RapiData 2008, Brookhaven, USA, 6–11 April.

International School on Mathematical and Theoretical Crystallography, Gargnano, Italy, 27 April – 3 May.

12th International Workshop on Protein Crystallization, Quintana Roo, Mexico, 6–9 May.

Fourth Moroccan School of Crystallography, Rabat, Morocco, 26–29 May.

From Molecules to Medicines: Integrating Crystallography into Drug Discovery, Erice, Italy, 29 May – 8 June.

ACA Annual Meeting, Knoxville, USA, 31 May – 5 June.

European Charge Density Meeting, Gravedona, Italy, 6–11 June.

Crystallization: Focus on Membrane Proteins, Brookhaven, USA, 10–14 June.

Structure Determination from Powder Diffraction Data: a Hands-on Workshop on X-rays, Synchrotron Radiation and Neutron Diffraction Techniques including Experimental and Computational Aspects, Villigen, Switzerland, 18–22 June.

The Zürich School of Crystallography – Bring Your Own Crystals 2008, Zürich, Switzerland, 22 June – 5 July.

10th International Conference on Quasicrystals (ICQ10), Zürich, Switzerland, 6–11 July.

First K. H. Kuo Summer School of Electron Microscopy and Crystallography: Cryo-Electron Microscopy of Macromolecular Complexes, Beijing, People’s Republic of China, 14–16 July.

European Powder Diffraction Conference (EPDIC-11), Warsaw, Poland, 19–22 September.

3. Executive Committee

The membership of the Executive Committee, including new members elected at the General Assembly in 2008, is as follows: President: Professor S. Larsen (France/Denmark); Vice-President: Professor P. Colman (Australia); General Secretary and Treasurer: Professor S. Lidin (Sweden); Immediate Past President: Professor Y. Ohashi (Japan); Ordinary members: Professor E. Boldyreva (Russia), Professor L. T. J. Delbaere (Canada), Professor G. R. Desiraju (India), Professor C. J. Gilmore (UK), Professor C. Lecomte (France), Professor J. M. Perez-Mato (Spain).

4. Publications

Volume 64 of *Acta Crystallographica*, Volume 41 of *Journal of Applied Crystallography* and Volume 15 of *Journal of Synchrotron Radiation* were published.

5. 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].

6. Work of the Commissions

6.1. Commission on Journals

6.1.1. Overview. The total number of articles published in IUCr Journals in 2008 was 4795 (*Acta Crystallographica* Section E alone: 3556), which compares with 6637 in 2007 (Section E: 5181) and 5376 (Section E: 3991) in 2006. The number of pages published was also lower (11 295 compared with 16 138 pages in 2007 and 17 524 pages in 2006); this decrease is a result of the move of Section E to open access and also the change to a new short-format style for Section E. Of the total, 5448 pages were published electronically only.

In 2008, 702 pages were printed for Section A (510 in 2007), 791 for Section B (940 in 2007), 1197 for Section C (1510 in 2007) and 1294 for Section D (1283 in 2007). Section E published 4261 electronic only pages (8375 in 2007) and Section F published 1187 electronic only pages (1090 in 2007).

The average length of Full Articles was 10.0 pages for Section A, 9.3 pages for Section B, 3.6 pages for Section C, 9.1 pages for Section D, 1.2 pages for Section E and 4.0 pages for Section F. Average publication times were as follows: Section A 5.3 months, Section B 5.0 months, Section C 1.8 months, Section D 4.4 months, Section E 0.8 months and Section F 2.6 months. The rejection/withdrawal rates were: Section A 33%, Section B 35%, Section C 60%, Section D 20%, Section E 16% and Section F 9%.

The number of Full Articles published in *Journal of Applied Crystallography* (JAC) in 2008 was 120 (124 in 2007). The number of pages decreased from 1895 in 2007 (when the SAS 2006 Proceedings were published) to 1197. The average review time was 4.4 months and the technical-editing time 1.5 months; the overall publication time was 5.8 months. The rejection/withdrawal rate was 39%.

The number of Full Articles published in *Journal of Synchrotron Radiation* (JSR) in 2008 was 106 (64 in 2007). The number of pages increased to 666 in 2008 (535 in 2007). The average review time was 3.9 months and the technical-editing time 2.5 months; the overall publication time was 6.4 months. The rejection/withdrawal rate was 24%.

IUCr journals continue to be highly ranked amongst crystallographic journals, occupying four of the top six positions in crystallography. JAC had the highest impact factor at 3.6. Sections A, B and C, and JAC had cited half-lives of >10 years.

A Special Issue entitled *Crystallography Across the Sciences* 2 was published in Section A to mark 60 years of *Acta Crystallographica* and the IUCr. Proceedings of the 2nd International Symposium on Diffraction Structural Biology (ISDSB2007) were published in JSR, Proceedings of the CCP4 Study Weekend on Molecular Replacement were published in Section D and the Osaka Congress Abstracts were published in Section A.

Commission on Journals meetings were held in Osaka, Japan, just before the IUCr Congress, and were attended by over 80 editors and Chester staff. There was a plenary meeting and ten additional smaller meetings that covered individual journals or groups of journals. Topics discussed at the meetings included refereeing standards, publication ethics, author rights and open access, as well as promotion

of the journals, and developments in the submission and review system.

The conversion of Section E to an open-access journal has been successful, with over 250 articles submitted each month. The journal is healthy and still growing, but is now able to finance itself. Open access has become increasingly popular across the journals, and 90 (apart from Section E) open-access articles (about 7% of all possible) were published in 2008. All open-access articles are published with a Creative Commons Licence and are deposited in PubMed Central.

Two new online tools for authors were launched in 2008: a JMol toolkit for the preparation of enhanced figures, and *publBio*, which can be used to prepare the experimental data tables, the text and the figures for biological articles.

At the end of the year, more than 150 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 wellbeing of the journals and highly appreciated. The year marked the retirements of a number of Section Editors: George Ferguson retired from Section C to be replaced by Tony Linden; Bill Clegg and David Watson retired from Section E to be replaced by Bill Harrison, Jim Simpson and Matthias Weil; Mitchell Guss retired from Section F to be replaced by Manfred Weiss; and Denny Mills retired from JSR to be replaced by Gene Ice. Their contributions and those of the numerous retiring Co-editors mentioned in the individual reports are gratefully acknowledged.

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

G. Kostorz, Chair

6.1.2. *Acta Crystallographica* Section A. Section A published 702 pages in 2008, up from 510 in 2007. In addition, the Abstracts of the Osaka Congress comprise 642 pages. The increase is due to the publication, in January 2008, of a 271-page special celebration issue entitled *Crystallography Across the Sciences* 2 on the occasion of the 60-year anniversary of the IUCr, edited by Guest Editor Henk Schenk. The other 5 issues were regular ones. These contained 406 pages devoted to Research Papers and Short Communications, down from 440 for the 6 issues of 2007. The average publication time for regular papers remained constant at 5.3 months; the average review time decreased from 3.8 to 3.3 months.

There were 66 full papers, including 24 feature articles in the Special Issue, giving an average of 10 pages per article. The average numbers of full Research Papers per regular issue are similar for 2008 (8.4 with 8.9 pages) and for 2007 (7.8 with 9.1 pages). There were 6 Short Communications, and no Topical Reviews or Lead Articles in the regular issues. The proportion of withdrawn plus rejected manuscripts remained nearly unchanged at 33%. There is no backlog in the editorial offices. In general, the statistics look favourable compared to last year's thanks to the Special Issue, and average values are stable. However, absolute numbers of regular research papers, 42 in 2008 against 47 in 2007, differ.

Section A is a high-level journal with a very diverse range of topics. In the five regular issues, 52% of the papers treat phasing, refinement, charge density and electron crystallography, 36% are on topics in group theory, tensors, topology and crystal chemistry, and 12% are in the field of diffraction physics. Papers may also be classified as methodological, mathematical, of interest to materials science or to macromolecular crystallography. The impact factor increased to 2.385. The geographical distribution of the origins of the articles (counted as integral or half-integral numbers) is still dominated by Europe 56% (−1), followed by the Americas 26% (+7) and

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
A60	2004	644	96	78	7.8	18	2.0
B60		763	87	84	8.9	3	3.3
C60		1694	556	554	3.0	2	4.0
D60		2406	511	462	4.9	49	3.0
E60		4676	1811	1803	2.6	8	1.6
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	6247	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	4514	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

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
37	2004	1041	170	110	7.7	27	4.0	33	2.3
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

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
11	2004	512	119	85	5.5	3	3.3	31	1.0
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

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

Asia+Australia 18% (–6). 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 Sue Barnes and Nicola Ashcroft.

In the pipeline for 2009 and 2010 are two Special Issues and four Lead Articles.

D. Schwarzenbach, Editor of Section A

6.1.3. Acta Crystallographica Section B. Section B continues to publish articles of very high quality. Many articles report work on several related compounds or phases using a variety of techniques, some of which are still being developed. The results reported and conclusions drawn will be of lasting importance.

The number of pages printed for Section B decreased from 940 in 2007 to 791 in 2008. This change is probably partly a consequence of the drop in the impact factor that occurred when the highly cited papers of the 2002 special database issue were no longer included in the three-year running average. It may also be that authors of Section B articles are including more work in each paper. The average length of a Research Paper has been about nine pages for many years, but the average for 2008 was marginally higher at 9.3 pages. It seems likely that the average length would be even greater if the supplementary material were not so easily available. Authors now deposit many results in order to keep the printed articles more focused and easier to read.

The impact factor in 2007 (2.2) was the same as in 2006. The 2003 jump in the number of rejected manuscripts that accompanied the spike in the impact factor continued for several years, but the number of unsuitable submissions now seems to be dropping to more normal levels.

Given the content of most manuscripts it is remarkable that the time to publication decreased again last year (from 6.3 to 5.8 to 5.0 months in the period 2006–2008). At least part of this improvement is a result of the software developments in the Chester office.

The fractions of papers dealing with inorganic/metallic structures and with organic structures are so variable ($\pm 10\%$ relative to the means) that no trend can be discerned. The fraction of metal-organic (organometallic) papers is much smaller (*ca* 10%) and more constant.

During 2008 Co-editors Sandy Blake, Lee Brammer, Gautam Desiraju, Finn Krebs Larsen, Lynne McCusker and Bill Stallings retired from the board, some after many years of service. We are grateful to them all.

C. P. Brock, Editor of Section B

6.1.4. Acta Crystallographica Section C. The editorship of Section C passed from George Ferguson to me during the Osaka Congress. George is most warmly thanked for his sterling stewardship over the last nine years. Section C continues to specialize in the rapid publication of high-quality studies of novel and challenging crystal and molecular structures. In 2008, Section C published 328 papers (32 inorganic, 114 metal-organic and 182 organic) in a total of 1197 pages, which is down from the 447 papers (-27%) and 1510 pages produced in 2007 (-20%). In the same period, the number of submitted papers also fell from 928 to 751 (-20%). The proportion of inorganic (13%), metal-organic (35%) and organic papers (55%) remains within the bands of previous years. The citation impact factor, after being nearly 0.90 in 2006, fell to 0.72 in 2007, which is more in line with 2003–2005. Average publication times improved to slightly under two months for the first time. Approximately 60% of submissions to Section C in the past year were either subsequently withdrawn by the authors or rejected – an 8% increase over 2007 and the highest ever, although close to the rate in 2005.

The decrease in the number of papers submitted to Section C in 2008, combined with the high rejection/withdrawal rate, is cause to watch these trends closely. The number of submitted papers was slightly down and fairly constant during the second half of 2008, but low during November and December. Whether the trend continues, was some sort of seasonal effect, or is somehow related to the changes for Section E, remains to be seen. The high rejection/withdrawal rate

is primarily related to the quality of the submissions we receive. While the structure determinations are usually carried out competently, many papers are poorly written in terms of language or the depth and logic of the discussion. The large proportion of submissions from authors for whom English is a second language compounds the language issues and makes considerable work for the Co-editors, who often spend significant time essentially rewriting papers – well above the call of duty. At the other end of the scale, very high quality studies with some interesting outcomes often find their way into other journals.

How we address these problems is an open question. Section C continues to require high-quality work and significant discussion in the Comment section that goes well beyond just stating the basic features of the structure. The acceptance of briefer papers would seem to muddy the distinction between Sections C and E. In order to improve the perception of the journal in the community, the *Notes for Authors* for 2009 have been modified slightly to make it clearer that Section C considers papers reporting challenging structures, when the difficulties are adequately documented. It has also been announced that the journal will publish previously reported structures where the earlier report said little about the crystal structure itself (such as in a chemistry journal). My editorial in the January 2009 issue also highlighted these points and it is hoped that these policies bear fruit. In addition, one of the Editors of Section E, Jim Simpson, and I are working on a paper to help educate people that validation is a useful tool and is not designed as a ‘firewall’, to help counter misconceptions in that area.

Co-editors report frequent difficulties finding good and thorough referees who respond within a respectable timescale. We ask for responses in 7–10 days, if possible, otherwise the fast publication times cannot be maintained. Part of the problem is that a lot of good referees are now Co-editors themselves, and that people everywhere are constantly bombarded with review requests from many journals to the point where they simply ignore requests that they do not wish to act upon.

Improvements during 2008 for Sections B, C and E include the validation of structure-factor files, which is able to detect things like overlooked twinning and has revealed that the submitted structure-factor files are sometimes not the ones corresponding with the refinement used to prepare the submitted CIF. A new feature of IUCr Journals in general is the ability to generate additional enhanced crystallographic diagrams online either before or at the time of submission. It is hoped that use of this facility will increase during 2009.

It is a pleasure to welcome Len Barbour (University of Stellenbosch), Ulli Englert (RWTH Aachen), Phil Fanwick (Purdue University), Andreas Goeta (University of Durham), Maciej Kubicki (Adam Mickiewicz University), Vratislav Langer (Chalmers University of Technology), Peter Müller (MIT) and Hidehiro Uekusa (Tokyo Institute of Technology) as new members of the Section C Editorial Board. In addition, Alexander Blake has been appointed as Deputy Section Editor to assist with reading of the proofs. 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: Leonid Aslanov, Nobuo Ishizawa, Shigeru Ohba, Maryjane Tremayne and Madeleine Helliwell. I would also like to take this opportunity to thank all the current Section C Co-editors and the Chester Editorial Office staff for their outstanding efforts on behalf of Section C and for the support they have given me as a newly appointed Section Editor.

A. Linden, Editor of Section C

6.1.5. *Acta Crystallographica* Section D. Section D focuses on two main aspects of biological crystallography: new developments in crystallographic methods and novel biological structures. In 2008 these were evenly balanced, with approximately 45% of the articles published featuring aspects of methodology and the remainder presenting new structures. All structural papers were expected to provide new insights into biology, chemistry or structure. A small number of articles that did not meet this criterion, but which otherwise met the required standards of quality, were transferred to the partner journal, Section F.

An important development during 2008 was the increase in the impact factor for Section D, from 1.69 in 2006 to 2.62 in 2007. 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 stand-out feature of each year is the CCP4 Special Issue, usually published as the first issue of the year. The January 2008 issue, the latest in this series, focused on molecular replacement. It is now nearly 50 years since the basis of the molecular-replacement method was presented by Rossmann and Blow, in a classic paper in *Acta Crystallographica* (1962), and the power and importance of this approach to phasing has continued to grow in a spectacular way. We thank the Guest Editors for this issue, Garib Murshudov, Frank von Delft and Charles Ballard, for bringing together 17 articles that nicely cover the present state of the art. These articles are of enormous benefit to the macromolecular crystallography community.

Both the number of articles published during 2008, and the total number of pages, were similar to 2007: a total of 135 Full Articles, 13 Short Communications, and 3 Commentaries (Editorial comments or Letters to the Editor). The total number of pages was 1294, slightly more than in 2007, with the average length of full articles being 9.1 pages. Publication times remain good, at an average of 4.4 months and the electronic submission system works well.

We thank three retiring Co-editors, Felix Frolov, Glaucius Oliva and Bill Stallings, for their excellent contributions to the journal, and we welcome three new Co-editors, Mark Bartlam, Gerard Kleywegt and Elspeth Garman. Gerard and Elspeth bring outstanding expertise in methods, in different areas, while Mark will be our first Co-editor in the People's Republic of China. We see China as an important area of future expansion. Finally, we thank the Chester office for the outstanding technical quality of the journal production, and we are 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

6.1.6. *Acta Crystallographica* Section E. In August of 2008, the founding Section Editors of the journal, Bill Clegg and David Watson, retired. They were replaced by Bill Harrison from Scotland, Jim Simpson from New Zealand and Matthias Weil from Austria at the Osaka Congress. It is appropriate to begin this report by acknowledging the fantastic contribution made by these former Section E Editors. They brought the journal from a concept to an extremely successful reality, oversaw changes to the new short-format papers and steered the journal through the process of moving to open-access status. Throughout these changes and developments they ensured that papers appearing in the journal maintained a high degree of quality and consistency, and handed over an extremely efficiently managed operation to the new Section Editors. Their work for the journal is acknowledged with sincere thanks.

As the year progressed it became obvious that the move to open access for Section E had not only been successful, but had also allayed the fears of many sceptics who felt that the requirement to pay for publication would lead to the journal's demise. The present funding model appears secure and there are no plans to increase the open-access charge for the journal in 2009. As Section Editors, we will do all that we can to maintain and build on this successful outcome.

Following a decline in submissions in the first three months after the journal became open access, the number of papers submitted each month has increased gradually to a level approaching that of 2006. The number of papers submitted in 2008 was 3846, down 40% from the number in 2007. The deluge of papers that flooded into the submission system in October and November of 2007, prior to the move to open access, accounts largely for the change. Nonetheless, the steady increase in submissions throughout 2008 augurs well for the future of the journal. The total number of papers published in 2008 was 3556, compared with 5181 in 2007, 3991 in 2006 and 2887 in 2005. Of these, 63% described structures of organic, 34% structures of metal-organic and 3% structures of inorganic compounds. 51% of authors were from the People's Republic of China, 6% from India, 5% from the USA, 4% from Germany, 4% from Malaysia, 3% from Iran and 2% from Pakistan, with smaller percentages from other countries. The number of papers withdrawn or rejected for a variety of reasons remains similar to previous years at 16%, while the journal's impact factor is 0.5.

As new Section Editors we are delighted to have inherited a cohort of hardworking Co-editors whose knowledge and expertise is of enormous benefit to us, the journal and the small-molecule crystallographic community. Dr J. Low, Professor A. Roodt, Professor A. M. Z. Slawin and Professor B. M. Yamin retired as Co-editors during last year and we are very grateful to them for their work on behalf of the journal. There are currently 52 Co-editors including the three joint Section Editors. We expect that there will be a small number of additions to the Co-editorial board in 2009 to accommodate the steady increase in submissions and to spread the load among the Co-editors.

The *checkCIF* software continues to be developed thanks to the efforts of Ton Spek and Mike Hoyland. Recently, some new checks on submitted structure-factor files have been incorporated into the submission process. These additional checks effectively compare values reported in the CIF with the contents of the structure-factor file and other metrical information that can be calculated directly from the reflection data. Missing reflections out to θ_{\max} and reflections that may be affected by the beamstop are also indicated. One of the results of these additional checks has been a disturbing increase in evidence for manual editing of CIF files to report better *R* factors or to alter parameters such as minimum and maximum difference peaks that generate alerts requiring additional input from the authors. In such cases our policy has been to deal directly with the authors and, if a suitable explanation is not forthcoming, to reject the article with no right of re-submission. Other difficulties have arisen with authors being dropped from or added to papers with no satisfactory explanation, or added simply because they had funding to pay the open-access fee. The statement on authorship in the *Notes for Authors* has been modified in an attempt to minimize such occurrences.

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 and to Peter Strickland for his ready availability with sound guidance and wise counsel.

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

6.1.7. *Acta Crystallographica Section F*. The fourth year of publication of Section F continued the maturation process for this relatively young journal as a venue for rapid publication of structure and crystallization communications on biological macromolecules. In 2008 the number of articles published was 302 and the number of pages published was 1187. The average time from submission to publication, including peer review, remained a very rapid 2.55 months.

2008 was marked by several important milestones. First and foremost, founding Section Editor J. Mitchell Guss retired at the conclusion of the Osaka Congress and is replaced by Manfred S. Weiss. All who worked with Mitchell, and that includes most prominently the current Section Editors, enjoyed his comity and good humour as well as his wise advice and guidance, and all thank him for his service and wish him well. Second, the streamlining project, long a featured development project of Section F, was officially declared completed. In fact, as the project matured, its goals morphed into a much more ambitious effort that simply outstripped the goals of streamlining and became a much bigger project, the results of which will be launched in 2009. The product of that more ambitious project includes a template-based web portal to guide and assist authors in entering data and assembling a draft article and will produce as a by-product an mmCIF file of the data that will be freely available to databases. Thanks go to Gernot Kostorz, 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. Third, in summer 2008 we received our first impact factor. The value, 0.645, is small, but is higher than expected when one considers that the bulk of our articles are crystallization communications, which typically have small citation rates. Fourth, 2008 saw the introduction of a new service that allows authors to create enhanced illustrations of molecular structures; the first illustration prepared in this way appeared in the article of Mueller-Dieckmann *et al.* [*Acta Cryst. (2008)*, F64, 156–162] on the crystal structure of mouse ADP-ribosylhydrolase 3. Finally, approval was granted to assemble a panel of experienced referees to provide reviews at a rate of about one a month, each review returned within a two-week review period. We have made great progress in reducing our average time between submission and publication. We believe this is the next step needed to assure that more of our reports are completed in a timely fashion and with high standards of quality. The referee panel will begin its work about mid-year 2009 and we are very much looking forward to working with the panel members.

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

6.1.8. *Journal of Applied Crystallography*. The number of Full Articles published in *JAC* in 2008 was 120; this is similar to 2007 when 124 Full Articles were published. The number of pages decreased from 1895 in 2007 (when the SAS 2006 Proceedings were published) to 1197. The number of manuscripts submitted was 258, compared with 258 in 2007 and 399 in 2006 (when the numbers were boosted by submissions for the SAS 2006 Proceedings). There was an increase in the impact factor to 3.6, making *JAC* the highest ranked IUCr journal; the journal also has a long cited half-life (>10 years).

Online submission and a new policy to put articles online as soon as they have been technically edited, have kept publication times down. The average review time was 4.4 months and the technical-editing time decreased to 1.5 months; the overall publication time decreased to 5.8 months. The average publication time for Short Communications was 3.9 months.

The *JAC* board met just before the Osaka Congress; it was considered that as *JAC* articles are widely read it is important that they are written in a style that is accessible across the crystallographic community. The publication of Special Issues, and Lead and Feature Articles was also discussed. It is planned that the journal will publish a Special Issue on crystallographic education in 2010.

The year saw the retirement of Doug Ohlendorf as Co-editor and Cryocrystallography Editor; I thank Doug for his hard work on the journal. It is a pleasure to welcome Elspeth Garman (University of Oxford) as a new Co-editor. I also thank the Chester editorial staff for all the work they do on the journal.

A. Pyzalla, Editor of *JAC*

6.1.9. *Journal of Synchrotron Radiation*. In 2008, *JSR* published 106 Research Papers and a total of 666 pages in the six issues. This was an increase in both articles and pages as compared to 2007 primarily due to a large Special Issue. This Special Issue on Diffraction Structural Biology was published in March (Volume 15, Part 3) with Noritake Yasuoka serving as Guest Editor. We continue to 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 2008. 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 2008 increased to 3.9 months (3.5 months in 2007) and the technical-editing time to 2.5 months (1.5 months in 2007) resulting in an overall publication time of 6.4 months (5.0 months in 2007). This increase was mainly due to the publication of the large Special Issue. We are happy to report that the impact factor increased to 3.0 *versus* 2.4 for 2007.

Denny Mills retired as Editor at the Osaka Congress and is replaced by Gene Ice. We thank Denny for his work.

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

6.2. Commission on International Tables

The Commission discussed the current status and future developments of the *International Tables* series extensively in Closed and Open Commission Meetings during the Osaka Congress.

A review of progress with **International Tables Online** was presented by Nicola Ashcroft. Several future improvements were proposed and were accepted by the Commission.

The new Editor of Volume A, Mois Aroyo, presented his ideas for the sixth editions of Volume A and the Brief Teaching Edition of Volume A. The new edition of Volume A will include important modifications of the contents and a rearrangement of the tabulated material of the fifth edition. The text and the data will be grouped into three main parts:

(1) Part 1: Introduction to space-group symmetries. The aim of the introductory part will be 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 of *International Tables*. The main topics to be treated in Part 1 are: a general introduction to group theory, crystallographic symmetry operations and their representations by matrices, coordinate-system transformations, a general introduction to space groups and their description in the

tables, reflection conditions, sections and projections of space groups, subgroups and supergroups of space groups and relations between Wyckoff positions for a group–subgroup pair of space groups.

(2) Part 2: Tables of plane and space groups. This part will start with the guidelines and examples necessary for the presentation of the tabulated data followed by the tables of plane and space groups. For each plane- and space-group type the following symmetry items will be listed: headline block with the group symbols, space-group diagrams, origin of the unit cell and asymmetric unit, symmetry operations, generators, general and special Wyckoff positions, reflection conditions and symmetry of special projections. The maximal subgroup and minimal supergroup data, available in part in the fifth edition of Volume A, will be omitted. (Complete data on maximal subgroups and minimal supergroups form part of Volume A1.)

(3) Part 3: Advanced topics in space-group symmetry. The following, more specialized, aspects of space-group symmetry will be discussed in this part: the mathematical approach to space groups, crystal lattices, point groups and crystal classes, symbols for space groups, lattice complexes and normalizers of space groups.

The main purpose of the new edition of the Brief Teaching Edition of Volume A is to provide an introduction to the space-group data in Volumes A and A1. It will consist of two parts. The first part includes a series of introductory lectures on the symmetry items that appear in both Volumes A and A1. The text of this part will be an extended version of the corresponding part of the sixth edition of Volume A with additional illustrative examples and exercises to provide the reader with practical experience in the use of the crystallographic symmetry data of Volumes A and A1. The second part of the Teaching Edition will focus on the presentation of the tabulated symmetry data of Volumes A and A1. It will contain descriptions of the symbols and terms used in the tables and detailed guides for their use. The new edition will also include selected plane-group and space-group examples of varying complexity useful for teaching of symmetry.

The first edition of Volume A1 (Editors Hans Wondratschek and Ulrich Müller) was published in 2004. The second edition is in preparation and is expected to be published in 2009. The volume contains a complete list of maximal subgroups of the space groups. For the second edition, all detected errors will be corrected and local improvements will be introduced.

Part 1 deals with group-theoretical aspects of space groups, group–subgroup relations and the underlying mathematical background. In the new edition, the mathematical background will be extended to the theory of the minimal supergroups of the space groups. A new section will be added which gives instructions on how to build trees of group–subgroup relations for crystal structures that can be derived from a high-symmetry structure type (aristotype). Trees of this kind are useful to show crystallographic relations between crystal-structure types and between the polymorphic forms of a compound. A new section on the Bilbao Crystallographic Server will also be added with descriptions of the databases and computer programs that are related to the subjects of the volume.

Part 2 contains complete listings of all maximal subgroups for each space group, including their general positions or their generators, their conjugacy relations and transformations to conventional settings. The new edition will contain a detailed discussion of the listed supergroup data, and a procedure for the complete derivation of the minimal supergroups from the listed (complete) data on maximal subgroups will be added.

Part 3 lists the relations between the Wyckoff positions for every maximal subgroup of every space group, including the cell transfor-

mations and coordinate transformations. In both Parts 2 and 3, the infinitely many isomorphic subgroups have been included in a parametrized form.

2008 was marked by the completion and the publication in August of the third edition of Volume B, edited by Uri Shmueli. A new chapter on modern extensions of the Ewald method for Coulomb interactions in crystals and three new sections on electron diffraction and electron microscopy in structure determination, describing point-group and space-group determination by convergent-beam electron diffraction, three-dimensional reconstruction, and single-particle reconstruction, were included. The chapters on space-group representations in reciprocal space, direct methods, Patterson and molecular replacement techniques, and disorder diffuse scattering were substantially revised and several other chapters were updated. Following the publication of the third edition, Uri announced his retirement as Editor of the volume. The Commission and the community of crystallographers extend their warmest thanks to him for the fruitful work he has done over the years.

Volume C (Editor Hartmut Fuess) is under revision. Most of the existing authors are willing to contribute to the new edition. Some chapters have to be rewritten.

A second edition of Volume E (Editors Vojtech Kopský and Danny Litvin) is in preparation. Typographical errors will be corrected and additional information will be 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 crystallographic 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 will be added below the corresponding international notation.

Daniel Himmel joined Michael Rossmann and Eddy Arnold as Editors of Volume F. The preparation of a second edition is well under way; the new edition will include around 30 new articles and should be on sale in 2010.

There are no immediate plans for new editions of Volume D (Editor André Authier) or Volume G (Editors Sydney Hall and Brian McMahon), although some chapters in each volume may be updated in **International Tables Online**.

Plans for new volumes on powder diffraction and materials were discussed at the Commission meetings, but no decision was reached.

The online series has been well received and continues to sell well (77 subscriptions to institutions and large consortia were sold in 2008). Sales of the print volumes in 2008 were 213 copies of Volume A, 195 copies of the Teaching Edition, 63 copies of Volume A1, 30 copies of the second edition of Volume B, 114 copies of the third edition of Volume B, 80 copies of Volume C, 67 copies of Volume D, 39 copies of Volume E, 65 copies of Volume F and 43 copies of Volume G.

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

6.3. Commission on Aperiodic Crystals

The Commission has continued actively to promote aperiodic crystallography in 2008, in organizing meetings and workshops as well

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

As part of these activities, the Commission continued to promote aperiodic crystallography at national, regional and international meetings. The 10th International Conference on Quasicrystals, organized by W. Steurer, took place in Zürich, Switzerland, 6–11 July. A satellite meeting on the Mathematical Aspects of Aperiodic Order took place, 3–5 July 2008, at the University of Bielefeld, Germany [organized by D. Lenz (Chemnitz) and C. Richard (Bielefeld)]. During the Osaka Congress, two Keynote Lectures and four Micro-symposia in the area of aperiodic order have been organized. A workshop on Combinatorial and Computational Aspects of Tiling was organized at London Imperial College, UK, 30 July – 6 August, by E. Harriss and J. Lamb.

The most important upcoming meeting for the Commission is Aperiodic 2009 to be held in Liverpool, UK, 13–18 September 2009 (<http://www.aperiodic09.org/index.html>). The meeting is organized by R. McGrath and U. Grimm, and is shaping up to be a very exciting meeting. Other upcoming activities include the 6th Workshop on the Structural Analysis of Aperiodic Crystals organized by S. van Smaleen, 5–8 March 2009 at the University of Bayreuth, Germany.

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

M. de Boissieu, Chair

6.4. Commission on Biological Macromolecules

The Commission has continued to support the vitality of the biological crystallography community, particularly through recommending and supporting IUCr proposals to hold meetings, workshops and schools. Numerous meetings of this type will be held in Africa, South America, Europe, North America and Southeast Asia in 2009.

A key activity of the Commission was contributing to the Osaka Congress. Structural biology was represented at all levels, with the revelation of spectacular novel macromolecular structures and evolving methods described in plenary talks, invited presentations, topical sessions and posters. A large number of students attended and participated from all corners of the world and the travel of many young scientists was sponsored by the IUCr.

Regional meetings with biologically relevant content sponsored by the IUCr in 2008 included in April: the RapiData course (Brookhaven, USA) and an International School on Mathematical and Theoretical Crystallography (Gargnano, Italy); in May: 12th International Workshop on Protein Crystallization (Quintana Roo, Mexico), Fourth Moroccan School of Crystallography (Rabat, Morocco), From Molecules to Medicines: Integrating Crystallography into Drug Discovery (Erice, Italy), and the Annual American Crystallographic Association Meeting (Knoxville, USA); in June: Crystallization: Focus on Membrane Proteins (Brookhaven, USA); in July: First K. H. Kuo Summer School of Electron Microscopy and Crystallography: Cryo-Electron Microscopy of Macromolecular Complexes (Beijing, People's Republic of China); and in September: the European Powder Diffraction Conference (EPDIC-11, Warsaw, Poland). These meetings, schools and workshops provide

tremendous value in training in and dissemination of novel scientific methods.

E. Arnold, Chair

6.5. Commission on Charge, Spin and Momentum Densities

The most important event of the Commission was at the time of the Osaka Congress. A Keynote Lecture was given by C. Lecomte, former (2002–2005) Commission Chair, on experimental charge density modeling, where he illustrated a number of interesting frontier examples covering the study of the charge and spin density of long-living metastable states, the analysis of charge-transfer mechanisms in charge-transfer complexes and the first charge-density studies of subatomic resolution protein structures. Five Micro-symposia (MS24, MS37, MS68, MS75, MS82) were organized by our Commission, while another two were jointly organized with the Commission on Electron Crystallography (MS48) and the Commission on XAFS (MS94). Emphasis has been placed on new research directions (photo-excited-state crystallography, MS24), on the use of charge-density research to extract physical and chemical properties (MS68), and on the complementary information for materials science coming from the proper combination of charge, spin and momentum density studies (MS75) or from integrated electron and X-ray diffraction experiments (MS48). Latest advances in magnetic Compton scattering have been reported in MS82, particularly in new collaborations with high-pressure and neutron-scattering experiments. Progress in the complementary use of accurate charge-density studies and quantum calculations (MS37) have also been addressed. The emerging field of X-ray Raman scattering was discussed in MS94, with particular emphasis on the detection of short- and long-range structural changes in amorphous phases of water. Owing to the truly interdisciplinary character of all the topics discussed and to the diversity of the application fields involved, a large audience attended these sessions and, in general, a quite vivid discussion took place.

The Commission met during the Congress and approved its nominations for new members. During the Commission meeting, the next Sagamore meeting to be held in the USA in August 2009 was discussed; the decision to promote (basic) schools to disseminate charge, spin and momentum density (CSMD) research knowledge among the new generations of crystallographers (which was proposed by C. Lecomte and other Commission members) was taken. An intermediate report on the Constrained Experimental Wavefunction Commission Project was presented by D. Jayatilaka.

Another important activity of the Commission was the 5th European Charge Density Meeting (ECDM-V), <http://www.ecdm5.istm.cnr.it/ECDM-Introduction.html>), which took place in Gravedona, Italy, on the shores of the Lake Como, 6–11 June, as a continuation of analogous meetings held in Nancy, France (1996), Sitges, Spain (1999), Sandbjerg Estate, Denmark (2003), and Brandenburg on the Havel, Germany (2006). The meeting was this time organized by C. Gatti, P. Macchi and R. Destro, with help from many colleagues at the University of Milan, the University of Insubria (Como) and CNR-ISTM Milan, and under the scientific supervision of a Scientific Committee and an International Advisory Committee comprising, among others, many Commission members. ECDM-V had an innovative format, since the usual ECDM conference had been joined with the DFG-1178 annual meeting, where DFG-1178 is the acronym of an impressive programme funded by the Deutsche Forschungsgemeinschaft (DFG) to spread the word of charge-density analysis in both the chemistry and the materials science communities. Participation and the programme schedule exceeded any expectation

and were much larger than in all previous editions of this series of conferences. 170 registered participants attended the meeting, from more than 20 countries and 4 continents. 11 Keynote Lectures, 38 talks (in 11 Microsymposia) and 70 posters were presented during the meeting.

C. Gatti, Chair

6.6. Commission on Crystal Growth and Characterization of Materials

The Osaka Congress was a busy time for the Commission. We had the rare opportunity to meet in person and to discuss our plans and activities. The main concern at our meeting on Tuesday 26 August was the organization of the future international schools and conferences in the area of crystal growth, as well as the future membership of the Commission.

Commission members were very active at the Congress. On the first day of lectures J. M. Garcia-Ruiz presented an excellent Keynote Lecture (chaired by K. Tsukamoto) on Growth of Silica Biomorphs: Self-Assembled Crystal Aggregates with Non-Crystallographic Morphologies. Later, there were four Microsymposia organized directly by this Commission, all four well received and well attended:

MS4: Hydrothermal Growth of Crystals, organized and chaired by K. Byrappa and S. Feng;

MS13: Growth of Single Crystals for Neutrons and X-rays by Floating Zone Technique, by H. Dabkowska and I. Tanaka;

MS38: Self-Organization and Self-Assembly, by D. Pawlak and P. Metrangolo;

MS49: Wide Gap Semiconductors for Health, Energy and Environment, by K. Kakimoto and D. Bliss.

The reports from these Microsymposia will be published in the *IUCr Newsletter*.

Following the Osaka Congress, four new members and five new consultants joined the Commission. They replaced the members and consultants who have stepped down. I would like to take this opportunity to welcome J. Anwar, A. Glikin, C. Klemenz, D. Klimm, A. Pyzalla, J. Ng, E. Talik, K. Tuskamoto and A. Zappettini to our group and to thank R. Fornari, T. Ohachi, P. Rudolf, A. Pajaczkowska, P. Dryburgh and A. Voloshin for their strong input to the work of this Commission during their terms.

In 2008, the IUCr, following Commission recommendations, supported two important meetings, both related to crystallization of biological materials:

The 12th International Conference on the Crystallization of Biological Macromolecules (ICCBM-12), in conjunction with the International School on Biomacromolecular Crystallization (ISBC-12), took place in Mexico, 2–9 May 2009. There were 150 attendees from different countries for ICCBM-12, and additionally 40 invited professors, instructors and trainers for the workshop. It was organized and reported by A. Moreno.

The second meeting, Crystallization: Focus on Membrane Proteins 10–14 June 2008, was organized in Brookhaven, USA, by V. Stojanoff. Thanks to IUCr support it was possible to assist five students from around the world to take part in this venue. More information about this workshop can be found at <http://www.nsls.bnl.gov/newsroom/events/workshops/2008/crys/>.

In 2008 I received requests for writing letters of support for several local and international meetings in 2009 [applications for meetings in Romania, Malaysia, Italy, Brazil (two), Ukraine, USA, UK, Japan and Poland]. I send letters of support for meaningful meetings related to crystal growth.

On another note: it is my pleasure to report that A. Glikin has published the book *Polymineral-Metasomatic Crystallogenesis* (Springer): <https://www.springer.com/materials/book/978-1-4020-8982-4>.

As in previous years many of the Commission members and consultants (S. Baldochi, H. Dabkowska, T. Duffar, K. Kakimoto, A. Moreno and E. Vlieg) were involved in the ongoing work of the International Organization for Crystal Growth.

H. A. Dabkowska, Chair

6.7. Commission on Crystallographic Computing

Prior to the Osaka Congress, the traditional Crystallographic Computing School took place in the Kansai Seminar House, Kyoto, Japan, 18–23 August 2008. The School had the theme of Sharing our Knowledge and included an emphasis on the issue of Age Concern, where a significant number of crystallographic software developers are either formally retired or soon to retire. The School's Organizing Committee were A. L. Spek (Chair), Min Yao (local contact), H. Powell, R. Grosse-Kunstleve, A. Nakagawa and L. M. D. Cranswick. The School was structured to foster the exchange of ideas via formal lectures and a wide selection of tutorials in the afternoon. Lecturers were L. Bourhis, Hai-fu Fan, C. Farrow, R. Grosse-Kunstleve, R. Hooft, G. Murshudov, G. Oszlányi, J. Pflugrath, H. Powell, A. L. Spek, D. Svergun, T. Terwilliger, B. Toby, C. Vonrhein, D. Watkin and Min Yao. School information, including abstracts and photographs, can be found via the Commission web page at <http://www.iucr.org/resources/commissions/crystallographic-computing/>. The presentation notes were collated, and are also available on the Commission web site as *CompComm Newsletter* No. 9, October 2008. Thanks are especially owed to Min Yao as local contact and R. Grosse-Kunstleve for organizing and coordinating the tutorials.

Nine sessions were organized by the Commission for the Osaka Congress, and were generally well attended. The Chairs and Co-Chairs for all the sessions are thanked for their organizing work. There were a number of lectures related to developments of the 'charge flipping' algorithm for *ab initio* structure determination and for space-group determination. This included a Keynote Lecture on Charge Flipping by G. Oszlányi. A session on Crystallographic Algorithm Libraries was organized by J. Wright and L. Palatinus in honour of P. Jane Brown, who is one of the Cambridge Crystallographic Subroutine Library developers. As has occurred since the 1999 Glasgow Congress, a non-commercial Crystallographic Software Fayre was held at the Osaka Congress, 26–29 August. The local organizers are thanked for providing facilities for the software fayre.

The main priority for the coming triennium is the organization of the traditional Crystallographic Computing School prior to the 2011 Congress in Madrid. Planning is already underway for holding this in Mieres, Northwest Spain (about 3 to 5 hours from Madrid), 15–21 August 2011. The Organizing Committee comprises L. M. D. Cranswick (Chair), S. Garcia-Granda (local contact), H. Powell (speakers programme), R. Grosse-Kunstleve (tutorials programme), A. L. Spek, Min Yao and J. Rius. Preliminary costings have been provided by the local Chair and a web page for promoting the school is being organized.

L. M. D. Cranswick, Chair

6.8. Commission on Crystallographic Nomenclature

Meeting in Osaka. The Commission held a closed meeting at the Osaka Congress on 25 August 2008.

Online Dictionary of Crystallography. A new Editor-in-Chief, G. Chapuis, has been appointed. The present Board of Editors is: A. Authier (Founding Editor), G. Chapuis (Editor-in-Chief), H. M. Einspahr (Editor for Biocrystallography), H. Flack (Editor) and B. McMahon (Administrator). The Online Dictionary may be consulted at http://reference.iucr.org/dictionary/Main_Page.

Nomenclature issues. Following the debate in Osaka on the ‘non-crystallographic symmetry’ issue raised by M. Nespolo, there is an ongoing email discussion among members of the Commission on the definitions of ‘non-crystallographic symmetry’ and ‘local symmetry’, in particular in the context of biocrystallography.

A. Authier, Chair

6.9. Commission on Crystallographic Teaching

For 2008 the activity of the Commission has been focused on the organization of the Summer School on Mathematical and Theoretical Crystallography held in Gargnano, Lake Garda, Italy, 27 April – 2 May 2008. The School was planned in collaboration with the Commission on Mathematical and Theoretical Crystallography and the programme, after a first part devoted to introductory lessons on crystallographic symmetry, included group theory applied to crystallography, the symmetry principle in crystal chemistry, the role of symmetry and energy in structural phase transitions, how intermolecular energies determine crystal symmetry and intermolecular geometry. Emphasis was also placed on computer tools for crystallography.

The students numbered about 40 coming mainly from Europe but also from India, the Philippines, Japan, Armenia, Turkey and the USA. They were very interested and motivated, and enjoyed working until late in the evening with tutorials and exercises. The lecturers were very collaborative and were available to help students all the time. Villa Feltrinelli, the location chosen for the School, was very much appreciated by the students and could be a good candidate for future similar activities.

In July 2008 the second Zürich Crystallography School – Bring Your Own Crystals was held, again organized by A. Linden and H.-B. Bürgi with the help of G. Chapuis. The School was planned in a similar way to the first, trying to improve the organization of the tutorials to make them more fruitful for students. The attendance was limited to about 20 students and in this way the ratio lecturers/tutors/students was very good.

Commission members K. Ogawa, E. Boldyreva and L. M. D. Cranswick with the help of P. Spadon also actively worked as members of the International Programme Committee for the Osaka Congress. In particular the Commission was involved in the organization of MS11: Pitfalls and Successes in Crystallographic Teaching, MS44: Teaching Macromolecular Crystallography (together with the Commission on Biological Macromolecules), MS25: Crystallographic Teaching using New Computer and Internet Based Approaches (with the Commission on Crystallographic Computing). In addition, the Commission organized a pre-conference workshop on Teaching Crystallography in the 21st Century that was very successful and gathered together a lot of crystallographers for one day. The contributions were highly varied and very interesting, and there was a great deal of discussion at the end of the workshop.

The Commission members (old and newly nominated) met during the Osaka Congress in order to discuss future activity and to assign tasks. The final decision was to try to organize a school in collaboration with the Commission on Aperiodic Crystals, targeted at newcomers in the field of aperiodic crystals and people outside the

field interested in aperiodic crystals, the level of the school thus being intended to be introductory. In addition, the Commission will try to organize, in collaboration with crystallography colleagues at Granada, a Pre-Conference School on Crystallization as a satellite meeting of the Madrid Congress in 2011.

P. Spadon, Chair

6.10. Commission on Crystallography in Art and Cultural Heritage

The Commission was approved by the General Assembly at the Osaka Congress. It covers two main issues: crystallography and symmetry in art, and crystallographic analysis (e.g. diffraction-based) of artworks and ancient materials.

The Commission has set up a web site at <http://www.crystallography.fr/crysac/> and has submitted an article to the *IUCr Newsletter*.

A Workshop on X-ray Techniques in Investigation of the Objects of Cultural Heritage, Chair: A. Rafalska-Lasocha, was held in Cracow, Poland, 18–19 September 2008, in association with EPDIC-11, Warsaw, Poland, 19–22 September 2008. The aim of the Workshop was to promote the development and use of X-ray techniques in order to extract information from the objects of cultural heritage and to have scientists and conservators present advanced methods of investigation in this area.

There will be a satellite meeting of the 25th European Crystallographic Meeting (ECM-25) entitled Symmetry and Crystallography in Turkish Art and Culture, Chair: M. Nespolo, Istanbul, Turkey, 14–16 August 2009 (<http://www.crystallography.fr/mathcrys/istanbul2009.php>). This satellite (organized by the Commission on Mathematical and Theoretical Crystallography in cooperation with the Commission on Crystallography in Art and Cultural Heritage) is devoted to the analysis of crystallographic aspects of art and culture in Turkey and neighbouring countries and regions like Middle Asia, Caucasus, Iran, Anatolia and the Middle East, including carpet ornaments and kilim frames.

The programme proposed by the Commission on 15 August is as follows:

I. Nakai: X-ray Diffraction and Fluorescence Analysis of Archaeological Anatolian Artifacts by Portable Equipment;

M. 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.

ECM-25 will also contain a Microsymposium on Crystallography in Art and Archaeology, Chair: E. Dooryhée, Co-Chair: P. Bezdička, on 18 August 2009, with the following programme:

L. Sawyer: Crystallography and Industrial Design: Past, Present and Future;

M. Schreiner: The Hoard of Beçin – the Silver Content of the Akce Coins and the Monetary History of the Ottoman Empire;

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

A. M. Thalal: Multi-Grids Method Construction of Moroccan Geometric Patterns;

A. Haake: The Javanese Colleagues of Karagöz and their Dress.

There will also be a variety of posters.

Forthcoming actions. The Commission has agreed on the preparation/publication of a monograph focused on the different aspects covered by the Commission, describing the many connections between crystallography and crystallographic methods/techniques on the one hand, and the world of art and cultural heritage on the other.

E. Dooryhée, Chair

6.11. Commission on Electron Crystallography

The year 2008 was an active one for the Commission. At the Osaka Congress a lively Open Meeting with about 30 representatives was held. As part of this a number of Sub-committees were established, and their reports are given below. At this meeting the Commission voted unanimously to change its name to the Commission on Electron Crystallography, with a definition of 'electron crystallography' as 'the branch of science that uses electron scattering to study the structure of matter', which more accurately reflects the areas of interest of the Commission. The terms of reference of the Commission are:

To strengthen links and interactions among electron crystallographers, and to promote a common language;

To promote the presence at IUCr meetings of scientists working in the field of electron crystallography;

To promote the publication of electron crystallography papers in the journals of the IUCr;

To encourage the development and dissemination of mathematical and theoretical methods, software and databases for the solution of electron crystallographic problems;

To promote the use of precise measurements based upon electron scattering;

To promote and organize symposia of interest to electron crystallographers during IUCr Congresses and meetings of Regional Associates, in cooperation with other Commissions of the Union;

To promote and organize meetings, workshops and schools in electron crystallography, particularly targeting post-graduate students and young scientists.

The Commission established a Sub-committee on Updating the *International Tables for Crystallography* regarding the electron crystallography related paragraphs, chaired by J. Hadermann. The aim is to have all electron crystallography related paragraphs updated where necessary in the next revision of *International Tables*. The Sub-committee has reviewed the paragraphs related to electron crystallography and has submitted its recommendations for changes, removals and updates to H. Fuess, Chair of the Commission on *International Tables*. When approval to make the changes is received, scientists with the correct expertise will be solicited for the actual writing.

The Commission established a Sub-Committee on Dynamical Scattering, chaired by J. Etheridge, with the aim to raise the level of knowledge and understanding of dynamical electron scattering and its role in electron crystallography. In the first instance, the Sub-committee will organize research schools covering the theory, implications and applications of dynamical scattering. These will target postgraduate- and postdoctoral-level researchers and will be held as satellites to relevant international conferences. The Sub-committee will also encourage the publication of relevant review and teaching articles.

The Commission established a Sub-committee on Software for Electron Imaging, Diffraction and Crystallography. As part of this, J. M. Zuo is revitalizing the electron crystallography software database, and W. Sinkler has started work on establishing a repository for electron crystallographic data.

The Commission was involved in organizing a satellite meeting for the Osaka Congress, on the Development of Advanced Instruments for New Electron Microscopy and Diffraction.

This meeting was aimed at discussing various topics in advanced instrumentation, newly developed techniques and their applications to nanomaterials covering the following topics: precession electron diffraction; fast diffraction; advanced electron microscopy; diffractive

imaging; charge density in electron microscopy; surfaces; environmental cell; EELS – atom by atom; image processing.

The Commission was involved in a Tsinghua-FEI Workshop on Cs-Corrected Transmission Electron Microscopy (TEM) held in Tsinghua University, Beijing, People's Republic of China, 15–17 October 2008, organized by Jing Zhu, Director of the Beijing National Center for Electron Microscopy, which hosts the first Cs-corrected transmission electron microscope in mainland China. The workshop aimed to provide basic and in-depth descriptions and recent advances in Cs-corrected microscopy, including fundamental theory, principles of operation, recent technical developments, qualitative and quantitative data interpretation, as well as applications in physical sciences, material science and biological sciences. Lectures were given by well known pioneers and experts in the field, including K. Urban (Germany), M. Haider (Germany), C. Kisielowski (USA), Cunlin Jia (Germany), Jianmin Zuo (USA), R. E. Dunin-Borkowski (Denmark), Lijun Wu (USA), Fanghua Li (People's Republic of China) and Jianghua Chen (People's Republic of China). Jing Zhu (People's Republic of China), Hengqiang Ye (People's Republic of China) and Rong Yu (People's Republic of China) gave pre-lectures for the introduction of basic knowledge on Cs-corrected EM. Over 160 persons attended the Workshop.

At the Commission meeting, plans for future meetings/workshops were reviewed. It was noted that the Commission had not hosted a meeting on the African continent and in view of its commitment to training and outreach A. Kirkland was asked to investigate the possibility of hosting a workshop in South Africa. Subsequently Professor Kirkland has had extensive discussions with the National Science Foundation in South Africa, who have indicated strong support for such a meeting and moreover have agreed to provide provisional funds of USD 10 000 and to assist with local organization. At the current time we are discussing suitable dates in 2010 together with venues and a final meeting format. Subsequently, we anticipate having a full proposal for consideration by the IUCr in mid-2009 together with an accurate funding model.

At the satellite meeting held in Nagoya, Japan, immediately after the Osaka Congress, it was agreed by the participants that the electron microscopy community was lacking a robust definition of resolution for both transmission and scanning transmission modes. A. Kirkland agreed to set up a working group to discuss this topic and ultimately to provide a set of working definitions.

A Symposium on Electron Crystallography for Materials Research was organized by P. Moeck at the Spring MRS meeting in San Francisco, USA, with invited talks by P. Midgley, W. Sinkler, J.-P. Morniroli, Z. D. Zuo, U. Kolb, H. Klein, C. Tang, W. Neumann, L. D. Marks, J. M. Zuo and J. McKeown.

J. Zuo and L. D. Marks are organizing a session for the Microscopy & Microanalysis 2009 Meeting (<http://www.microscopy.org/events/annualmeeting09/index.cfm>) on Electron Diffraction and Imaging Techniques for Quantitative Structure Determination, with invited talks from P. Midgley, S. Nicopolous, X. Kou, J. Tao, F.-R. Chen and S. Marchesini.

The Commission's home page is maintained by L. D. Marks, and can be found at http://www.numis.northwestern.edu/IUCR_CED.

L. D. Marks, Chair

6.12. Commission on High Pressure

Crystallography at high pressure continues to gain prominence within condensed-matter science: Science at Extreme Conditions is one of the five key science areas of the upgrade programme at the European

Synchrotron Radiation Facility (ESRF, France). The High Pressure Synergetic Consortium (HPSync) at the Advanced Photon Source (APS, USA) has recently been established to promote cutting-edge high-pressure science using synchrotron radiation. The extreme conditions diffraction beamline I15 at the Diamond Light Source in the UK was among the first seven beamlines that have opened to users. The field of neutron diffraction has also seen major new developments with the completion of the SNAP high-pressure beamline at SNS, Oak Ridge, Tennessee, USA, the formation of a consortium to construct an extreme conditions beamline at the new Japanese neutron source J-PARC in Tokai as well as the completion of the second target station at the ISIS neutron source in the UK. The aim of the Commission is to provide platforms that help the dissemination and exchange of new techniques, ideas and scientific achievements in this field. The main tools for achieving this goal are special workshops in each of the two years between the triennial IUCr Congresses.

Commission members. A major reshuffling of the Commission took place in 2008 because the Chair, Secretary, Treasurer and four other Commission members had reached the limit of their terms: M. Kunz, J. S. Loveday, J. Tse, N. Hamaya, M. Mezouar, S. Tolbert and R. Winter. In part, they have been replaced by previous consultants (R. Angel and P. Dera). As before, the Commission aims to have all current subfields of high-pressure crystallography represented (neutron and X-ray diffraction, material science, biology and soft matter, computational crystallography etc.).

Osaka Congress. The Commission organized six Microsymposia, two of these jointly with other Commissions:

Biological and Soft Condensed Matter under Pressure: Chair: F. Fabbiani (UK), Co-Chair: R. Winter (Germany). Jointly with the Commission on Structural Chemistry.

Computational Crystallography at Extreme Conditions: Chair: R. Ahuja (Sweden), Co-Chair: J. Tse (Canada).

High Pressure Studies on Advanced and Nano-Materials: Chair: N. Dubrovinskaia (Germany), Co-Chair: V. Solozhenko (France).

Phase Transitions and Physical Properties at High Pressure: Chair: R. Benedetti (USA), Co-Chair: G. Shen (USA).

Liquids and Amorphous Systems at High Pressure: Chair: M. Guthrie (UK), Co-Chair: Y. Katayama (Japan).

Crystallography of Planetary Materials at Extreme Conditions: Chair: T. Yagi (Japan), Co-Chair: J.-B. Parise (USA). Jointly with the Commission on Inorganic and Mineral Structures.

Two Keynote Lectures were presented by high-pressure scientists – G. Galli (USA) on Quantum Simulations of Liquids and Solids under Pressure: Synergy between Theory and Experiment and S. Klotz (France) on Advances in High-Pressure Neutron Scattering. The lecture on neutron scattering was to have been given by Igor Goncharenko, but he tragically died in late 2007 and Stefan Klotz kindly agreed to take his place. Numerous posters on high-pressure research were presented under various topics in all three poster sessions. Finally, the Congress organizers offered an excursion to the SPring-8 synchrotron radiation facility, which is one of the leading facilities for high-pressure synchrotron X-ray diffraction. A closed Commission meeting was held during the Congress. E. Boldyreva, P. Dera, F. Fabbiani, Y. Katayama, A. Katrusiak, I. Loa, J. Loveday and V. Solozhenko were present. The main topics were: the handover of affairs for the next triennium; progress reports on the preparations for the 2009 Commission Workshop in Harbin, People's Republic of China, as well as the 2009 Crystallographic Course in Erice, Italy; the proposition to hold the 2010 Commission workshop in Oak Ridge, Tennessee (USA) at the new Spallation Neutron Source facility and the relaunch of the Commission's web site.

Web site. The Commission web site has been renewed from the ground up to offer up-to-date information to both researchers in the field and outsiders. In order to ensure continuing updates, it was suggested at the 2007 workshop in Oxford that an institution should take responsibility for the web site and delegate the work to one of its members. The Centre for Science at Extreme Conditions at Edinburgh University volunteered to take on this responsibility, and the current webmaster is the Commission secretary, I. Loa. The web site is presently accessible at <http://www.ph.ed.ac.uk/~iloa/IUCr-HP>, but it is planned to integrate this with the new IUCr web site in the future.

2009 Commission Workshop. The workshop in 2009 will be held in Harbin (Heilongjiang Province, People's Republic of China). Commission member H. Liu is acting as head of the Local Organizing Committee. The Commission regards this workshop as an opportunity to intensify scientific exchange with the Chinese high-pressure crystallography community.

Summer School. Commission members E. Boldyreva and P. Dera are directing a Summer School on High-Pressure Crystallography in June 2009 in Erice, Italy. This is a follow-up to the very successful summer school organized in 2003.

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

6.13. Commission on Inorganic and Mineral Structures

A major reconfiguration of the Commission (CIMS) occurred during the Osaka Congress, as several members had reached the end of their term and had to be replaced and some consultants expressed their wish to discontinue their service. The new composition of CIMS can be found on the IUCr web site (<http://www.iucr.org/iucr/commissions/cims.html>). Every effort has been made to make the repartition of the members and consultants of CIMS as fairly distributed as possible with respect to sex, geographical location and scientific interests. M. Nespolo has agreed to continue as consultant and webmaster of the Commission-maintained web site (<http://www.crystallography.fr/cims/>). The Osaka Congress saw various activities of members or consultants of CIMS: P. A. Thomas was a member of the Programme Committee, T. J. White gave a Keynote Lecture, L. B. McCusker, S.-L. Wang, G. Ferraris, J.-B. Parise, D. Pandey and W. Depmeier served as Chairs or Co-Chairs at various sessions.

During the Congress two poster prizes for mineralogical crystallography [sponsored by the European Mineralogical Union (EMU) and restricted to young scientists up to 35 years of age] and for inorganic crystallography (sponsored by *Zeitschrift für Kristallographie*) were awarded.

During the General Assembly a new Commission on Crystallography in Art and Cultural Heritage was approved with W. Depmeier and M. Nespolo as consultants.

Apart from the Osaka Congress, and occasional other meetings, the members and consultants of the Commission communicated mostly via email, or by using the web site.

CIMS was involved in the following meetings held in 2008:

VI International Symposium 'Mineralogical Museums', St Petersburg, Russia, 17–20 June 2008. The meeting was jointly organized by St Petersburg State University, Russia, and Kiel University, Germany. W. Depmeier was Chair of the Symposium (<http://www.mineral.pu.ru/confer.html>).

II International Workshop on 'Layered Materials: Structure and Properties', Vercelli, Italy, 28–29 March 2008 (<http://www.layeredmaterials.mfn.unipmn.it/>). G. Ferraris was a member of the Organizing Committee, W. Depmeier, G. Ferraris and D. Pandey were members of the Scientific Committee and J. Rocha was an invited

speaker. An outcome of this workshop is a Special Issue (5/2009) of *Zeitschrift für Kristallographie* on Layered Materials (Guest Editor: G. Ferraris; <http://www.oldenbourg-wissenschaftsverlag.de/olb/de/1.c.335324.de>).

CIMS has supported the application for financial support by the IUCr of the following meetings planned to be held in 2009:

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

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). CIMS member H. Effenberger is Secretary of EMU (European Mineralogical Union). It is intended to further the cooperation between EMU and CIMS.

Symposium on Crystallography of Inorganic Materials at High Pressure at AIRAPT2009, the International Conference on High Pressure Science and Technology, Odaiba, Tokyo, Japan, 26–31 July 2009 (<http://www.prime-intl.co.jp/airapt22/>). The symposium was proposed by Commission member T. Nagai who is also convener of the symposium. CIMS consultant J.-B. Parise is an invited speaker.

International Conference on the Chemistry of the Organic Solid State (ICCOSS IX), 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.

Besides the activity given above, members of CIMS have reported to the Chair the following personal activity related to the purposes of the Commission.

H. Effenberger presented a Keynote Lecture at the Joint Seminar of the Australasian Mineral Societies (Structural Aspects of Copper Minerals, Tasmania, Australia, 3–7 November 2009). He is also a representative of EMU on the Managing Committee of the *European Journal of Mineralogy*.

D. Pandey has been appointed a Co-editor of *Zeitschrift für Kristallographie*.

O. Yakubovich is Chair in the organization of the Microsymposium on Minerals as Treasury for Advanced Materials for ECM-25, Istanbul, Turkey.

G. Ferraris is an author of *Crystallography of Modular Materials* by G. Ferraris, E. Makovicky and E. Merlino, IUCr/OUP Monograph on Crystallography No. 15 (paperback edition), published in 2008.

D. Pushcharovsky was elected Academician of the Russian Academy of Science.

R. Withers is also a consultant of the Commission on Aperiodic Crystals (CAC). CIMS and CAC jointly organized a Microsymposium on Modulated Structures as part of the Osaka Congress.

In terms of promoting inorganic and mineral crystallography while a consultant, C. Cahill has lectured in the UK (Cardiff, Sheffield, Cambridge, Belfast), Ireland (Dublin) and Germany (Karlsruhe, Stuttgart and Siegen) while on sabbatical as a Fulbright Scholar. He is also a member of the US National Committee for Crystallography.

W. Depmeier, Chair

6.14. Commission on Mathematical and Theoretical Crystallography

Scientific activity in 2008. The Commission on Mathematical and Theoretical Crystallography (MaThCryst) organized the following activities:

(1) A school at the University of Gargnano, Lake Garda, Italy, 27 April – 2 May 2008, organized in cooperation with the Commission on Crystallographic Teaching. The school was held over five days and was attended by 40 participants from 13 countries. The first day was

devoted to fundamentals of group theory to give all the participants, having a rather heterogeneous background, a common level necessary to achieve a detailed understanding of the topics treated in the following days. Day 2 was entirely dedicated to mathematical aspects of crystallography in direct space (dimensionless definitions, space-group classification, normalizers). The third day gave the participants the fundamental knowledge of group–subgroup relations between space groups and presented applications. On the fourth day the participants could apply what they had just learnt to derivative structures, twins and phase transitions. On the last day, the knowledge acquired was complemented by exercises on the Bilbao Crystallographic Server, where several tools are offered free of charge to extract interactively the information the participants had learnt to obtain by hand calculation. The school ended with a presentation of organic crystal packing and the intermolecular relations in organic crystals. Participants were lodged directly at the venue (Palazzo Feltrinelli, owned by the University of Milan) or in a building of the University within walking distance of the venue. This logistic allowed the participants to stay together the whole five days and evening sessions were also organized on request, for additional exercises and revision sessions. A poster session was also held, where the participants had the occasion to present their research topics and results. Didactic material from the school and abstracts of the poster presentations are available from the school web site (<http://www.crystallography.fr/mathcryst/gargnano2008.htm>).

(2) At the Osaka Congress:

KN29: Keynote Lecture on Metal-Organic Materials: Strategies toward Functional Porous Materials, by M. Eddaoudi, Chair S.-L. Wang, in cooperation with the Commission on Structural Chemistry.

MS89: Microsymposium in Honour of E. Ascher and J. J. Burkhardt, Chairs H. Grimmer and M. Nespolo.

An Evening Session on Art and Crystallography, in cooperation with the newly formed Commission on Crystallography in Art and Cultural Heritage, Chairs M. Nespolo and K. Ohsumi.

Commission renewal. MaThCryst was approved by action of the IUCr General Assembly in Florence, 25 August 2005. The first three-year term came to its end on the occasion of the General Assembly in Osaka, August 2008. The number of members has been increased by one and the membership may be found at <http://www.iucr.org/iucr/commissions/cmtc.html>.

Scientific Activities in 2009 and later. Forthcoming activities at present include:

Crystallography Online: International School on the Use and Application of the Bilbao Crystallographic Server, Lekeitio, Spain, 21–27 June 2009 (see <http://www.crystallography.fr/mathcryst/bilbao2009.php>).

A satellite conference of ECM-25 on ‘Symmetry and Crystallography in Turkish Art and Culture, Istanbul, Turkey, 14–16 August 2009 (see <http://www.crystallography.fr/mathcryst/istanbul2009.php>).

A school on Topological Crystal Chemistry: Theory and Practice, Nancy, France, 28 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>).

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

An ‘African tour’ in Spring 2010 to promote fundamental and mathematical crystallography: this is expected to be a three-week tour including two schools in South Africa (in the north and south of the country) followed by a school in Tunisia. We are waiting for action by the local organizers.

A second school in Nancy, immediately preceding the one mentioned above, devoted to Irreducible Representations of Space Groups, with a possible exchange in the order of the two schools. The link between the two schools would allow most of the participants to be retained and would ease the organizational logistics. Commission members M. Aroyo and B. Souvignier are finalizing the considerations about the possibility of realizing the project.

A workshop in India, under the responsibility of Commission consultant D. Pandey.

A contribution to an American meeting for which W. L. Duax has promised to help MaThCryst obtain logistic help in a region where it has greater difficulties in affirming 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 and J. Rutherford for publication as an IUCr Monograph on Crystallography jointly published by the IUCr and Oxford University Press (OUP). OUP has agreed to provide copies to 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 entitled *Geometric Algebra in Crystallography*, currently under consideration as an IUCr Monograph on Crystallography jointly published by IUCr and Oxford University Press.

Web-related activities. Didactic pages directly hosted on our server (twinning and OD structures) have been updated. We regret, however, the lack of activity and contribution from members and consultants to expand the existing pages and to creating new ones.

Other activities. M. Nespolo and B. Souvignier regularly contribute to the *Online Dictionary of Crystallography* (<http://reference.iucr.org>).

M. Nespolo, Chair

6.15. Commission on Neutron Scattering

The principal event for the Commission in 2008 was the preparation for the Osaka Congress and, in particular, the five Microsymposia coordinated by the Commission (together with three other Microsymposia held jointly with other Commissions). In addition to the direct work of the Commission two members played a crucial role in the preparation of the Congress: Y. Fujii (former Chair of this Commission) as Chair of the International Programme Committee (IPC) and T. Kamijama as Secretary of the IPC.

The Commission met during the Congress and the main discussion concerned the landscape of neutron sources worldwide. In fact, 2008 has seen the fruition of major projects of neutron radiation science facilities.

The end of May 2008 marked the arrival of the J-PARC MW pulsed neutron source with its first neutron production.

At the beginning of August 2008 the ISIS second target station project measured the first neutrons from the new target station in the INTER beamline and one month later both neutron targets were operated at full power. New instruments are being commissioned such as WISH (Wide angle In a Single Histogram): a long-wavelength diffractometer primarily designed for powder diffraction at long *d*-spacing in magnetic and large-unit-cell systems, with the option of enabling single-crystal and polarized-beam experiments.

The year 2008 marked as well a significant step in the ramp up to full power of the Oak Ridge Spallation Neutron Source (SNS),

building up to its eventual suite of 25 instruments for neutron analysis and with nine instruments already in their User Programme.

The existing neutron sources operated successfully over this period of time.

Over the eight years of the Millennium Programme, the Institut Laue–Langevin (ILL) has seen an increase in detection rate of flux by a factor of about 17 across its instrument suite and in 2008 three new or refurbished instruments were open to users: the cold-neutron multi-chopper time-of-flight spectrometer IN5 returned with a 60× higher detection rate; the high-resolution SANS instrument D11 with 2–3× more flux at the sample and a new detector that allows twice the resolution: ILL's first horizontal surface reflectometer, FIGARO.

FRM-II, the high-flux reactor source in Munich, Germany, has continued increasing its instrumental park and in 2008 offered 251 days to its users (this equals 100%).

OPAL restarted in May 2008 following approval of the new fuel design by Australia's independent nuclear regulator ARPANSA.

Six neutron beam instruments commenced 'user' operations in 2008 following granting of operation licences by ARPANSA.

In order to increase the neutron community and to make optimal use of these forefront facilities, a remarkably high number of conferences and workshops related to neutron techniques took place in 2008. For example, the fourth biennial American Conference on Neutron Scattering was held in Santa Fe, New Mexico, USA, sponsored by the Neutron Scattering Society of America.

The Indian Neutron Scattering Society (INSS) was formed on 11 June 2008 during a meeting of neutron users at Mumbai with an objective to promote the research and development activities of neutron scattering science and applications.

We can also welcome the formation of the Asia–Oceania Neutron Scattering Association, which is intended to act as a central body for coordination of activities of the neutron scattering societies of the member countries (currently Australia, India, Japan, Korea, Taiwan) and to liaise with the regional neutron scattering societies of Europe and North America on international activities.

The largest effort, nevertheless, has been put into training young researchers in neutron scattering techniques through more than twenty dedicated schools and training courses worldwide.

M. T. Fernandez-Diaz, Chair

6.16. Commission on Powder Diffraction

Commission meetings. The Commission (CPD) held its 2008 meeting during the Osaka Congress. Both the Chair and the Secretary retired, resulting in significant changes within the membership. The retiring members were thanked for their efforts over the previous years. It was decided to give members different particular responsibilities depending on their expertise and geographical location.

The 2009 CPD meeting is scheduled to take place during the ACA in Toronto.

Meeting sponsorship. The CPD received nine requests for support towards IUCr sponsorship. Meetings where support was given include the Indaba 6 meeting to be held in South Africa in late 2009, the 19th Brazilian Crystallographic Meeting in September 2009 and the Powder Diffraction and Rietveld Analysis School to be held in April 2010 in the UK.

Newspapers, web site and PR poster. CPD Newsletter No. 35 edited by S. Billinge should be available soon on the CPD web site. To reduce the significant workload required for the production of the *Newsletter* it has been decided to share the editorial responsibility for future *Newsletters* between two members. Hopefully this will

decrease the time between future issues. It was decided that the CPD needs to raise its profile, both within the mainstream powder diffraction community and the wider science community who use powder diffraction as a tool, e.g. solid-state chemists, mineralogists etc. It was decided to produce a small poster to display at various meetings to explain what the CPD does and how it contributes to the community, and to solicit suggestions on how to improve the impact of the CPD. The CPD web site was redesigned during 2008 and moved to www.iucr-cpd.org.

Projects. One of the CPD projects came to fruition during 2008 – the publication of the textbook *Powder Diffraction – Theory and Practice*, edited by R. Dinnebier and S. Billinge and published by the Royal Society of Chemistry. Together with the second edition of *Fundamentals of Powder Diffraction and Structural Characterization of Materials* (Pecharsky and Zavalij), and the publication of *Principles and Applications of Powder Diffraction* (Clearfield, Reibenspies, and Bhuvanesh) these should provide an excellent resource for everyone from undergraduate to researcher. Efforts towards producing an organic standard to assist in validation of structures solved from powder diffraction data is continuing. A number of potential compounds have been examined but none has so far been deemed suitable. With a similar aim, contact has been initiated with the Cambridge Crystallographic Data Centre to see whether a CPD-organized workshop on validation of organic structures solved from powder diffraction may be of interest.

P. Whitfield, Chair

6.17. Commission on Small-Angle Scattering

Commission meetings and communication. Commission members communicated by e-mail or during personal meetings at national and international conferences. The Osaka Congress, where most of the Commission members were present, gave an opportunity for the Commission to meet.

Activities. The Commission Chair, D. Svergun, and other Commission members were actively involved in the Osaka Congress. A Keynote Lecture on Advances in Micro- and Nano-SAXS was given by Commission member P. Fratzl. Four Microsymposia were suggested by the Commission and Co-Chaired by the following Commission members:

(1) Complementarity of SAXS and SANS with Other Structural Methods in Molecular Biology, Co-Chaired by J. Trewella.

(2) Micro-SAXS for Nanoscience and Medicine, Co-Chaired by P. Fratzl.

(3) Time Resolved and Coherent X-ray Scattering and Imaging, Co-Chaired by P. Thiagarajan.

(4) Advances in Grazing Incidence, Reflectivity and Diffuse Scattering, Co-Chaired by A. Allen.

A discussion was initiated and undertaken by G. Kostorz and D. Svergun with the International Advisory Committee of the SAS conference in Oxford (2009) about the new procedure for soliciting the applications for the venue of the next SAS conference in 2012. The modified rules were adopted, envisaging pre-selection of the venue by a Committee of internationally recognized scientists, Commission members and the previous SAS conference organizers. The procedure will be used for selecting the venues as of 2012.

D. Svergun organized the Commission meeting during the Osaka Congress.

The Commission discussed publication standard requirements for journal publications involving SAS. While no formal publication standard requirements are planned for the near future, it was agreed

to look into the matter further. Requirements for SAS contributions to the protein crystallography database were also discussed, and identified as potentially a more urgent issue.

Educational activities. The members of the Commission were actively involved in presenting seminars and tutorial lectures at various schools and workshops worldwide, explaining SAS methods to young students and researchers from different fields.

In particular, D. Svergun presented the lectures:

Small-Angle Scattering from Macromolecular Solutions at the Kyoto Crystallographic Computing School, Japan, 19 August 2008.

Ab initio Methods: How/Why Do They Work? at EMBO Practical Course on Solution Scattering from Biological Macromolecules, Hamburg, Germany, 12 October 2008.

Rigid Body Refinement (Basics) at EMBO Practical Course on Solution Scattering from Biological Macromolecules, Hamburg, Germany, 22 October 2008.

Small-Angle X-ray and Neutron Scattering at EMBL Predoctoral Course, Heidelberg, Germany, 13 November 2008.

A. Allen has supported the publication of ‘Probing Nanoscale Structures: The SANS Toolbox’ by B. Hammouda (NIST Center for Neutron Research), which was released online in 2008. It contains 670 pages, presents a great deal of tutorial information for SANS, and is available from the IUCr SAS listserver. Other new SAS guides have been prepared at the Advanced Photon Source for SAXS and USAXS.

P. Thiagarajan gave the lecture Introduction to Small-Angle Scattering at ACA Workshop 4, Structural Biology Without Crystals, Knoxville, Tennessee, USA, 30 May 2008. In addition, he organized the SAS short course Beyond R_g at the APS, ANL (30 participants). This course included Global Facilities Overview (30 June 2008) and BioSAXS (1 July 2008) as well as hands-on experiments and analysis by measuring data at the APS beamlines.

H. Yagi was involved in the summer school (intended for Japanese students) at SPring-8, 11–14 July 2008, during which he carried out a beamline practice on SAXS. There were 40 participants. He also contributed to a Cheiron school (International School on Synchrotron Radiation) that was held 29 September – 8 October 2008, at SPring-8, where he also undertook beamline practicals (<http://cheiron2008.spring8.or.jp/>). There were about 60 participants.

I. Torriani has been involved in counselling on experimental details of the projects executed at the SAXS Beamline of the Brazilian National Synchrotron Radiation Laboratory (LNLS), interaction with the LNLS users on data treatment and interpretation of results, and thesis advisory activities to PhD students from the University of Campinas, Brazil.

R. Serimaa gave a lecture on SAXS in the Nordic and European summer school on VUV and X-ray Research for the Future using FEL and Ultra-Brilliant Sources organized by MaxLab, Röstänga, Lund, Sweden, 26 May – 2 July 2008.

J. S. Pedersen was co-organizer of a one-day course on Particle Characterization, held at Aarhus University, 27 February 2008, under the auspices of the Danish Colloid and Interface Society. He was also part of the Organizing Committee of the 8th European Summer School on Scattering Methods Applied to Soft Condensed Matter, Bombannes, Gironde, France, 7–14 June 2008. He also presented lectures at the School.

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 and especially in the joint use of SAS with other structural techniques.

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

J. Trewella and D. Svergun organized a joint Open Meeting of the Commission with the representatives of the IUCr Commission on Journals and the Protein Data Bank at the Osaka Congress to discuss establishing standards for SAS publications and structural data deposition.

Following the NIST-hosted canSAS V workshop in 2007, A. Allen has continued to contribute to the development of standardized portable 1D data formats (both IUCr SAS CIF and SAS NeXus), and to the development of candidate standards for SAXS and SANS, as well as more general standardization issues. NIST is actively pursuing development of a small-angle X-ray diffraction wavelength standard reference material (SRM). An international round robin exploring the potential of glassy carbon as a SAXS (and possibly SANS) intensity standard reference material was initiated in 2008, and will remain ongoing in 2009.

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

Structural Analysis of Intrinsically Unfolded Proteins by Small-Angle X-ray Scattering, presented at the International Structural Genomics Conference, Oxford, UK, 24 September 2008 and at Soft Condensed Matter Days, Jülich, Germany, 12 November 2008.

Structure Studies of Biological Macromolecules in Solution by Small-Angle X-ray Scattering, presented at the Hellenic Crystallographic Conference, Athens, Greece, 26 September 2008.

Joint Use of SAXS and SANS with High-Resolution Methods for Macromolecular Solutions, presented at the NMR-Life meeting, Florence, Italy, 12 December 2008.

P. Thiyagarajan continued to provide a SAS analysis software package to the students and faculty who visit IPNS and APS for experiments. He also promoted small-angle scattering in his invited talks:

Phase Behavior of Block Copolymer/Inorganic Nanoparticle Composites, at the APS meeting, New Orleans, USA, 13 March 2008.

SANS and SAXS Characterization of Block Copolymer/Bioinspired Mineral Composite Gels, at ACA 2008, Knoxville, USA, 1 June 2008.

Characterization of Block Copolymer/Bioinspired Mineral Nanocomposite Gels (Plenary) at an IUCr satellite meeting, SPring-8, Japan, 22 August 2008.

Phase Behavior of Block Copolymer/Inorganic Nanocomposites, at the Osaka Congress.

N. Yagi has participated in several users meetings and talked about SAXS beamlines at SPring-8. He also supports SAXS users and guides them in selecting the optimum equipment and conditions for their measurements.

I. Torriani has been part of the Millenium Institute for the Study of Polymers group and participated in their annual meeting, presenting results of combined experimental and theoretical research on the structure of layered particles. The polymer groups in Brazil have increasingly become aware of the importance of SAXS-WAXS uses, as well the singular opportunity of performing combined-techniques experiments (SAXS-WAXS-DSC) and setups with magnetic or electric fields. At the SAXS Beamline of the Brazilian National Synchrotron Radiation Laboratory (LNLS), there has been a growth in the number of users with biological projects, and I. Torriani has offered continued support for performing experiments in proper conditions. Almost 40% of the projects at the beamline are from the macromolecular science community.

V. Volkov heads the SAS Laboratory in the Institute of Crystallography, where the staff in 2008 have supported specialists from about 12 scientific organizations in Russia who have performed investigations of about 200 samples of self-organized polymers, nano-disperse carbons with metal nanoparticles, liquid crystals, and protein molecules in solution.

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

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

Consultant activities. 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 Beamtime Allocation Committee at the NIST Center for Neutron Research, USA.

P. Thiyagarajan serves on the BioCAT Advisory Committee, APS, USA, and is a reviewer of the 12-ID SAXS facility upgrade proposal.

I. Torriani has acted as a consultant for the Brazilian pharmaceutical industry on the development of a self-nanoemulsifying drug-delivery system, and has collaborated with Argentinian groups carrying out industrial research on natural rubber blends.

R. Serimaa was a member of the EMBL Priority Committee (Synchrotron Radiation Research of Biological Systems, Hamburg Outstation, Germany) and reviewed SAXS proposals. She also participated in the ESRF Brainstorming Meeting, 15–16 December 2008, on the ESRF Upgrade Beamlines dedicated to time-resolved scattering/diffraction and ultra-small-angle scattering (UPBL9).

Organizational activities. D. Svergun organized an EMBO Practical Course on Solution Scattering from Biological Macromolecules in Hamburg, Germany, 19–26 October 2008. There were over 100 applicants, of which 20 were selected as full participants and 6 for lectures, representing over 20 countries from Europe and overseas. A team of 15 lecturers and tutors, including Commission members (J. S. Pedersen, J. Trewella), conducted the course.

P. Thiyagarajan co-organized the SAS short course Beyond Rg at the APS, ANL (http://small-angle.aps.anl.gov/short_course_2008.html), which had 30 participants with a good background in SAS. He also co-organized the workshop on SAXS and SANS Applications in Nano Materials and Nano Biology at the APS users meeting, May 2008, which had 60 participants.

N. Yagi participated in the organization of the satellite meeting of the Osaka Congress at SPring-8 entitled X-ray and Neutron Techniques for Nano-Structural Research, 20–22 August 2008 (http://xrm.spring8.or.jp/IUCr_satellite.html). There were about 60 participants. He was also a member of the International Programme Committee for the Osaka Congress.

I. Torriani participated in the International Programme Committee of the Osaka Congress as a member of the IUCr Executive Committee and as a representative of the Commission. She contributed to the organization of the Microsymposia and Keynote Lectures as well as to the judging of poster prizes.

J. S. Pedersen was a member of the Organizing Committee of the European Summer School entitled Scattering Applied to Soft Condensed Matter, Bombannes, Gironde, France, June 2008.

Technical activities. D. Svergun was involved in further development of the automation of a SAXS experiment and data analysis at

the EMBL synchrotron SAXS beamline (DESY, Hamburg, Germany).

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.

A. Allen has contributed to the work at NIST to issue three nanoparticle reference materials (RMs): NIST RMs 8011, 8012 and 8013, respectively, for nominal 10, 30 and 60 nm gold nanoparticles in aqueous suspension – for use primarily in biological research applications. ‘Reference values’ for mean particle diameter were provided for a number of techniques, including both SAXS (modified Rigaku laboratory instrument at NIST) and the USAXS instrument at APS. Details of the combined SAXS and USAXS measurements are included in the certificates (issued January 2008). A. Allen has also contributed to the on-going development of silver and titanium oxide nanoparticle reference materials (both for biomedical and for environmental health and safety applications), and this will also probably involve SAXS/USAXS measurements.

P. Thiagarajan has been active in the development of new capabilities for GISAXS, ASAXS, XPCS and the area detectors at the APS.

N. Yagi has contributed to the upgrade SAXS beamlines at SPring-8 and has participated in the design of a new SAXS beamline, which is due in autumn 2009.

During 2008, I. Torriani has been coordinator of the SAXS beamlines of the LNLS. Relocation of the SAXS1 to a new BM port has almost been completed. The SAXS2 beamline has undertaken the full load of external projects and installation of new experiments has to be postponed until 2009.

J. S. Pedersen, Chair, and **D. Svergun**, former Chair

6.18. Commission on Structural Chemistry

The key activity of the Commission (CSC) during the first semester of 2008 was contributing to the Scientific Programme of the Osaka Congress. All members and consultants of the CSC, together with a wide range of scientists around the world with interests covering all aspects of structural chemistry, were involved in a strong programme of Plenary Lectures, Keynote Lectures, Microsymposia and Chairs that ran through all the Congress, as well as in joint Microsymposia with other Commissions (High Pressure; Biological Macromolecules; Crystallographic Teaching; Crystal Growth and Characterization of Materials; Crystallographic Computing; Charge, Spin and Momentum Densities; Powder Diffraction). The topics covered included: Modelization of Structure of Molecular Compounds and Implications for Reactivity; Water Clusters in Molecular Crystals; Symmetry, Asymmetry and Chirality in Molecular Aggregation; Photochemistry and Solid-State Transformations of Molecular Solids; Uncommon Organic and Organometallic Structures and Functions; Electric and Magnetic Properties of Molecular Crystals; Crystal Design from Hydrogen Bond to Halogen Bond and Beyond; Host-Guest Crystal Chemistry; Chemical Recognition and Supramolecular Architectures; Co-Crystals: Theory, Synthesis and Use; Structure-Function Relationships of MOF (Metal Organic Frameworks); Understanding and Controlling Polymorphism; Design and Applications of Nanoscale Materials; Knowledge-Based Applications in Structural Chemistry. A Microsymposium in tribute to Pierre-Gilles de Gennes on Liquid Crystals and Crystallography was also held.

During the Osaka Congress the Commission organized an Open Meeting to collect opinions and ideas on new actions that could encourage the growing interest of the crystallographic community in

topics related to structural chemistry on the one hand, and that in parallel could encourage interdisciplinarity and links to other Commissions by stimulating exchanges of experiences with neighbouring communities. This issue was thoroughly discussed through the second semester of 2008 by the newly installed Commission; as a first action it was suggested that consultants could be shared between the Commission on Structural Chemistry and other Commissions with closely related interests. This issue will be carried on during 2009.

Some main tasks have been distributed among members and consultants to rationalize the activities of the next three years: A. Bacchi and S. R. Batten update the new CSC page on the IUCr web site; P. Bombicz, S. R. Batten and M. T. L. Duarte contribute to the contents of the IUCr Online Dictionary and link to the Commission on Crystallographic Nomenclature; A. Nangia, K. Ogawa, F. Lahoz and P. Mueller link to the IUCr/OUP Book Series; S. A. Bourne, P. R. Raithby, P. Mueller, J.-C. Daran and Shi Xiong Liu provide support and ideas for schools and link to the Commission on Crystallographic Teaching; F. Lahoz and A. Bacchi collect inputs for the programme of the next IUCr Congress in Madrid; A. Beatty links to the Commission on Inorganic and Mineral Structures; J. L. Flippin-Anderson links to the *IUCr Newsletter*.

A. Bacchi, Chair

6.19. 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. Two subcharges are to promote the development of crystallographic instrumentation technology and standards, and to promote synergies between classical storage rings and the LINAC-based next-generation sources such as X-ray free electron lasers (X-FELs) and energy recovery linacs (ERLs). In order to reach these goals we endorse relevant international meetings when IUCr financial support is requested, or in some cases become actively engaged in the organization of such international meetings and workshops as the best means to achieve our mission.

We endorsed the request for support of the Symposium on X-ray Techniques for Advanced Materials, Nanostructures and Thin Films – From Laboratory Sources to Synchrotron Radiation as part of the Spring Meeting of the European Materials Research Society (MRS) in Strasbourg, France, 8–12 June 2009. We considered that this symposium was important for the promotion of synchrotron use in materials research.

The Commission continued to support the RapiData course on automated data collection at NSLS, Brookhaven National Laboratory, USA. In particular, it supported the participation of scientists from South and Central America.

The Commission endorsed the request for financial support for the International Conference on Neutron and X-ray Scattering 2009, Kuala Lumpur, Malaysia, 29 June – 1 July 2009. The theme of the meeting is Neutron and X-ray Scattering in Materials Research Advancement.

In December 2008, the third Asia–Oceania Forum for Synchrotron Radiation Research (AOFSRR) was hosted by the Australian Synchrotron (AS). The meeting was held 4–5 December in Melbourne in conjunction with the AS Users Meeting. Two sessions, Next Generation Photon Science I and II, were organized on the potential scientific applications of next-generation sources (FELs and ERLs). The fourth AOFSRR workshop will be held on 31 November – 1 December 2009 in Shanghai, People’s Republic of China. A

special issue is being prepared for *Synchrotron Radiation News*. As one of the core activities of the AOFSRR, the second Cheiron School was held at SPring-8, Japan, 29 September – 8 October 2008. About 64 young students and post-docs attended from eight countries in Asia and Oceania. Members of the Commission were involved in the programme preparation and lecturing. Following this success, the third Cheiron School is scheduled to be held at SPring-8, 2–11 November 2009.

In addition to these meetings endorsed by the Commission, members of the Commission are involved in the triennial international Synchrotron Radiation Instrumentation meeting in Melbourne, Australia, September 2009 (SRI 2009). Members of the Commission will again be involved in developing the programme of SRI 2009. In particular, R. Garret serves as the Chair of the Technical Programme Committee of which H. Graafsma is also a member. G. Kulipanov and S. Wakatsuki are members of the SRI 2009 International Advisory Committee. Looking ahead, Biology and Synchrotron Radiation (BSR), another triennial international meeting where crystallography is a major field, is scheduled to be held in Melbourne, Australia, 15–18 February 2010. S. Wakatsuki will be involved in the BSR meeting as a member of the International Advisory Committee.

S. Wakatsuki, Chair

6.20. Commission on XAFS

Commission meetings and communication. Commission members communicated by e-mail or during personal meetings at national and international conferences. The annual meeting was held at the Osaka Congress, with old and new Commission members. A. Molenbroek reported on the meeting with the Executive Committee. The Commission activity has considerably increased in the last triennium and discussions were focused on the continuation of this activity and on further improvements. I. Ascone, K. Asakura, and B. Hedman were designated by the Commission as representatives on the International Programme Committee, to contribute to the suggestions and planning of topics for Keynote Lectures, Microsymposia and Chairs for the 2011 Madrid Congress. Moreover, it was agreed to continue informal joint activities with the International X-ray Absorption Society (IXAS) – for example, in the organization of sessions at the Camerino conference and at future IUCr Congresses.

The Commission web site hosted by Bologna University was updated in 2008 by F. Boscherini. It contains an exhaustive list of XAFS beamlines in the world, and recent information on European beamlines (especially BESSY, SRS/Diamond) has been included.

Activities. The Commission has contributed to the Osaka Congress – for example, by having a member on the International Programme Committee (A. Molenbroek) and by organizing and co-organizing four Microsymposia at the Osaka Congress, some in collaboration with other IUCr Commissions:

(1) MS35 on Combined XAFS and Diffraction of Inorganic Structures took place in cooperation with the Commission on Crystallographic Computing with K. Asakura and E. Holub-Krappe as organizers. Presentations demonstrated that combination of XAFS and XRD provides a powerful tool for disordered and dilute systems under high-pressure conditions and in the time-resolved mode.

(2) MS94 on Complementary Low-Z Element Absorption Spectroscopy by X-ray Raman Scattering; the Chair was U. Bergmann and the Co-Chair E. Holub-Krappe. The Commission on XAFS and the Commission on Charge, Spin and Momentum Densities jointly organized this symposium. Non-resonant X-ray Raman scattering is a valuable complementary, and in some cases unique, tool to study bulk

sensitive soft X-ray absorption edges with high-energy X-rays – in particular, if electrons or soft X-rays are difficult to use as a probe.

(3) MS55 on Surfaces was jointly organized by the Commission on Electron Crystallography and the Commission on XAFS; the Chair was D. Saldin and the Co-Chair F. Boscherini. The aim was to report state-of-the-art research on surfaces and interfaces, with particular reference to the contribution of diffraction and X-ray absorption methods.

(4) MS63 on XAFS in Biocrystallography; the Chair was I. Ascone and the Co-Chair T. Prange. Presentations showed examples where X-ray absorption spectroscopy has been used as a powerful tool for local structural determination of proteins, on single crystals (in synergy with crystallography) and in solution, providing structural and electronic details during protein function.

The Commission endorsed the meeting International Forum on Future Directions in Atomic and Condensed Matter Research and Applications, Melbourne, Australia, 22–23 September 2008. The Forum was a great success in terms of interactions, communications and discussions. The Forum began with experts on the fundamental side in theory and experiment and led towards diverse critical applications, finishing off with a Forum to discuss key recent advances, personnel and possible future linkages and efforts. The thread of Atomic and Condensed Matter Theory and Science is crucial to several developing applications and opportunities across different fields (from physics and chemistry, biophysics, biomedicine through synchrotron science), and this was a key focus. A number of invited plenaries gave critical reviews of diverse areas and linked up to issues wider than their particular fields of expertise.

Presentations concerned developments and challenges in (fundamental) scattering theory and experiment (R. H. Pratt), and scattering interactions in resonant X-ray diffraction studies (M. J. Cooper). Crystallography without crystals was the subject of a review by P. Colman.

Interleaved with this theoretical and experimental basis was the strong thread of XAFS basic theory including the new XAFS technique of XERT (X-ray Extended Range Technique) developed by the team of one of the authors of this report (C. T. Chantler). Advanced applications of such an approach concerned several domains, among them, biomedical, cultural heritage and biological fields.

The Forum, at the end, brought these superficially disparate threads together, and looked towards other potential future developments and exciting areas, which in part will be foci of the coming International Symposium on Radiation Physics, Melbourne, Australia, 20–25 September 2009, and the associated Workshop, 26–27 September 2009 (<http://www.memconferences.com/isrp11/>). The Workshop will be particularly focused on XAFS and related synchrotron analytical techniques and applications. The Commission supports both these initiatives.

The Commission has promoted educational activities. K. Asakura organized an XAFS Tutorial at KEK International Center, Photon Factory, Tsukuba, Japan, 20–23 August 2008, before the Osaka Congress. The purpose of the Tutorial was to give a general introduction and analytical methods for crystallographers and beginners in the field of XAFS. A total of 44 participants joined this workshop, co-organized by Photon Factory KEK, the XAFS Society of Japan, Precise Surface Design of Catalysts and the Japanese Society of Catalysis, and supported by the Accelerator Promotion Organization and the Chemical Society of Japan. Several Commission members (K. Asakura, F. Boscherini, A. Michalowitz and A. Molenbroek) presented lectures; other lecturers were selected as representative users of theoretical calculation programs (*FEFF*, *GNXAS*,

EXCURVE). Most of the lectures concerned *FEFF*. R. Strange prepared a manuscript that focused on data analysis using *EXCURVE* and this was given to all participants. Lectures covered the fundamentals of XAFS, data analysis and its principle, theory, and simulation of XAFS spectra with applications to biology, chemistry, physics and materials science. Finally, time-resolved XAFS was presented. The tutorials provided hands-on practice of EXAFS analysis and theoretical calculations using *REX* and *FEFF*.

The Commission supported the funding request for the 14th International Conference on X-ray Absorption Fine Structure (XAFS14), Camerino, Italy, 26–31 July 2009. This is a well established conference, now held every three years, with the first meeting in 1981. It attracts delegates from most parts of the world and from most science disciplines, ranging from material to biological sciences. This conference is relevant to the Commission's goals and missions. The Commission on XAFS and IXAS, the body that oversees the organization of this important conference, have jointly organized a Symposium at XAFS14 focused on combination of XAFS and XRD in material and biological science.

The co-organization of this symposium at XAFS14 and the XAFS Tutorial at the Osaka Congress allowed strengthening of the contacts with IXAS.

I. Ascone, Chair, **A. Molenbroek**, former Chair and **C. T. Chandler**, Secretary

7. 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 2008 the Executive Committee approved sponsorship of various schools and meetings, mostly with financial support. Those held in 2008 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 2009, but approved in 2008, are listed below.

Second African School and Workshop on X-rays in Materials: Some Established Techniques and Practical Applications, Dakar, Senegal, 19–26 January 2009.

Role of Synchrotron Radiation in the Advancement of Materials, Red Sea, Egypt, 1–5 February 2009.

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

XII Intensive Course on X-ray Structure Analysis, Durham, UK, 28 March – 6 April 2009.

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

Second International School on Biological Crystallization and International School on Crystallization: Drugs, Foods and Agrochemicals, Granada, Spain, 18–22 May 2009 and 25–29 May 2009.

High-Pressure Crystallography: From Novel Experimental Approaches to Applications in Cutting-Edge Technologies, Erice, Italy, 4–14 June 2009.

Symposium R on X-ray Techniques for Advanced Materials, Nanostructures and Thin Films – From Laboratory Sources to Synchrotron Radiation, Strasbourg, France, 8–12 June 2009.

2nd School and Workshop on X-ray Micro- and Nanoprobes, Palinuro, Italy, 11–19 June 2009.

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

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

Advances in the Characterization of Industrial Materials, Chania, Greece, 10–20 July 2009.

Advanced Crystallography at High Pressure, Harbin, People's Republic of China, 27–31 August 2009.

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 L. T. J. Delbaere. 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.

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

The continuation of this Committee will be discussed at the meeting of the Executive Committee in Toronto in 2009.

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

The central event for COMCIFS in 2008 was the Osaka Congress, where two closed meetings and one Microsymposium were held. New standards for writing CIF dictionaries (DDLm and dREL) were accepted in draft form at the meeting, subject to some technical refinements. DDLm represents a merging and enhancement of the original dictionary languages (DDL1 and DDL2). The new standards will, among other things, permit more modularity in dictionary construction and allow mathematical relationships between CIF data items to be expressed in a way that permits fully automated calculation of derived values.

imgCIF and the associated Crystallographic Binary Format (CBF) once again saw significant activity in 2008, including round-table technical discussions with manufacturers and software developers during the Osaka Congress. CBF is seeing increasing take-up, with manufacturers providing or developing CBF support for their detectors now including Pilatus, ADSC, Rayonix and Rigaku. Software support for CBF is also improving, with MOSFLM, ADXV and

XDS all supporting CBF input. Following work at a number of laboratories in 2008, programming libraries for CBF support now exist in all major programming languages used in handling diffraction images.

While technical development has been the focus of activity during the year, dictionaries also continue to be maintained and upgraded. An updated core CIF dictionary (version 2.4) was released in April, representing the culmination of several years' work. Following the publication of Volume A1 of *International Tables (Symmetry Relations Between Space Groups)*, G. Madariaga is leading a group which will resume work on updating and expanding the symmetry CIF dictionary to include information from this new volume.

As other scientific disciplines and organizations begin to tackle the problem of data portability and archiving, interoperability of CIF with other data frameworks is becoming important. NeXuS is a framework for raw data storage which has seen broad adoption in X-ray and neutron facilities. Working links with the NeXuS community were established this year, including a presentation to the NeXuS Advisory Committee (the equivalent of COMCIFS). Discussions on how best to interoperate are ongoing. COMCIFS has also established a working group to explore how CIF, and particularly mmCIF, might interact with the Open Biomedical Ontologies project (OBO), which aims to codify concepts and relationships in biological and medical fields.

The Osaka meeting also saw a changing of the guard, with N. Spadaccini and myself replacing outgoing members H. Berman, S. R. Hall, G. Madariaga and I. D. Brown. I. D. Brown also stepped down as Chair after 15 years of dedicated service, for which I would like to thank him on behalf of the Committee.

J. Hester, Chair

10. Committee on Crystallographic Databases

The role of the Committee will be discussed at the meeting of the Executive Committee in Toronto in 2009.

C. Lecomte, Chair

11. IUCr Newsletter

Four issues of the *IUCr Newsletter* were prepared in 2008 (Volume 16-1 to 16-4), with 16-4 being printed and mailed in early 2009. This report will cover all of Volume 16. Three of the four issues were 32 pages in length and the fourth contained 24 pages. 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 meetings calendar.

Each issue carried a President's column. The first two were written by Y. Ohashi and the last two were written by S. Larsen after the elections in Osaka. Editorial responsibilities were shared by W. L. Duax and J. Flippen-Anderson. P. Coley 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. The articles on crystallography in the various countries adhering to the Union were suspended for 2008 as there were no articles ready for publication in the first half of the year and the second half was dedicated to reporting on the Osaka Congress.

Volume 16 published reports on the annual meetings of all three IUCr Regional Associates and reported on the activities of a number of IUCr Commissions (Computing, Teaching, Mathematical and

Theoretical Crystallography) as well as on the formation of the new Commission on Crystallography in Art and Cultural Heritage.

Additional meeting and workshop reports were published covering activities in Poland, Croatia, Argentina, Germany, Italy, France, Canada, China, Portugal, Belgium and the USA.

The first issue of the year contained a two-page promotion for the Osaka Congress and photos from the Geneva Congress in the centrefold as part of our focus on 2008 being the year of an IUCr Congress.

The mailing list was 1% smaller than in 2007 with an average distribution of 18 353. 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; Å. Kvick, 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. R. 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

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

In 2008, 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 Texts on Crystallography were published: No. 10, *Advanced Structural Inorganic Chemistry*, by Wai-Kee Li, Gong-Du Zhou and T. Mak (publication date 27 March 2008); and No. 11, *Diffuse Scattering and Defect Structure Simulations*, by R. B. Neder and T. Proffen (publication date 20 November 2008).

A number of new books are in the production phase and others are in the pipeline. The Committee and the OUP editing staff reviewed a number of proposals and there are contacts with authors about possible new volumes.

The Committee is very interested in proposals for new volumes and encourages prospective authors to contact the Chair of the Committee (davide.viterbo@mfn.unipmn.it). Readers may suggest topics and/or authors as they know the subjects that are not well covered in the literature. Manuscripts covering important aspects of crystallography and related fields are very welcome.

D. Viterbo, Chair of Book Series Committee, and **H. Schenk**, former Chair

13. Regional Associates and Scientific Associates

13.1. American Crystallographic Association (ACA)

Since 2008 was the year of an IUCr Congress, the ACA meeting was an early meeting, Knoxville, Tennessee, USA, 31 May – 5 June 2008. The ACA Council had a combined Spring/Summer meeting on 30 May 2008 in Knoxville. J. Britten is the new Canadian Representative on the ACA Council. J. Britten is also the Programme Chair of the ACA 2009 meeting to be held in Toronto, Ontario, Canada, 25–30 July 2009. Multiple visas are required for some non-USA students for the ACA 2009 meeting. A crystallography school will be held at

McMaster University in Hamilton, Ontario, prior to the ACA 2009 meeting; this is important for the teaching of crystallography.

At the ACA 2008 meeting in Knoxville, there were four Workshops on 31 May 2008:

(1) Magnetic Structure Analysis by Neutron Diffraction Techniques.

(2) Neutron Macromolecular Crystallography from Expression to Refinement.

(3) Wise Use of Dose: Structure Solvability vs Structure Integrity.

(4) Structural Biology without Crystals: Small-Angle Scattering Methods.

Highlights of the ACA 2008 Programme are:

(a) Transactions Symposium on Complementary Methods for Structure/Function Studies of Biomolecules.

(b) The Etter Early Career Award to R. Custelcean and the following Symposium.

(c) The Patterson Award to Bi-Cheng Wang and the Symposium on Advances in Macromolecular Phasing and their Impact to Structural Biology.

The total number of participants at ACA 2008 was 634. There were 201 posters and 248 lectures at the meeting. A total of 15 students were provided with travel grants from the IUCr travel grant; all applicants from outside of the USA (Brazil, Germany, The Netherlands) received funds. Ten prizes were awarded to the best poster presentations in various areas of crystallography.

The 2008 Summer School Course on Small Molecule Crystallography was organized by C. H. Lake and B. M. Craven and was held at the Indiana University of Pennsylvania, 7–16 July 2008. Single crystal and powder diffraction were extensively covered in the course. A total of 19 students attended from Uruguay, Brazil and the USA. The course entailed lectures in the morning, workshops in the afternoon and computer tutorials in the evening, a day to tour Pittsburgh and a day of final student presentations. The course was rated very highly by the student evaluations. It is important that such crystallographic schools continue to be offered.

The 2008 Summer School in Macromolecular Crystallography was organized by A. J. Howard and was held at the Illinois Institute of Technology and the Advanced Photon Source, 14–25 July 2008. Crystallization techniques of macromolecules were taught by experts and employed by the students. At least three visits per student to beamlines at the APS were held to enable them to collect diffraction data on their own crystals. The students tried molecular replacement to solve protein crystal structures. A total of 11 students attended the School from Columbia and the USA. Macromolecular Crystallography Schools should continue to be offered.

L. T. J. Delbaere, IUCr Representative

13.2. Asian Crystallographic Association (AsCA)

During 2008, AsCA continued to be an active forum for scientific interaction among crystallographers in the Asian region. The Osaka Congress of course provided a wonderful opportunity for crystallographers worldwide to interact with their colleagues in Asia. Activities of AsCA in 2008 included planning for the meetings in Beijing, People's Republic of China, in October 2009, jointly with the Chinese Crystallographic Association, and in Busan, Korea, in November 2010. P. Colman is Chair of the International Programme Committee for the Beijing meeting and J. Martin is the Chair of the International Programme Committee for the Busan meeting. AsCA plans to use some of its accumulated reserves to fund access to these

meetings by young scientists in the region. The IUCr is also expected to provide support.

AsCA coordinated an initiative prompted by the IUCr President 2005–2008, Y. Ohashi, to establish a group of Asian nations who were not IUCr members to join the IUCr as a group. This proposal was accepted at the Osaka General Assembly. The first two triennia of membership are generously funded by the Society for Crystallographers in Australia and New Zealand (SCANZ) and the Crystallographic Society of Japan (CrSJ).

The trustees of AsCA are M. Spackman and C. Bond at the University of Western Australia. All the funds are currently held as cash deposits in Australian dollars. The total funds as of March 2009 are AUD 130 592.

G. R. Desiraju, IUCr Representative

13.3. European Crystallographic Association (ECA)

The present membership of the ECA Executive Committee is: President: J. R. Helliwell (UK); Vice-President: S. Larsen (Denmark); Secretary: P. Bombicz (Hungary); Treasurer: R. Kuzel (Czech Republic); Members: S. Garcia-Granda (Spain), L. Van Meervelt (Belgium), A. Roodt (South Africa) and ECA Webmaster M. Nespolo (France, *ex officio*).

Overview of supported meetings. The ECA supported the following meetings between September 2008 and August 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, Bialowieza, Poland, 4–11 July 2009 (EUR 1000).

Total sum support: EUR 7250.

A new rule was introduced in 2009: Dates of a conference must be outside of a blackout period of one month around the ECMs and IUCr Congresses. This was motivated by feedback from exhibitors at ECM-24 that there were too many conferences in the summer and these were actively encouraged by the formal Bursary Awards. Thus the large conferences such as the IUCr Congresses and the ECMs were not being respected. The Exhibitors preferred to focus on doing a good job at these bigger conferences. All the above meetings satisfied the new rule. Several applications unfortunately did not and had to be rejected.

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.

Future ECA meetings will be held as follows:

(1) ECM-25: Istanbul, Turkey, August 2009.

(2) ECM-26: Darmstadt, Germany, August 2010 (this will be held along with EPDIC-22).

(3) ECM-27 Bergen, Norway, 2012.

The organization of the Programme of ECM meetings now follows the Focus Areas subject themes approach as pioneered at ECM-21.

Candidates bidding to host ECM-28 in 2013 are Greece and the UK.

ECM-25 will feature a special celebration in a ‘Look Back, Look Forward’ evening session. L. B. McCusker is to be the recipient of the Max Perutz Prize and L. Palatinus is to be the recipient of the Bertaut Prize.

2009 is an election year whereby the ECA Executive Committee elections for Officers for the period 2009–2012 will take place in Istanbul.

The ECA leaflet that was prepared for the first time in 2008 year by R. Kuzel has been updated. The first edition of the leaflet resulted in a substantial increase in the number of Corporate Affiliate Members (CAMs) of the ECA to more than 20. The goal is to encourage the new CAMs to continue their membership for several years. As it is highly important to enlarge the number of individual members of ECA, a reminder was sent to all ECA individual members about the renewal of their membership and to consider the possibility of making a donation to the ECA.

C. J. Gilmore, IUCr Representative

13.4. International Organization for Crystal Growth (IOCG)

No formal meeting of the IOCG (<http://www.iocg.org/>) was planned or organized in 2008.

The IOCG President for 2007–2010 is A. A. Chernov (USA), with Co-Vice-Presidents T. Ohachi (Japan) and R. Fornari (Germany), Secretary T. F. Kuech (USA) and Treasurer V. Fratello (USA). The other members of the Executive Committee are H. Dabkowska (Canada), J. Derby (USA), T. Duffar (France), K. Kakimoto (Japan), S. Krukowski (Poland), K. Roberts (UK), P. Rudolph (Germany) and E. Vlieg (The Netherlands) with the Past President R. F. Sekerka (USA) and honorary principal founder M. Schieber (Israel).

The Sixteenth International Conference on Crystal Growth (ICCG-16) together with the Fourteenth International Conference on Vapor Growth and Epitaxy (ICVGE-14) will be held in Beijing, People’s Republic of China, 8–13 August 2010 (Chair Minhua Jiang, General Secretary Jiang Wang). Members and consultants of the Commission on Crystal Growth and Characterization of Materials are strongly involved in the work of Programme and Advisory Committees of both meetings.

The 14th International School on Crystal Growth (Chair Mu Wang) will be held in Dalian, People’s Republic of China, 1–7 August 2010.

Detailed information about both Conferences and the School will be posted on the IOCG web site.

The next General Assembly of the IOCG will take place in Beijing during ICCG-16.

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. Some examples are listed below.

Deutsche Kristallzuchtertagung der DGKK, Munich, Germany, 5–8 March 2008, Chair P. Gille (LMU) (<http://www.dgkk.de>).

4th Asian Conference on Crystal Growth, Sendai, Japan, 21–24 May 2008, Chair K. Nakajima (<http://www.cgct4.imr.tohoku.ac.jp/>).

22nd Conference on Crystal Growth and Epitaxy of the American Association for Crystal Growth – West, Stanford Sierra Camp, Fallen Leaf Lake, California, USA, 8–11 June 2008, Chair F. Ross (IBM) (<https://www.crystalgrowth.org/>).

4th International Workshop on Crystal Growth Technology (IWCCT-3), Beatenberg, Switzerland, 18–25 May 2008, Chair H. Scheel.

International Conference on Quasicrystals (ICQ10), Zürich, Switzerland, 9–14 June 2008.

Fifth School on Crystal Growth, Hotel Happy Star Hnanice-Znojmo, Czech Republic, 1–2 September 2008 (<http://www.fzu.cz/varia/cacg/DMS18/>).

International Symposium on Industrial Crystallization (ISIC 17), Maastricht, The Netherlands, 14–17 September 2008 (<http://www.ti.kviv.be/conf/isic17/>).

The extended list of past and future conferences and meetings relevant to the crystal growth community can be found at <http://iocg.org/>.

H. A. Dabkowska, IUCr Representative

13.5. International Centre for Diffraction Data

Two members of the Commission on Powder Diffraction (CPD) will attend the ICDD spring meeting at the end of March 2009. P. Whitfield was kindly invited by the ICDD board as CPD Chair and B. Toby was also in attendance. Formal linkages exist between the IUCr and the ICDD, as the CPD has a representative from the ICDD and the CPD Chair is the IUCr representative to the ICDD. Although J. A. Kaduk from the ICDD has attended CPD meetings regularly, geography has hindered this being a two-way process. With the current CPD chair based in Canada it is hoped that this relationship can be improved. The CPD poster described in §6.16 is now on display at the ICDD headquarters.

At the suggestion of the CPD Chair, the current President of the ACA, R. Von Dreele, was invited to the meeting. This year, the Denver X-ray Meeting (DXC), organized by the ICDD, was inadvertently scheduled at the exact same time as the ACA meeting. This demonstrated the need for improved communication between the two organizations, and the presence of a prominent powder diffractionist as ACA President presented an excellent opportunity to move things forward. I am delighted to report that this goal was achieved during the meeting spontaneously without any further external input. The result of these discussions is that a jointly sited and coordinated ACA-DXC meeting is currently being explored for 2013, which is excellent news for powder diffraction both in North America and elsewhere. The ICDD will once again fund ten USD 2500 Ludo Frevel scholarships in 2009.

The Powder Diffraction Files (PDF-2 and PDF-4) are important tools for researchers using powder diffraction. A number of motions were put forward to the ICDD board which will be of interest to many users of these databases. From the Ceramics Sub-committee it was proposed that initial studies on the creation of a sub-file on hydrogen-storage materials be started, and that the definition of bioceramics be revised. From the Minerals Sub-committee the most important motion was that the PDF continue using the current Shaller adjectives in the mineral sub-file rather than following the new guidelines from the International Mineralogical Association. The Organics Sub-committee proposed that the CSD chemical classes be used along with the current functional classifications in the sub-files. The Non-Ambient Sub-committee had an extended discussion on how to deal with conditions other than pressure and temperature (e.g. humidity) as well as patterns of materials such as quenched, metastable high-temperature phases taken at room temperature.

P. Whitfield, IUCr Representative

14. Representatives on Other Bodies

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

ICTNS continued its activities on behalf of IUPAC in reviewing and approving Technical Reports and Recommendations submitted to IUPAC for publication in *Pure and Applied Chemistry*, and also for approving, on behalf of IUPAC, publications emanating from international bodies on which IUPAC has representation.

The document *Towards Defining Materials Chemistry* under Technical Reports and Recommendations has been reviewed by referees chosen among IUCr members.

Several of the ‘colour’ books have undergone revision during the biennium, and these have been reviewed by ICTNS. They include:

Quantities, Units and Symbols in Physical Chemistry (Green Book), 3rd edition, 2007.

Terminology and Nomenclature in Polymer Chemistry (Purple Book), 2nd edition, 2008.

A. Authier, IUCr Representative

14.2. International Council for Scientific and Technical Information (ICSTI)

ICSTI offers a unique forum for interaction among organizations that create, disseminate and use scientific and technical information. ICSTI is a scientific associate of ICSU, the International Council for Science. ICSTI’s mission cuts across scientific and technical disciplines as well as international borders, to give member organizations the benefit of a truly global community. A developing emphasis in its events and Committee work, most prominently at its Public Conference held at the Korea Institute of Science and Technology Information (KISTI), Seoul, Korea, 11–12 June 2008 (see the detailed Conference Programme at http://www.icsti.org/conf2008/kisti_icsti_conf.htm) and with more planned for 2009, is on the need for readers of the results of scientific research to have a better connection with the primary data supporting these results. IUCr Journals is widely recognized as a leader in these matters, as recognized by the prize for technical innovation awarded by the Association of Learned and Professional Society Publishers (ALPSP) in 2006. An ICSTI Workshop in February 2009 will discuss aspects of identifying and citing data sets, and a public conference in Ottawa in June 2009 will cover a wider range of topics on this theme.

ICSTI’s Technical Activities Coordinating Committee (TACC) has initialized two projects: (1) Numeric Data: Citation Techniques and Integration with Text and (2) Multimedia Search and Retrieval, which are both of interest to the IUCr. The IUCr has offered to contribute to the data citation project with examples of our use of Digital Object Identifiers (DOIs) for citing supplementary CIF data sets, and examples of a DOI-based parameter-passing mechanism that could form a model for citing subsets or slices through data sets. The multimedia project aims to advance the integration of multimedia into traditional Science and Technical Information (STI) search and retrieval. It will explore the indexing of full spoken content in an audio or video file through voice-recognition technology. The IUCr has contributed some video materials to this project, including the W. L. Bragg Public Lecture by J. R. Helliwell [available from the IUCr web site, with detailed explanations of the lecture demonstrations in *J. Appl. Cryst.* (2009), **42**, 365]. This lecture (<http://www.iucr.org/education/teaching-resources/bragg-lecture-2001>) contains useful crystallographic technical terms suitable for subject-specialized voice-recognition training.

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

J. R. Helliwell, IUCr Representative

14.3. International Council for Science (ICSU)

ICSU was founded in 1931 as an organization composed of International Scientific Unions and National Scientific Councils. At present, there are 30 Scientific Union members and 97 National Council members. The IUCr is one of the member Scientific Unions. The activities of ICSU are closely correlated with those of the organizations of The United Nations, such as UNESCO (United Nations Educational, Scientific and Cultural Organization), UNEP (United Nations Environment Programme), CSD (Commission on Sustainable Development) and WMO (World Meteorological Organization), and those of TWAS (The Academy of Sciences for the Developing World), CAETS (International Council of Academies of Engineering and Technological Sciences Inc.) and ISSC (The International Social Sciences Council). The General Assembly is held every three years. The Executive Board, including President, immediate Past President or President-Elect, two Vice-Presidents, Treasurer, Secretary-General and eight Ordinary Members, usually comprises the Council.

I attended the 29th General Assembly (GA) of ICSU, which was held in Maputo, Mozambique, 21–24 October 2008, as the representative of the IUCr, since the Immediate Past President of the IUCr is traditionally assigned to the post. Each member of the Scientific Unions and National Scientific Councils has one voting right in the GA. However, since the total voting rights for both groups should be equal, each member of the Scientific Union has a weighted voting right of 97/30, a ratio of the numbers of their members.

Before the Opening Ceremony on 21 October, the Open Forum of the Scientific Union members was held from 9:00 a.m. to 4:00 p.m. The pre-discussions were performed for the important items in the GA. I think it very important to attend the Open Forum and understand the background to the important items in the GA. I displayed a poster showing the history and activity of the IUCr on the poster board and put the leaflets of the IUCr Journals and *International Tables* on a table in front of the poster. About two thirds of the Unions had poster presentations. Several Scientific Unions had beautiful posters that had been prepared previously and used in many meetings. In the Opening Ceremony from 4:00 p.m., the President of Mozambique, H. E. Armando Emilio Guebuza, made a welcoming speech.

On the second day, 22 October, the GA started from 9:00 a.m. at the Main Hall of the International Conference Center ‘Joaquim Chissano’ (CICJC). The Secretary General reported the activities over the last three years, especially the establishment of Regional Offices, the celebration of ICSU’s 75th anniversary in 2006 and the organization of the Young Scientists’ Conference in 2007. The reports from the Scientific Unions and National Councils Fora were presented.

The first ever ICSU Strategic Plan was approved at the 28th GA in 2006. The plan covered the six-year period 2006–2011. The implementation of the first three years was reported by the Executive Secretary, the representative of the Plan. The Strategic Plan is composed of four Projects:

- (1) International Polar Year (IPY);
- (2) Integrated Research on Disaster Risk;
- (3) Ecosystem Change and Human Well-being; and
- (4) Health and Well-being in the Changing Urban Environment.

All the reports were accepted and were encouraged to continue for the next three years.

Finally, the presentations by candidates for Officers were held. There were two candidates for President-Elect, two for Vice-Presidents (Internal and External), but only one candidate for Secretary General and one for Treasurer.

On the third day, 23 October, the Global Environmental Change Programmes, as part of the Strategic Plan, were reviewed. The following programmes were reported by the Executive Secretary and the representatives of the programmes:

- (1) International Human Dimensions Programme (IHDP);
- (2) Earth System Scientific Partnership (ESSP);
- (3) International Geosphere–Biosphere Programme (IGBP); and
- (4) World Climate Research Programme (WCRP).

The discussions continued very intensively. The proposed decisions were modified so that the planning group of ICSU (CSPR: Committee on Scientific Planning and Review) should organize the high-level meeting and outline the overall framework after this.

Then the activity of the Scientific Commission on Problems of the Environment (SCOPE) was discussed. This Commission was reviewed last year since several environmental organizations had made their own scientific assessments and provided competition for SCOPE's assessments. Finally, the decision was accepted that after a suitable transition period of no more than two years SCOPE will cease to be an ICSU Interdisciplinary Body.

The report of the Committee on Freedom and Responsibility in the conduct of Science (CFRS) was presented by the Chair. After the discussion, it was decided that the CFRS booklet *Freedom, Responsibility and Universality of Science* should be endorsed.

In the Strategic Plan, ICSU will increasingly seek productive collaboration in the area of Social Sciences, where it lacks expertise. To encourage this Plan, the Scientific Unions were divided into four groups in the 28th GA: (1) Physical, Chemical and Mathematical sciences; (2) Biological Sciences; (3) Earth and Space Sciences; and (4) Social Sciences. One member of the Executive Board should be elected from each group.

After lunch, the Election of Officers was performed. The results are as follows: President-Elect: Yuan-Tsueh Lee (China, Taipei); Vice-President for Scientific Planning and Review: K. Raivio (Finland); Vice-President for External Relations: R. Kuroda (Japan); Secretary-General: M. Tchuente (Cameroon); Treasurer: H.-R. Ott (Switzerland). The President, C. Brechignac (France), had already been elected as the President-Elect at the previous GA.

The reports from the Strategic Committee on Information and Data (SCID), from Regional Offices (Africa, Asia and Pacific, Latin America and the Caribbean), and from the Policy Committee on Developing Countries (PCDC) were given. All the reports were accepted. Then the dinner party was held.

On the fourth day, 24 October, the reports on the other Strategic Activities and Planning for the next Strategic Plan 2012–2017 were presented.

The report on Dues Structure and the Recommendation from the Executive Board was then given. At the previous 28th GA it had been decided to form a working group to modify the dues structure. The following structure was accepted:

- (1) Dues to be based on a model based on raw GDP figures.
- (2) Ten bands to be used, rather than the current 51.
- (3) A minimum payment of EUR 1000 to be required.
- (4) A cap to be placed on the top band amount (currently paid by the USA).
- (5) In-kind contribution to ICSU to be encouraged and recognized in some way.

(6) Four bands be created for Scientific Union dues.

(7) Scientific Unions to be assigned to bands that would be based on their declared income from dues.

(8) The dues for Scientific Associates be maintained at EUR 500.

(9) The new dues structure to be regarded as a 'lower bound' by each member, with higher voluntary payments being encouraged.

(10) Members may voluntarily move to a higher subscription band.

(11) The new mechanisms for National Members, Scientific Unions and Scientific Associates become operative from 2012.

Since the dues will be based on raw GDP figure, the payment of the USA will become very high. Therefore, item (4) was introduced. Probably the payment of Japan or China will be most greatly increased. Last year the working group proposed a plan in which the Scientific Union dues should be based on the total income of the Scientific Union. This indicated that the IUCr should pay EUR 30 000 per year. Objections to the plan were sent to the working group from 14 Scientific Unions including the IUCr. The plan was withdrawn and the above dues structure was proposed. From the above proposed list, the IUCr will be included in the third band (declared income less than EUR 100 000 per year) and the payment would be EUR 2500 per year from 2012. The IUCr currently pays EUR 6002 per year. The new dues for the IUCr should be decided considering the items (9) and (10).

Another problem was the weighted voting. This was strongly supported by the large countries, such as USA and Japan. The developing countries strongly supported the equal voting policy adapted currently. No decision was made, so that the equal voting will continue.

The election of the Ordinary Members of the Executive Board was held. Four members were elected from the National Council members and four members were elected from Scientific Union members. The following members were elected: from Scientific Union members: B. Henry (IUPAC), D. Jaron (IUPESM), B. Overmier (IUPsyS), U. Shamir (IUGG); from National Council members: Fu Congbin (China), M. Iaccarino (Italy), S. Pastrana (Cuba), Abdul Hamid Zakri (Malaysia).

The Executive Secretary was recommended by the Executive Board and was accepted as follows: Deliang Chen (University of Gothenburg, Sweden, and Beijing Climate Center, China).

It had already been decided that the next GA would be held in Rome, Italy, in 2011. However, the location for the GA in 2014 was not decided at the GA but a city in China, Taipei was introduced. The decision will be made by the new Executive Board and will be announced in the near future.

All the business was complete at 6:00 p.m. on 24 October.

Y. Ohashi, IUCr Representative

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

The major event for CODATA during 2008 was the biennial Conference and General Assembly held in Kyiv, Ukraine, 5–8 October 2008.

CODATA Conference. The theme of the 21st International CODATA Conference: 'Scientific Information for Society: from Today to the Future' continued the focus on the information society that has emerged in the last few biennial meetings. The 2008 meeting took as its keynote the importance of engaging the younger generation of scientists to lead future developments in a world community increasingly dependent upon information and scientific data.

Presentations of interest to the IUCr were delivered in some of the Plenary Lectures (Information and Knowledge as a Tool in Facing Global Challenges; Interdisciplinary Scientific Data for Sustainable Development Global Simulation; Curating Data? What about Curating Services and Workflows?) and in the meeting sessions:

Long-term data and knowledge management;

Physical science: data quality and database; and

Data visualization approaches, at which the IUCr representative gave a presentation demonstrating the IUCr approach to the interactive visualization of data as a feature of online crystallography journal articles.

A full meeting report is available at <http://www.iucr.org/resources/data/meeting-reports/codata-2008>.

General Assembly. During the course of the 2008 CODATA Conference, two special sessions were held to reduce the burden spent on reporting directly to the General Assembly, and to allow greater involvement of conference members. The first was on 'Collaboration with ICSU Organizations and Report from the ICSU *ad hoc* Strategic Committee on Data and Information (SCID)'. Its main purpose was to discuss the recommendations contained in the report of the ICSU *ad hoc* Strategic Committee on Data and Information. This Committee, following on from the ICSU Priority Area Assessment Report of 2004, was formed to implement the key recommendations from that report relating to the reforms of ICSU's own structures. It acknowledged CODATA's development of a Strategic Plan, recommended that CODATA be closely involved with a new *ad hoc* ICSU Strategic Coordinating Committee, and recommended that CODATA should work closely with the World Data System (a proposed reorganization of the World Data Centres and Federation of Astronomical and Geophysical Data Analysis Services). The second special session allowed National and Union members of CODATA to report on their relevant activities in the previous two-year period.

The General Assembly noted the SCID Report. It was commented that the advisory role recommended by the Report for CODATA reflected the fact that it was still developing focus within its evolving Strategic Plan, and might later become more closely involved in managing the World Data System. The General Assembly reviewed progress with the CODATA Strategic Plan, and noted the urgent need to finalize the Plan and roll out energetic work plans within each of its three major initiatives [the Global Information Commons for Science Initiative, the Scientific Data Across the Digital Divide Programme, and the Advanced Data Methods and Information Technologies for Research and Education (ADMIRE) project].

A report of the activities of the Secretariat described the upheaval during the period involved in relocating the office to its new premises at 5 rue Auguste Vacquerie in Paris, but also described the many projects in which it had been actively involved in spite of the disruption. The General Assembly greeted this report with acclamation.

The 2008 CODATA Prize for outstanding achievement in scientific and technical data was awarded to Liu Chuang, Professor and Director of the Global Change Information and Research Center at the Institute of Geography and Natural Resources, Chinese Academy of Sciences, who has been very actively involved as Co-Chair with the CODATA Task Group on the Preservation and Archiving of Scientific and Technical Data in Developing Countries, and who served on the ICSU Priority Area Assessment (PAA) Panel on Scientific Data and Information.

The General Assembly also appoints or re-confirms Task Groups and Working Groups to further the objectives of CODATA. The Task Groups approved by the 26th General Assembly for 2008–2010 are as

follows (those marked with an asterisk are continuations of existing Task Groups):

Anthropometric Data and Engineering (*);

Biodiversity: Observation and Specimen Records (*);

Data Exchange and Interoperability of Heterogeneous Data;

Resources for Material Science and Education (*);

Data on Natural Gas Hydrates (*);

Data Sources for Sustainable Development in South African Development Community (SADC) Countries (*);

eGY Earth and Space Science Data Interoperability;

Fundamental Constants (*);

Global Information Commons for Science – GICSI/EU;

International Polar Year Data Policy and Management Subcommittee (*); and

Preservation of and Access to Scientific and Technical Data in Developing Countries (*).

Australia and the UK were formally welcomed as National Members of CODATA. Italy has withdrawn its membership.

The Officers of CODATA (terms of office in parentheses) are: President: K. Lal (India; 2006–2010); Vice-Presidents: S. Rossouw (South Africa; 2006–2010), G. Wood (Canada; 2006–2010); Secretary General: R. Chen (USA; 2008–2012); Treasurer: M. Sabourin (Canada; 2008–2012). Ordinary Members of the Executive Board are listed on the CODATA web site at <http://www.codata.org>.

Other activities. CODATA European activities expanded under the COMMUNIA network signed with the Politecnico of Turin, Italy, on the 'Public Domain in the Digital Age'. This is a European-funded Thematic Network. CODATA is taking the lead, in collaboration with other partners of the network, on the second international conference in 2009 on Global Science and the Economics of Knowledge-Sharing Institutions (G-SEKSI). The first International Conference, in which CODATA participated, took place in June 2008 in Louvain, Belgium.

CODATA built on work that started in 2006 as scientific lead on GEO Task DA-06-01: 'Review of GEOSS Data Sharing Principles'. This culminated in a special side event organized by CODATA in conjunction with the GEO-V Plenary in Bucharest, Romania, in November 2008, focusing on Implementation Guidelines of the GEOSS Data Sharing Principles prepared by CODATA.

The IUCr CODATA Representative continues to work closely with the ICSTI Representative, Professor J. R. Helliwell, on matters of common interest.

B. McMahon, IUCr Representative

14.5. ICSU Committee on Space Research (COSPAR)

The majority of COSPAR activities are devoted to space topics, such as astronomy, space travel and exploration, and climate research.

The 37th Assembly of the Committee on Space Research (COSPAR, <http://cosparhq.cnes.fr/>) was held in the Congress Center, Montreal, Canada, 13–20 July 2008. The Local Organizing Committee of the 37th Assembly, headed by G. G. Shepard (University of Toronto, Canada) did an excellent job. The official participation statistics supplied by the local organizers is as follows: Full participants: 1856; students: 343; exhibitors: 32; guests: 104; IAA day: 42; accompanying: 87; total: 2464. 3775 abstracts were submitted by 2874 authors for the 94 events creating the scientific programme.

The 50th Anniversary Lectures were presented by P. Willmore, University of Birmingham (COSPAR's First 50 Years), by S. Vitale, University of Trento and INFN (Space and the Spacecraft as a

Precision Laboratory) and by L. A. Fisk, University of Michigan (The Impact of Space on Society). The Chair and Chief Executive Officer of Arianespace, J.-Y. Le Gall, talked about Service and Solutions for Scientific Endeavours. The detailed scientific programme of the Montreal Assembly may be viewed at <http://cosparhq.cnrs.fr/>.

The COSPAR President for the period 2006–2010 is R.-M. Bonnet (France) and the Vice-Presidents are W. Hermans (The Netherlands) and E. C. Stone (USA). Members of the Bureau are: M.-H. Jiang (China), M. E. Machado (Argentina), G. G. Shepherd (Canada), R. Sridharan (India), L. Zelenyi (Russia) and J. B. Zielinski (Poland).

The most interesting division of COSPAR for the IUCr is the Scientific Commission on Materials Science in Space (MSS), which deals with scientific experiments in materials and fluid performed in reduced gravity. Different experiments on the growth of crystals in microgravity were, at some point, an important part of these programmes. The MSS Commission reviews fundamental theoretical and experimental approaches to this research, recommending promising avenues for the future and coordinating the exchange of information on scientific subjects. The Commission is chaired by V. Shevtsova (Belgium) with the Vice-Chairs W.-R. Hu (China), S. Amiroudine (France) and S. Yoda (Japan).

Advances in Space Research (ASR), the official journal of COSPAR, covers all areas of space research including – but not limited to – space studies of the earth's surface, meteorology, climate, fundamental physics in space, materials physics in space, space debris, weather and earth observation of space phenomena. The journal home page is at <http://ees.elsevier.com/asr>. ASR is included in the Web of Science and has an impact factor of 0.774.

As the 23rd IUCr Congress will be held in Montreal in 2014 in the same Palais des Congress it is good to know that all the participants were very much impressed with both the scientific programme and the beauty of the city itself. They also had an opportunity to visit Niagara Falls, Toronto and the very picturesque rural provinces of Ontario and Quebec.

The full report from the Montreal Assembly was recently published in the *IUCr Newsletter* (2008, Volume 16, No. 3). A copy of this *Newsletter* was recently delivered to the COSPAR secretariat and the article will be kept there as part of press clippings from the Montreal Assembly.

The next COSPAR Assembly will be held in Bremen, Germany, in 2010.

H. A. Dabkowska, IUCr Representative

15. Finances

Extracts from the full financial statements, namely the Income and Expenditure account, Balance Sheet and Summary of Fund Accounts, are given in Tables 2, 3 and 4, respectively.¹ For comparison, the figures for 2007 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 2008 have been translated into CHF in the balance sheet at the rate operative at that date. For the income and expenditure accounts

¹ The full audited accounts are available from the IUCr electronic archives (Reference ES0372). Services for accessing these data are described at the back of the journal.

transactions have been translated into CHF by applying the rates appropriate to the individual dates of these transactions. As a consequence of the fluctuation in exchange rates, overall an apparent loss has arisen on the assets of the Union, in terms of CHF, amounting to CHF 1 193 529. In the accounts this loss has been assigned as 'Realized' (CHF 349 133) and 'Unrealized' (CHF 844 396). The loss attributable to investment activities has been assigned to the General Fund and the loss attributable to trading activities has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 2008. It should be noted that this overall loss in CHF is not a real loss of money, but rather a loss on paper resulting from the accounts being expressed in CHF.

Investments are noted in the balance sheet at their market value at 31 December 2008.

The balance sheet shows that the assets of the Union, including the loss resulting from fluctuations in rates of exchange, have decreased during the year, from CHF 5 019 330 to CHF 3 023 501. The movement in market value of the investments was CHF –972 646 in 2008 (CHF –244 032 in 2007). The significant loss in value of the investments in 2008 is a result of the well known market situation that developed in 2008 and the fall in value of the British pound.

In 2008 the Executive Committee decided to merge the individual journal funds [*Acta Crystallographica* Fund (containing six journals), *Journal of Applied Crystallography* Fund and *Journal of Synchrotron Radiation* Fund] into a single Journals Fund.

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 75 000 to the *Newsletter* Fund; CHF 25 000 to the President's Fund; and CHF 40 000 to the Ewald Fund.

The following comments refer to figures in the full accounts. When comparing figures for 2008 with those for 2007 it should be borne in mind that in the period 31 December 2007 to 31 December 2008 the Swiss Franc (in which these accounts are expressed) strengthened by 33% against the British pound (in which the majority of the IUCr's expenses are incurred).

The General Fund account shows a deficit of CHF 347 375, as compared with a deficit in 2007 of CHF 190 250. The administrative expenses were CHF 440 098 in 2008 as compared with CHF 506 617 in 2007. Of this amount, CHF 198 044 was charged to the publications of the Union.

The expenses of the Union Representatives on other bodies were CHF 14 279. The cost of the Finance Committee meetings held in 2008 was CHF 22 818, while the Executive Committee meeting cost CHF 85 035. The income from the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 17 132. The subscriptions from Adhering Bodies were CHF 159 353. Interest on bank accounts and investments credited to the General Fund was CHF 135 282.

In 2008 the Executive Committee decided to assign all investment interest to the General Fund.

Grants totalling CHF 12 418 were paid from the President's Fund in 2008.

The Journals Fund account for 2008 shows a surplus of CHF 1 068 593 before the transfer of CHF 620 000 to the other fund accounts, as compared with a surplus of CHF 958 436 in 2007 before the transfer of CHF 535 000 to the other fund accounts.

The subscription rates were increased for 2008. In 2008, the number of paid subscriptions were as follows: *Acta Crystallographica*: Section A 607 (624) including 49 (48) personal subscriptions (values for 2007 are given in parentheses); Section B 600 (602) including 41

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Table 2

Income and Expenditure Account (in Swiss Francs) for the year ended 31 December 2008.

	2008	2007
Income		
Membership subscriptions	159 353	152 000
Sales		
Journals, back numbers and single issues	4 334 082	4 881 772
Books	268 897	396 541
Open Access Grant	46 284	46 684
Investment income		
Income from investments	102 284	129 916
Bank interest	32 996	34 966
(Loss)/Profit on sale of investments	<u>(22 993)</u>	<u>112 287</u>
Other income		
Royalties and copyright fees	13 744	10 206
Advertising income	227 689	264 486
STAR/CIF income	7 793	<u>37 991</u>
Total income	5 170 129	6 061 290
Expenditure		
Journals		
Publication costs	641 289	993 593
Editorial expenses	249 213	372 273
Technical editing	1 624 148	1 764 307
Subscription administration	<u>122 410</u>	<u>62 992</u>
Books		
Publication costs	33 566	58 657
Editorial expenses	72 304	103 317
Technical editing	<u>228 159</u>	<u>205 628</u>
Newsletter		
Publication costs	105 873	159 019
Editorial expenses	<u>121 678</u>	<u>126 809</u>
President's Fund and other Grants and Young Scientists' support	93 642	235 986
General Assembly costs	89 119	9 181
Committee meetings and expenses	119 870	118 966
Publications and journals development		
General	673 563	658 734
Editors' meetings	4 466	16 790
STAR/CIF	42 686	26 100
Promotion	<u>245 389</u>	<u>196 392</u>
Subscriptions paid	12 237	11 609
Visiting Professorship Programme	8 994	559
Administration expenses:		
General Secretary and Treasurer: Honorarium to Treasurer	13 302	9 829
Audit and accountancy charges	61 756	83 333
Legal and professional fees	12 032	17 807
Travelling expenses	4 795	8 012
Bank charges	<u>2 514</u>	<u>2 389</u>
Executive Secretary's office:		
Salaries and expenses	341 547	381 062
Travel expenses of IUCr Representatives on other bodies	14 279	231
Sponsorship of meetings	6 621	29 867
Congress costs	25 541	74 424
IUCr/FIZ agreement	<u>(17 131)</u>	<u>(19 147)</u>
Bad debts	—	4 000
Depreciation	<u>45 921</u>	<u>47 774</u>
Total expenditure	4 999 783	5 760 493

Table 2 (continued)

	2008	2007
<i>Surplus of income over expenditure (before realized exchange losses)</i>	170 346	300 797
Realized fluctuations in rates of exchange		
Exchange movement on trading activities	(349 133)	—
(Deficit)/surplus of income over expenditure (after realized exchange losses)	(178 787)	300 797
Movement in market value of investments in year	<u>(972 646)</u>	<u>(142 019)</u>
Unrealized fluctuation in rates of exchange		
Exchange movement on trading activities	28 347	(61 365)
Investment activities	<u>(872 743)</u>	<u>(182 667)</u>
Total recognized losses relating to the year	(1 995 829)	(85 254)
Opening fund accounts at 1 January 2008	<u>5 019 330</u>	<u>5 104 584</u>
Closing fund accounts at 31 December 2008	3 023 501	5 019 330

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.

Table 3

Balance sheet (in Swiss Francs) as at 31 December 2008.

	2008	2007
Fixed assets		
Tangible fixed assets	43 124	45 456
Investments at market value	<u>1 797 102</u>	<u>3 663 796</u>
	1 840 226	3 709 252
Current assets		
Stock	182 162	200 701
Cash at bank and in hand		
Current accounts	49 463	28 811
Deposit and savings accounts	601 391	637 242
Cash with Union officials	<u>17 108</u>	<u>17 161</u>
	667 962	683 214
Debtors, accrued income and payments in advance	674 538	878 821
Subscriptions due from Adhering Bodies	<u>13 000</u>	<u>39 000</u>
Total current assets	1 537 662	1 801 736
<i>Creditors: amounts falling due within one year</i>	<u>(354 387)</u>	<u>(491 658)</u>
Net current assets	<u>1 183 275</u>	<u>1 310 078</u>
Total funds	3 023 501	5 019 330

(36) personal subscriptions; Section C 573 (581) including 32 (30) personal subscriptions; Section D 571 (607) including 72 (86) personal subscriptions; *Journal of Applied Crystallography*: 526 (555) including 60 (64) personal subscriptions; *Journal of Synchrotron Radiation*: 189 (200) including 40 (47) personal 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 1 510 701 [for 11 295 published pages (4795 papers)] as compared with CHF 1 766 679 in 2007 [16 136 published pages (6637 papers)]. The smaller number of pages and papers in 2008 were a result of the change to a new short-format style for *Acta E* and the launch of *Acta E* as an open-access

only journal in 2008. Submissions to *Acta E* steadily increased during 2008 and present submission levels are approaching those for 2007. The Journal Fund has also been charged with administration expenses as in previous years as shown in the General Fund.

The *International Tables* account shows a deficit of CHF 127 969, as compared with a deficit of CHF 39 829 in 2007. The net sales income was CHF 198 829 in 2008 as compared with CHF 293 430 in 2007.

The *Newsletter* Fund account received a transfer of CHF 75 000 from the Journals Fund in 2008. The cost to the Union of producing the *Newsletter* in 2008 was CHF 52 353.

In the Publications and Journals Development Fund account, the computing and promotion expenses are divided between the General

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Table 4

Summary of Fund Accounts (in Swiss Francs) as at 31 December 2008.

	As at 1 January 2008	Transfers between funds	(Deficit)/ surplus of income over expenditure for the year	Decrease in market value of investments	Fluctuations in exchange rates		Balance at 31 December 2008
					Trading	Investments	
Fund accounts							
General Fund	247 595	—	(347 375)	(972 646)	81 579	(872 743)	(1 863 590)
President's Fund	91 583	25 000	(12 418)	—	(7 924)	—	96 241
Journals Fund	2 357 821	(620 000)	1 068 593	—	(213 482)	—	2 592 932
<i>International Tables</i>	(201 479)	—	(127 969)	—	25 061	—	(304 387)
Publications and Journals Development Fund	901 099	120 000	(104 254)	—	(69 743)	—	847 102
Research and Education Fund	984 254	160 000	(109 958)	—	(78 678)	—	955 618
Ewald Fund	529 974	40 000	(38 579)	—	(40 423)	—	490 972
Newsletter Fund	74 015	75 000	(52 353)	—	(7 353)	—	89 309
General Assembly and Congress	34 468	200 000	(105 341)	—	(9 823)	—	119 304
	5 109 330	—	170 346	(972 646)	(320 786)	(872 743)	3 023 501

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 has been charged to this Fund. In 2008, CHF 45 541 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 89 143 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 2008 this Fund incurred expenses totalling CHF 105 341 and received a transfer of CHF 200 000 from the Journals Fund.