

## Report of the Executive Committee for 2006

## 1. Meetings

The IUCr sponsored the following meetings held during 2006:

International Workshop on Crystal Growth and Characterization of Advanced Materials, Chennai, India, 9–13 January.

Fourth European Charge Density Meeting (ECDM-IV), Brandenburg, Germany, 25–29 January.

RapiData 2006, Brookhaven, USA, 23–28 April.

Third Moroccan School of Crystallography, Agadir, Morocco, 8–12 May.

Structure and Solution of Large Molecular Assemblies, Erice, Italy, 9–18 June.

International School on Biological Crystallization, Granada, Spain, 18–24 June.

Fourth National Crystal Chemical Conference, Chernogolovka, Russia, 26–30 June.

Thirteenth International Conference on Small-Angle Scattering, Kyoto, Japan, 9–13 July.

ACA Annual Meeting, Hawaii, USA, 22–27 July.

23rd European Crystallographic Meeting (ECM-23), Leuven, Belgium, 6–11 August.

Sagamore XV: Electron Charge, Spin and Momentum Densities, Warwickshire, UK, 13–18 August.

Structural Chemistry – Indaba 5, Kruger National Park, South Africa, 20–25 August.

IUCr Teaching Commission Intensive School on Single-Crystal X-ray Structural Analysis, 27 August–2 September.

Structural Analysis by X-ray Diffraction, Crystallography under Perturbation, Nancy, France, 28 August–2 September.

10th European Powder Diffraction Conference (EPDIC X), Geneva, Switzerland, 1–4 September.

XX Conference on Applied Crystallography, Wisna, Poland, 11–16 September.

Use of Monte Carlo Techniques for Design and Analysis of Radiation Detectors, Coimbra, Portugal, 15–17 September.

Aperiodic 2006, Miyagi, Japan, 18–22 September.

Crystallography at High Pressure (Neutron, X-ray and Related Studies), Dubna, Russia, 28 September–1 October.

Fundamentals of Modern Methods of BioCrystallography – BioCrys2006, Oeiras, Portugal, 6–13 October.

Joint Conference of the Asian Crystallographic Association and the Crystallographic Society of Japan, Tsukuba, Japan, 20–23 November.

Workshop on Synchrotron-Light Applications in Biological Materials, Cairo, Egypt, 27–30 November.

The Executive Committee met in Leuven, Belgium, in August. The Finance Committee met in Jersey, Channel Islands, in March, and in Leuven to prepare its advice and recommendations on finances, establishment and staff matters. The most important items of business

dealt with by the Executive Committee at its meeting, and in email ballots, were:

editorial policy, pricing policy and subscription rates, approval of appointments of Co-editors, electronic publishing, archival policy, Special Issues, open access, alternative financial models for *Acta E/F*, education papers, language improvement of submitted papers, and other matters concerning the IUCr journals;

contract with Blackwell Munksgaard;

approval of the audited accounts for the previous year;

General Fund estimates;

status of membership subscriptions;

Joint National or Regional Committees for Crystallography;

investment policy;

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

Visiting Professorship Programme;

sponsorship and financial support for meetings, young scientists' support;

Journal Grants Fund;

cooperation with external databases;

progress with Volumes A, A1, B, C, D, E, F and G of *International Tables* and development of associated software, development work to make *International Tables* available online;

review of contract with Springer;

*IUCr Newsletter*;

World Database of Crystallographers;

Online Dictionary of Crystallography;

promotional activities;

Ewald Prize;

discussion of the arrangements for the 2008 General Assembly and Congress;

nomination procedures.

Other items dealt with in this way were:

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

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

crystallography in Africa;

relations with other Scientific Unions;

review of the activities of the Commissions;

review of the activities of Regional Associates;

review of the reports of IUCr Representatives on other bodies;

review of report of the Committee on Crystallographic Databases.

Items concerning the Chester office were:

pension scheme, upgrading of office technology, provision of internet services.

## 2. Publications

Volume 62 of *Acta Crystallographica*, Volume 39 of *Journal of Applied Crystallography* and Volume 13 of *Journal of Synchrotron Radiation* were published.

## 3. Adhering Bodies

A list of Adhering Bodies of the Union, with names and addresses of the Secretaries of the National Committees for Crystallography, was published as Annex IV to the Report of the Twentieth General Assembly and International Congress of Crystallography [*Acta Cryst.* (2006), A62, 465–526].

## 4. Work of the Commissions

### 4.1. Commission on Journals

**4.1.1. Overview.** Overall, 17,254 pages were published in IUCr Journals in 2006, compared with 14,869 in 2005 and 11,728 in 2004. This represents an increase of 16% on the 2005 level; of this total, 11,143 pages were published in electronic form only.

In 2006, 528 pages were printed for *Acta Crystallographica* Section A (622 in 2005), 1,138 for Section B (730 in 2005), 1,450 for Section C (1,412 in 2005) and 1,571 for Section D (1,681 in 2005). Section E published 9,843 electronic only pages (7,439 in 2005) and Section F published 1,300 electronic only pages (1,102 in 2005).

The average length of Full Articles was 10.1 pages for Section A, 9.3 pages for Section B, 3.3 pages for Section C, 8.6 pages for Section D, 2.5 pages for Section E and 3.8 pages for Section F. Average publication times were as follows: Section A 5.0 months, Section B 6.3 months, Section C 2.1 months, Section D 5.1 months, Section E 0.9 months and Section F 2.3 months. The rejection/withdrawal rates were: Section A 31%, Section B 34%, Section C 50%, Section D 23%, Section E 17% and Section F 9%.

The number of Full Articles published in *Journal of Applied Crystallography* (*JAC*) in 2006 was 89 (111 in 2005). The number of pages decreased from 1,045 to 928. The average review time was 4.6 months and the technical-editing time 2.0 months; the overall publication time was 6.6 months. The rejection/withdrawal rate was 21%.

The number of Full Articles published in *Journal of Synchrotron Radiation* (*JSR*) in 2006 was 58 (115 in 2005). The number of pages decreased to 496 in 2006 (838 in 2005). The average review time was 4.8 months and the technical-editing time 1.7 months; the overall publication time was 6.5 months. The rejection/withdrawal rate was 23%.

IUCr journals continue to be highly ranked amongst crystallographic journals; *JAC* occupied the top ranking in Crystallography with an impact factor of 5.25.

Proceedings of the International School on Mathematical and Theoretical Crystallography (MaThCryst) and the 23rd European Crystallographic Meeting (ECM-23) Abstracts were published in Section A. Special themed issues published in Section D in 2006 included the Proceedings of the CCP4 Study Weekend on Data Collection and Analysis, Get-Phases Beijing 2005 and SPINE (Structural Proteomics in Europe). *JSR* published a themed issue on Detectors.

At ECM-23 in Belgium, the IUCr Executive Committee took the decision that Section E should be made an open-access journal from

the start of 2008. Considerable work has since been undertaken to examine how the editorial workload and production costs for this journal can be reduced so that the open-access charge can be as low as possible. New procedures will be introduced early in 2007. Work has also been continuing on streamlining procedures for Section F. A tool that will create experimental tables for inclusion in manuscripts from mmCIF files is under development.

The Commission held two informal meetings – at the American Crystallographic Association meeting in Hawaii and at ECM-23 in Belgium. Ethics in science publishing and open access were topics of general concern.

At the end of the year, 158 Section Editors and Co-editors worked on IUCr journals, with allocated papers ranging from 1 to 303. The work of all these dedicated colleagues and of the competent and equally dedicated staff at Chester is highly appreciated.

**G. Kostorz**, Chair

**4.1.2. *Acta Crystallographica* Section A.** Section A published 528 pages in 2006, down from 622 in 2005 (down from 644 in 2004). In addition, the Abstracts of ECM-23 in Leuven, Belgium, comprise 311 pages. Five issues were regular ones. In March, a 99 page Special Issue on Mathematical and Theoretical Crystallography was published, edited by Guest Editor M. Nespolo. The number of pages devoted to Research Papers and Short Communications decreased from 531 to 447 (down from 619 in 2004); without the Special Issue, the decrease is from 410 to 348 pages. The average publication time for regular papers decreased marginally from 5.1 to 5.0 months; the average review time was 3.1 months.

There were 43 full Research Papers (55 in 2005), including 10 in the Special Issue, giving an average of 10.1 pages per article. This continues a yearly increase of about 1 page per year. There were five short communications, and no Topical Reviews and Lead Articles. The portion of 31% of withdrawn and rejected manuscripts remains high, but has decreased to the level of 2004. I have warned in my 2005 report that 'Section A shrinks alarmingly' and this is clearly evidenced by the number of pages and papers published in 2006. The January issue comprised only three papers! But this trend is now levelling off – compared to 2005, the number of submitted papers is unchanged, while the number of accepted papers is somewhat larger. There is no backlog in the Editorial Office.

Section A is a high-level journal with a very diverse range of topics. About half of the papers may be classified as mathematical (including twinning, topology, crystal chemistry). Other topics are crystal physics, materials science (thin films and nano particles), diffraction and structure determination, electron diffraction and microscopy, electron density, and single-particle imaging (one excellent paper). The geographical distribution of the origins of the articles (counted as integral or half-integral numbers) remains nearly unchanged with Europe 61% (+1), the Americas 27% (+4) and Asia+Australia 12% (–5). The Co-editors perform well, but the work is very unequally distributed: 40% of the submissions are handled by two Co-editors, a third Co-editor adds 8% and the Book Review Editor 11%. But all editors do very important work since many papers are difficult to handle.

In the pipeline for 2007 is a Lead Article (March 2007 issue). The second part of the Special Issue on Phase Transitions (Guest Editor D. Pandey) is commissioned. In addition, there is the Special Anniversary Issue planned for January 2008.

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

**4.1.3. Acta Crystallographica Section B.** The number of pages printed for Section B was up sharply in 2006; the total number increased from 730 in 2005 to 1,138 in 2006, which is a record high. The number of full papers increased by a slightly smaller factor (1.42 rather than 1.56) but the average length of a paper went from 8.5 to 9.3 pages. One Feature Article was published.

The content of individual papers continues to grow; many of the papers report very large amounts of work. There has been a slight increase in time to publication in the last year (5.8 to 6.3 months) but given the complexity of many of the papers this increase causes little concern.

The fraction of manuscripts withdrawn or rejected has decreased slightly. Everyone connected with the journal is very pleased with the quality of the submissions. The fraction of papers dealing with inorganic and metallic structures (currently 44%) seems to be increasing but this percentage has fluctuated in the past. The existence of a trend is possible but not certain.

The only negative result for the year was a decrease in the impact factor from 5.4 to 1.9. The drop was, however, predictable: it was a consequence of the highly cited articles of the 2002 database issue no longer being included in the calculation. The current impact factor is about the same as those for the several years before the database issue had an effect.

Finally, all those connected with Section B were very pleased to receive an e-mail in November from S. C. Abrahams, longtime Editor-in-Chief, who wrote:

'I would also like to register my deep satisfaction with the most recent issue of *Acta B*. It has taken about a quarter century of steady progress to have reached this moment but the contents of this issue (even more than most) exactly mirror the kinds of connection between structure and the larger aspects of the physical and chemical sciences that I had hoped for in proposing to split the old *Acta B* into two parts.'

During 2006, Co-Editor C. Lecomte retired after nine years on the board. We thank him for his fine service.

We also thank the Chester editorial staff, and especially Jill Bradshaw, for all they do to help authors with their manuscripts and to produce a quality journal. Anybody turning the pages of Section B or looking at the web version can quickly see that it has been put together carefully by people who are skilled copy editors and who know how to make pages visually attractive.

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

**4.1.4. Acta Crystallographica Section C.** Section C continues to specialize in the rapid publication of high-quality studies of novel and challenging crystal and molecular structures. In 2006, Section C published 444 papers (38 inorganic, 182 metal-organic, 224 organic) in a total of 1,450 pages – a small increase in papers over 2005. Publication times fell slightly in 2006 with the majority of technically correct and well written papers appearing on line (<http://journals.iucr.org/c>) within two months of submission. After review some 50% of submissions to Section C in the past year were either subsequently withdrawn by the authors or rejected – an 8% decrease over 2005. This change reflects a better understanding from authors that 'the text of the paper must provide significant added value to the numerical data freely available in the CIF', and improvements made to the submission system during the year.

I must also acknowledge and warmly thank P. D. Robinson and O. Q. Munro, who have now retired from the Section C Editorial Board, for their services to Section C and to the crystallographic community.

The high standard of Section C papers is due in no small part to the careful work of Co-editors, referees and the Chester staff; once again I very much appreciate the fine work done by these colleagues.

**G. Ferguson**, Editor of Section C

**4.1.5. Acta Crystallographica Section D.** Section D maintained a steady flow of high quality articles throughout 2006. In this year, 12 issues were published, including three Special Issues. In total, 184 articles were published, accounting for 1,555 pages. The large majority of these articles (176) were full Research Papers, the remainder comprising 7 Short Communications and one Feature Article. The latter, by D. E. Danley, focused on the preparation of protein–ligand complexes for crystallographic analysis, a subject of great interest for structure-guided drug design in particular. Three Book Reviews were also published. Publication times have remained at approximately 5 months.

The three Special Issues published during 2006 were strongly focused on crystallographic methods. The January issue contained the traditional proceedings of the 25th CCP4 Study Weekend held in Reading, UK, in January of the previous year, this time devoted to data collection and analysis. The August issue had contributions from the International Workshop on Recent Advances in Phasing Methods for High-Throughput Protein Structure Determination (in short, the Get-Phases meeting), held in Beijing, People's Republic of China, in October/November of the previous year. The October issue was devoted to descriptions of achievements of the SPINE (Structural Proteomics IN Europe) consortium, obtained over the previous three years. Each of these issues was prepared by Guest Editors, to whom we offer a special debt of gratitude. The CCP4 issue was handled by G. Evans and M. Walsh (the workshop organizers), the Get-Phases issue by Xiao-Dong Su and T. C. Terwilliger (again, the meeting organizers), and the SPINE issue by J. M. Guss.

Overall, the papers published during 2006 included 95 methodological publications (828 pages) and 89 structural papers (727 pages). Section D remains recognized as the main venue for publishing methodological papers relevant to macromolecular crystallography, but it is pleasing to see a large number of high-quality structural papers as well.

We were sorry to lose the services of one of our long-serving Co-editors during 2006, when Professor L. A. Aslanov, of Moscow State University, Russia, stepped down. We wish Leonid well, and thank him very warmly for his years of service. We also welcome two new Co-editors who were appointed during 2006. Professor T. Yeates, of the University of California, Los Angeles, USA, has an outstanding background in crystallographic methods as well as in structural biology. Dr V. Lunin, Head of the Laboratory of Macromolecular Crystallography at the Russian Academy of Sciences, likewise brings a strong background in crystallographic theory and methods.

All articles published in 2006 were submitted online and the texts were transferred between the authors, editors and the Chester Editorial Office electronically. This system is efficient and works very well, making the whole publication process easy for all involved. Several articles that were submitted to Section D were subsequently identified as more appropriate for other journals (Section F or *JAC*). The transfer processes work well, but the judgements involved are more subjective. The editors are extremely grateful to Louise Jones and Simon Glynn in Chester for their unfailingly excellent support.

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

**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
A58	2002	630	102	65	8.0	37	2.8
B58		1088	132	115	8.9	17	1.1
C58		1570	535	531	2.6	4	1.8
D58		2243	457	425	5.0	32	2.3
E58		2374	922	918	2.3	4	2.4
A59	2003	628	83	58	7.9	25	8.8
B59		821	88	81	9.8	7	2.1
C59		1482	482	478	2.8	4	2.2
D59		2385	466	429	5.2	37	3.4
E59		3419	1305	1297	2.5	8	1.8
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	

*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
35	2002	760	128	83	7.2	25	4.0	20	1.6
36	2003	1505	282	225	5.9	26	3.8	31	1.7
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

*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
9	2002	413	93	68	5.5	2	4.0	23	0.7
10	2003	475	108	77	5.5	5	2.2	26	0.8
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

† Including Lead Articles and Topical Reviews for Sections A, B, D and F. ‡ Including Addenda & Errata, Letters to the Editor, IUCr Notices, Notes & 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, Cryocrystallography Papers, Computer Program Abstracts, IUCr Notices, Notes & News, Book Reviews, Books Received, Obituaries, Crystallographers, Commission Reports, New Products, Abstracts, Current Events and Editorials.

**4.1.6. Acta Crystallographica Section E.** The year 2006 has seen yet another sustained period of growth for Section E.

The number of papers submitted rose by 39%; 4,183 (83%) were accepted, 566 (11%) rejected and 325 (6%) withdrawn. The number

of pages published was 9,843, an increase of 32% over 2005. The average length of papers was 2.5 pages. The average publication time rose slightly to 0.9 month. The proportions (%) of papers published in each category were: inorganic 4, metal-organic 33 and organic 63.

The People's Republic of China accounted for 51% of the papers, followed by India with 6% and USA with 5.8%. The journal's impact factor has risen from 0.491 to 0.581.

During 2006, the number of Co-editors was 48 but, for various reasons, three Co-editors have resigned during the year, *viz.* K. A. Abboud, L. J. Barbour and R. D. Gilardi. We thank them for their contribution to the success of the journal. The continued substantial growth of the journal has put increasing pressure on Co-editors and, towards the end of the year, a further batch of nominations was submitted to the IUCr Executive Committee for approval, with the successful candidates due to take up their duties early in 2007.

The web interface for the submission of manuscripts and files and for communication between authors and Co-editors, introduced during 2006, is now fully functional and there have been very few problems regarding its use. It has made editorial work much easier and more consistent, and it provides a firm foundation for further changes now being introduced.

Another new tool has been provided by the technical staff in Chester, *viz. pubCIF*. This provides facilities for the composition and checking of papers and has proved very popular with authors and Co-editors alike. We encourage its wider uptake; it can be downloaded from <http://journals.iucr.org/e/services/authorservices.html> and installed under Windows, Linux and MacOS. A description of the program will be published in due course.

At the 23rd European Crystallographic Meeting in Belgium and since then, there has been considerable debate about the future direction of our journal; an article by the IUCr President appeared in the *IUCr Newsletter*. This has been prompted by two pressures in particular. First, the journal is currently financially unsustainable in the view of the IUCr Finance Committee and the Executive Committee, because it generates very little direct income (most of its readers have free or very low cost access to it as a result of subscribing to Section C or *via* consortial arrangements) and its production costs have been steadily climbing with its popularity. Second, as noted above, the submission of papers continues to increase without any sign of abating, and this is making life very difficult for the editorial staff, the Section Editors, and existing Co-editors; we cannot just keep appointing more Co-editors and allow the journal to grow without limit.

The Finance Committee have asked those responsible for the journal production to examine the possibility of making the journal completely open access, which would mean free access without any subscription or reader's fee, with the production costs being met by a charge to authors. In practice, this is likely to be the only possible way forward in financial terms; there appear to be no viable alternatives if the journal is to continue operation. In this case, it is important to make the open-access charge as low as possible. This means reducing the production costs as much as we can. To satisfy these linked demands, we have been developing a new format for the PDF version of the published articles, so that much less of the submitted results would appear in this format, the bulk of the material being available through a new PDF supplement to the article, as well as *via* the archived CIF, structure factors *etc.* The PDF version of the article will consist of the title, authors, key indicators, an Abstract (longer than most of the present ones, but with a length limit), a new 'Related literature' section, Experimental data sections (Crystal data, Data collection, and Refinement), very brief table(s) if any at all, a chemical scheme, acknowledgements, and References. A small working party has reviewed the items that appear in the Experimental data sections, and some of these will be removed, not only in Section E papers, but also in Sections B and C for consistency; they will, however, be in the PDF supplement and the CIF, together with

many other items that have never appeared in the 'old-style' paper, and will therefore be fully available to readers. The Experimental text sections and Comment will still be provided by authors for the PDF supplement and the CIF; it will not need as much editorial attention or any time-consuming typesetting. Figures will also be available through the PDF supplement of the paper. We stress that each publication consists of the complete package supplied by authors – CIF, structure factors, graphics and any other submitted supplementary files – together with the generated paper and supplement, and this still represents a richer collection of material than is provided by publishers of other journals.

Much time and effort of the editorial staff in Chester, together with the Section Editors, was taken up in the final months of 2006 in developing and testing the new procedures, which are being introduced early in 2007. Changes include revision of the Notes for Authors, updating of CIF templates and examples, and new Notes for Co-editors, in addition to the web interfaces seen by authors and Co-editors and the very considerable programming effort that lies behind these. We are convinced these major changes will lead to a more efficient and more cost-effective publication process for Section E, and will be welcomed by authors and readers.

Finally we again thank the editorial staff in the Chester office for all their help and dedication. In particular, we are indebted to Gillian Holmes, Sean Conway, Sarah Froggatt and Lisa Stephenson who look after Section E on a daily basis, and to Mike Hoyland, David Hoare and David Holden who have been particularly involved in the development of new procedures under the direction of Peter Strickland.

**W. Clegg and D. G. Watson**, Editors of Section E

**4.1.7. Acta Crystallographica Section F.** 2006 was the second year of publication of Section F: *Structural Biology and Crystallization Communications*. This purely electronic journal for biological crystallography made significant progress in 2006 with almost 350 articles and 1,300 pages published, an 18% increase in the number of pages published over the first year.

One of the primary reasons for launching the journal was to allow authors in fields such as structural genomics and macromolecular crystallization to benefit from the fast turnaround of electronic-only publication. In its second year, the journal has worked very hard to maintain speedy publication with a low average time from submission to publication, including peer review, of 2.3 months. The journal has continued to work on a streamlined route from database deposition to publication. Early in the year, volunteers completed testing of a version of a RCSB program to harvest data identified as required or recommended from output files. The responsibility for further development and implementation of streamlining is now in the hands of IUCr personnel and under active development is a tool that will create experimental tables for inclusion in manuscripts from mmCIF files. Implementation of the first phase of the streamlined process is expected before the end of 2007.

The remarkable success of Section F has continued into its second year of publication. This is due in no small measure to the dedication and hard work of the editorial staff in Chester and of our excellent team of Co-editors, to whom we are very grateful. We have again found it necessary to expand the Editorial Board and we thus welcome J. M. Newman (CSIRO, Australia) and J.-P. Renaud (AliX S.A., France) as new members.

**H. M. Einspahr and J. M. Guss**, Editors of Section F

**4.1.8. Journal of Applied Crystallography.** *JAC* published 928 pages in 2006 (1,045 in 2005). The number of full articles was 89 in 2006 (111 in 2005). Shorter items like Short Communications, Laboratory Notes, Letters to the Editor *etc.* increased to 36 from 24. The number of manuscripts submitted was 399, compared with 196 in 2005 and 226 in 2004. This increase was mainly due to the submission of manuscripts from the SAS 2006 meeting, held in Kyoto in July 2006. 143 SAS 2006 manuscripts will be published separately as a Special Issue (electronic version only) in 2007. The impact factor was 5.25 in 2005 (3.53 in 2005).

On-line submission is now almost exclusively used and works well. The publication time increased slightly to 6.6 months (4.6 months for editors/reviewers and 2.0 months for production). It has again been a pleasure to interact with the Chester staff who handled all matters arising with great competence and kindness.

**G. Kostorz**, Editor of *JAC*

**4.1.9. Journal of Synchrotron Radiation.** In 2006, *JSR* published 58 articles and a total of 496 pages in six issues. This was a decrease in both articles and pages as compared to 2005 due primarily to fewer Special Issues. In 2006, one Special Issue was published in March (Volume 13, Part 2) on detectors, with H. Graafsma serving as Guest Editor. We continue to believe that the publication of selected papers from workshops is an important service to the synchrotron-radiation community and we plan to continue this in the future.

The Facility Information pages where one page per issue is devoted to each of the three-third generation hard X-ray sources (APS, ESRF, and SPring-8) was also continued in 2006. These pages provide an opportunity for these facilities to communicate important news and updates to the international community of synchrotron-radiation users.

We are happy to report that the average review time for 2006 was reduced from 6.1 months in 2005 to 4.8 months and that the average editing time was reduced from 2.7 months in 2005 to 1.7 months in 2006 resulting in an average publication time of 6.5 months. In addition, the impact factor increased to 2.4.

**Å. Kvikvick, D. M. Mills and T. Ohta**, Editors of *JSR*

## 4.2. Commission on International Tables

Work on the different volumes of *International Tables* progressed smoothly during 2006. All eight volumes became available online in html and pdf formats on the IUCr's **International Tables Online** web site at <http://it.iucr.org> and pdfs for all chapters were supplied to Springer for hosting on SpringerLink. It is anticipated that access to **International Tables Online** will start to be sold by Springer during 2007.

**4.2.1. Volume A. Space-Group Symmetry; Editor Th. Hahn.** Corrected reprints of the fifth edition of both Volume A and the Brief Teaching Edition were published in the summer of 2005. Since then, all corrections of printing errors and small modifications of which the Editor has become aware have been collected and sent to the Technical Editor. Many of these have already been included in the online version. Chapter 10.2 on point-group symmetry and physical properties of crystals has also been revised. Volume A sold 300 copies in 2006 and the Brief Teaching Edition sold 264 copies.

**4.2.2. Volume A1. Symmetry Relations between Space Groups; Editors H. Wondratschek and U. Müller.** Volume A1 was published in 2004. 104 copies were sold in 2006. The second edition, in which all known errors will be corrected and local improvements will be introduced, is now in preparation.

The volume contains a complete list of maximal subgroups of the space groups. Part 1 deals with group-theoretical aspects of space groups, group-subgroup relations and the underlying mathematical background. In the second edition, the mathematical background to the theory of the minimal supergroups of the space groups is extended. 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 for showing 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 a description of those databases and computer programs that are related to the subjects of this 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 second edition will contain a detailed discussion of the listed supergroup data; 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 transformations and coordinate transformations. In both Parts 2 and 3, the infinitely many isomorphic subgroups have been included in a parameterized form.

**4.2.3. Volume B. Reciprocal Space; Editor U. Shmueli.** The second edition sold 78 copies in 2006. The Editor's work on the preparation of the third edition of Volume B was virtually complete by the end of the year. Chapters on all the topics that were announced in the 2005 report have been completed and all but one are with the Technical Editor in Chester. Information on the revised and new contributions to Volume B, and their status, can be found on the home page of the Commission on International Tables at <http://crystal.tau.ac.il/xtal/comit/index.html>.

**4.2.4. Volume C. Mathematical, Physical and Chemical Tables; Editor H. Fuess.** The third edition sold 104 copies in 2006. Work on the fourth edition is due to start early in 2007. Many chapters will need complete revision.

**4.2.5. Volume D. Physical Properties of Crystals; Editor A. Authier.** Volume D is doing well with about half the stock sold so far. 76 copies were sold in 2006. The availability of the volume online is great news and will make it more readily accessible. From the enquiries received so far, it can already be seen that it has spurred the interest of new readers.

The volume has 536 pages and 18 chapters distributed within three parts: (1) Tensorial aspects of physical properties; (2) Symmetry aspects of excitations; (3) Symmetry aspects of structural phase transitions, twinning and domain structures. It is accompanied by a CD-ROM with two items of software: *TenChar* (calculations with tensors and characters) and *GI-KoBo-1* supporting Part 3 on structural phase transitions.

A number of small errors and misprints have been found and **International Tables Online** has provided a good opportunity for correcting them. A number of chapters need updating and this will be done progressively. Updates for Chapters 1.1 and 1.3 have been sent to the Technical Editor, and more are in preparation.

A chapter on the tensorial aspects of dielectric properties was planned for the first edition but was not submitted in time; this is a very important topic in which there are new developments and new applications. A chapter on thermoelectricity and one on the tensorial nature of the susceptibility for the interaction of X-rays with matter

would also be timely. When and if a second edition is considered, new chapters on these topics should be commissioned.

**4.2.6. Volume E. Subperiodic Groups; Editors V. Kopsky and D. B. Litvin.** This volume has two parts: Part 1 provides tables of symmetry information for 7 frieze groups, the 75 rod groups and the 80 layer groups. Part 2 contains scanning tables for each of the 230 space groups. 45 copies were sold in 2006 leaving a stock of 176.

**4.2.7. Volume F. Macromolecular Crystallography; Editors M. G. Rossmann and E. A. Arnold.** Work during the year focused on the preparation of the online version of Volume F and the planning of the second edition, which is expected to go to press in 2009. 84 copies of the first edition were sold during 2006 and 438 copies remain.

**4.2.8. Volume G. Definition and Exchange of Crystallographic Data; Editors B. McMahon and S. R. Hall.** Volume G was published in late 2005 and represents the authoritative documentation of the Crystallographic Information Framework. A number of favourable reviews were received in 2006 and 94 copies of the volume were sold. In common with the other volumes in the series, Volume G has been converted to an interactive online form, where perhaps its most useful feature is in the presentation of searchable and hyperlinked CIF dictionaries.

**H. Fuess, Chair**

### 4.3. Commission on Aperiodic Crystals

The Commission has continued to be active in the promotion of aperiodic crystallography, in organizing meetings as well as coordinating activities between the quasi-crystalline and incommensurate structure communities.

As part of these activities, the Commission continued to promote aperiodic crystallography at national, regional and international meetings. During 2006, the triennial flagship meeting of the Commission, Aperiodic 2006, was held at the Miyagi Zao Royal Hotel in Zao, Miyagi prefecture, Japan, 17–22 September. Aperiodic 2006 was very ably organized by A. Yamamoto, A. P. Tsai, K. Saitoh, Y. Gotoh, Y. Miyazaki and Y. Michiue to whom the aperiodic community is indebted for such a stimulating and enjoyable meeting. The Conference Chairs were An Pang Tsai and A. Yamamoto. 128 delegates attended the conference, coming from 21 different countries. Over half the delegates were from Asia with 60 from Japan alone. It was decided at this meeting that Aperiodic 2009 would be held in Liverpool, UK, probably in mid-September 2009 and would be organized by R. McGrath and U. Grimm (see <http://www.aperiodic09.org>).

Further to the activities associated with Aperiodic 2006, a Microsymposium on Structure Determination of Modulated and Aperiodic Structures as well as a Plenary Lecture on Incommensurate High Pressure and High Temperature Structures in Group VI Elements were given as part of the 23rd European Crystallographic Meeting, ECM-23, held in Leuven, Belgium, 6–11 August. In addition, a Microsymposium on Crystal Chemistry and Complex Superstructures, co-organized by S. van Smaalen, was held during the German Crystallographic Association meeting held in Freiburg, Germany, 3–6 April.

Important upcoming activities for the Commission include the meeting Quasicrystals – the Silver Jubilee to be held in Tel Aviv, Israel, 14–19 October 2007 (see <http://www.congress.co.il/quasicrystals07/>). This meeting is organized by R. Lifshitz (Chair), D. Shechtman (Honorary Chair) and S. Ben Abraham. Other upcoming activities include the 5th Workshop on the Structural

Analysis of Aperiodic Crystals organized by S. van Smaalen to be held at the University of Bayreuth, Germany, 1–4 March 2007.

The Commission maintains internet pages at the web site of the IUCr at <http://www.iucr.org/iucr-top/comm/capd/index.html>. A web site on all aspects of the crystallography of aperiodic crystals is maintained by the Special Interest Group on Aperiodic Crystals of the European Crystallographic Association. It is maintained by M. Dusek (Prague, Czech Republic), and can be found at <http://www-xray.fzu.cz/sgip/aphome.html>.

**R. Withers, Chair**

### 4.4. Commission on Biological Macromolecules

The Commission has continued to support the vitality of the biological crystallography community, particularly through recommending and supporting IUCr proposals to hold meetings, workshops and schools. Several meetings of this type will be held in Europe, the USA, Russia and Southeast Asia in 2007. Also the Commission is working with various groups within the community to develop recommendations for an updated set of crystallographic publishing standards that will require structure-factor deposition (compliance is already well over 90%) and to remove the option for delaying the release of PDB structures following publication.

A key activity of the Commission was contributing to the planning of the Osaka Congress in 2008. Structural biology will be 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. Hopefully, a large number of students will attend and participate from all corners of the world and the travel of many young scientists will be sponsored by the IUCr. Three members of the Commission (E. Arnold, A. Podjarny and T. Tsukihara) met with the International Programme Committee to develop suggestions for Plenary Lectures, Keynote Lectures, topic-oriented Microsymposia and Chairs for all of the suggestions.

Regional meetings with biologically relevant content sponsored by the IUCr in 2006 included: in April, the RapiData course (Brookhaven, USA); in June, an Erice (Italy) Workshop on the Structure and Function of Macromolecular Assemblies, an International School for Biological Crystallography in Granada (Spain), and an Electron Crystallography School in Bangalore (India); in July, the 13th International Conference on Small-Angle Scattering in Kyoto (Japan), and The Annual American Crystallographic Association (Honolulu, USA); in October, Fundamentals of Modern Methods of Biocrystallography – BioCrys 2006 in Oeiras (Portugal); and, in November, The Joint Conference of the Asian Crystallographic Association and the Crystallographic Society of Japan at Tsukuba (Japan), and a Workshop on Synchrotron-Light Applications in Biological Materials in Cairo (Egypt). These meetings, schools and workshops provide tremendous value in training in and dissemination of novel scientific methods.

**E. Arnold, Chair**

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

The Sagamore meeting, the Gordon Research Conference (GRC) and the European Charge Density Meeting (ECDM) are the major conferences of the community. The year 2006 started with the 4th ECDM held in Brandenburg, Germany, 26–29 January. Sagamore XV was held in Warwickshire, UK, 13–18 August.

The 4th ECDM was organized by the group of U. Pietsch (Potsdam, later Siegen) and was held in Germany for the first time. It received high acceptance by the European charge-density community. High-ranking scientists accepted invitations to report on actual developments in experimental and theoretical charge-density analysis by presenting invited talks on electron localization in organometallic compounds (W. Scherer), light-induced metastable states (S. Pillet), photoisomerization (J. M. Cole), evaluation of thermodynamic values from X-ray data (A. O. Madson), ELF (electron localization function) topology (B. Silvi), extension of the program code *CRYSTAL* (B. Civalleri) and new developments based on density functional theory (H. Rosner). The programme was completed by an additional 16 oral talks and 21 posters. Fortunately, 37 from a total of 96 participants were students contributing by talks and discussions to the success of the conference. Considering the large number of students, the conference programme included two tutorial talks (P. Luger, D. Stalke) at the beginning. The conference took place in Bollmannsruh, a pleasant place near Beetzsee in Brandenburg. Good but cold weather and perfect organization were the basis for the success of the conference.

Sagamore XV was the first Sagamore Conference to be held in the UK. The organization was led by M. J. Cooper from Warwick University and the meeting attracted 100 scientific participants (plus 20 accompanying members) from 16 different countries, the largest contingents (more than 10 active participants) being from France, Germany, Japan, UK and USA. It was held under the auspices of this Commission and received IUCr sponsorship and young scientist support. The conference was based around eight themes which were treated in twelve oral sessions, supplemented by two poster sessions. The themes were: (1) Density Functional Theory for Charge and Momentum Density; (2) Charge Density in Macromolecules; (3) Charge Density and Chemical Interaction in Large Molecules; (4) Strongly Correlated Electrons; (5) The Nano Interface and Spin Densities in Nano Structures; (6) Characterization of Chemical Bonds; (7) Rare Earth and Actinide Magnetism and (8) Fermiology and Fermi-Surface Driven Phenomena. The oral presentations were largely from invited internationally leading speakers but under each topic a number of submitted papers were selected for oral presentation. Poster sessions were well attended. Several students were invited to give a 5 min presentation for their posters. There was also an open meeting of the Commission, which was used to discuss the nature and location of future Sagamore meetings.

The Conference venue was well suited to the conference group size and the countryside location provided a relaxed environment to encourage informal discussion outside of the organized sessions.

The majority of the Commission members attended the Sagamore XV meeting; both a closed and an open Commission meeting were held during the meeting. Future important events were discussed and continued by email communications: (1) the main themes of the GRC meeting on Electron Density Distribution and Chemical Bonding: Dynamic and Static were discussed; (2) the 5th ECDM will be organized by C. Gatti, P. Macchi and R. Destro early in June 2008; (3) the location of Sagamore XVI was discussed, three locations being proposed. Details of proposals were circulated among the members later in the year and the final decision was made before the end of the year. Sagamore XVI will be held in Santa Fe, USA, in August 2009; (4) nomination of the Osaka Programme Committee member on behalf of this Commission, Yu Wang being nominated.

**Yu Wang**, Chair

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

In 2006, the Commission continued its work mainly *via* email communication.

The first major activity was the International Workshop on Crystal Growth and Characterization of Advanced Materials, Chennai, India, 9–13 January 2006. 37 international and local invited speakers interacted successfully with 77 students and researchers mostly from India but also from Bangladesh. Commission member R. Fornari was one of the Co-Chairs of the workshop and the IUCr sponsored the event.

The International School on Biological Crystallization (ISBC) was held in Granada, Spain, 22–26 May 2006, under the auspices of the IUCr through the Commission. Commission member J. M. Garcia-Ruiz was the organizer. This School was oriented toward postgraduate or postdoctoral students and research scientists from industry and academia who work on crystallization every day, but seek fundamental knowledge of the crystallization phenomenon and the behaviour of crystallizing solutions. ISBC focused on crystallization from solution and its applications to crystallization of biological materials. The list of teachers and the full programme are available at <http://www.isbcgranada.org>. A. Moreno, a consultant to the Commission, was among the 22 experts teaching at this School. The detailed report from the meeting was published in the *IUCr Newsletter* [(2006), **14**(2), p. 17]. This School had a high profile and was so much appreciated in the area that Professor Garcia-Ruiz is considering the organization of a similar meeting in 2008. The Commission received and carefully considered applications for support for meetings (Conferences, Schools and Workshops) from crystallographers and crystal growers from Venezuela, Poland (two), Russia and USA (two). These applications covered various topics in crystal growth and characterization from crystal genesis to organic and biological crystallization.

The request from the International Organization of Crystal Growth for support of the International Summer School on Crystal Growth, Park City, USA, in August 2007 (<http://www.crystalgrowth.us/isscg13/index.php>) was very strongly supported by all Commission members and consultants as it is the major event for the crystal growth community and covers all aspects of crystal growth and characterization. Three members of the Commission (E. Vlieg, P. Rudolf and K. Kakimoto) will be teaching at this School. Commission member D. Bliss, who is also a President of the American Association for Crystal Growth, is among the organizers. For the fast-approaching Osaka Congress, E. Vlieg is representing the Commission on the International Programme Committee.

As in previous years, many of the Commission members and consultants (T. Ohachi, T. Duffar, R. Fornari, K. Kakimoto, S. Baldochi, J. Wang and A. Moreno) were involved in the work of the International Organization of Crystal Growth; K. Byrappa was elected General Secretary of the International Solvothermal and Hydrothermal Association.

**H. A. Dabkowska**, Chair

#### 4.7. Commission on Crystallographic Computing

One of the activities of the Commission is the maintenance of its web site: <http://www.iucr.org/iucr-top/comm/ccom/>. A regular *Newsletter* is produced. The latest *Newsletter* (issue No. 7) entitled Understanding Crystal Structures collects a wealth of articles by various authors and was edited by Commission members S. Parsons and L. M. D. Cranswick.

The Commission also assembled a list of computing-related proposals for Microsymposia as part of the Osaka Congress.

There is a significant overlap of the active members of the IUCr Commission and those of the ECA computing commission. In the ECA context, several computing sessions in Marrakech, Morocco, in 2007 have been organized.

As a general comment, it should be remarked that the various restraints that are imposed on the selection of Commission members make its functioning suboptimal. Some Commission members never responded to e-mails when asked for input and suggestions.

**A. L. Spek**, Chair

#### 4.8. Commission on Crystallographic Nomenclature

(1) Online Dictionary of Crystallography. Following the approval by the Executive Committee of the pilot project based on the principle of Wikipedia and the appointment of the Chair of this Commission as Chief Editor, work has progressed by extending the number of terms included. Discussions are under way to appoint a Board of Editors on specific topics and subtopics. The present stage of the project can be seen at the web page: [http://reference.iucr.org/dictionary/Main\\_Page](http://reference.iucr.org/dictionary/Main_Page)

As soon as the number of entries is considered sufficient, the online dictionary will be open to the public.

(2) Discussion of a proposal for the definition of 'family' and 'clan' in relation to structure types. The suggestion was that the set of all structures belonging to the same structure type be called a family, and that all structure types derived from the same aristotype be called a clan. Such definitions are already used in many classifications for protein structures. A long discussion involving many members of the Commission ensued, the result being that the proposal was eventually withdrawn as it was feared that it would introduce confusion with existing terms as defined in H. Megaw's book.

**A. Authier**, Chair

#### 4.9. Commission on Crystallographic Teaching

During the meetings held at the Florence Congress, the Commission widely discussed the general need for basic crystallographic courses, because basic crystallographic curricula are regressing in the academic bachelors and masters courses. This led to the decision to organize an International School on Basic Crystallography.

The Commission organized a Basic Crystallographic School, which was held in Pontignano, near Siena, Italy, August 2006, with G. Chapis (coordinator, EPFL, Lausanne, Switzerland), A. J. Blake (Nottingham, UK), A. Gavezzotti (Milan, Italy) and R. Neder (Wuerzburg, Germany) forming the Programme Committee and M. Mellini (University of Siena, Italy) and P. Spadon (University of Padova, Italy) as Local Organizers.

The students attending the course numbered 44, coming from 14 different countries; 20 were financially supported by the organization and obtained reduced fees. The total number of applicants was much higher but many of them could not participate because the organizing committee was not able to provide them with full travel support. There were 11 lecturers/tutors from different European countries and the sessions were organized in such a way that the time was nearly equally distributed between lectures and tutorial sessions. At the end of the school, a questionnaire was distributed to students which gave a satisfactory result: the course was generally well accepted, the alternation between lectures and tutorials was much appreciated but it was also stressed that there was a need for more time to be dedi-

cated to point and space groups and symmetry; students in the field of powder diffraction complained because the time allocated to the subject was insufficient. All the teaching material was made available before the course on the web site of the School.

In addition, the Commission decided to collaborate with the Commission on Mathematical and Theoretical Crystallography (M. Nespolo, Chair) concerning the organization of a School in Cuba. This School is planned for July 2007.

The Commission also agreed on the need to reformat and update its web site and edit an online Commission *Newsletter*. L. M. D. Cranswick volunteered to coordinate this work and the first issue is already on the web.

G. Chapis and P. Spadon were also involved in the organization of MS45, Communicating and Educating Crystallography, ECM-23, Leuven, Belgium, August 2006.

**P. Spadon**, Chair

#### 4.10. Commission on Electron Diffraction

The major event of 2006 was the 16th International Microscopy Congress, 3–8 September, Sapporo, Japan. This meeting was attended by over 2,000 scientists from 55 countries and had major components involving electron crystallography in both the physical and the biological sciences.

In terms of schools, a satellite meeting to the European Crystallographic Meeting was X-EI 2006: a school on structure determination by the combination of X-ray powder diffraction and electron crystallography, 1–4 August 2006, Antwerp, Belgium. This was attended by about 70 students and teachers.

One other major effort of the Commission was the establishment of the Gjønnnes medal in electron crystallography. This medal will be an award made to a scientist for life-time achievement in electron crystallography, presented at the IUCr triennial Congress. The first Gjønnnes Medal will be awarded to J. Gjønnnes at the Osaka Congress.

Future events with which the Commission has been actively involved include a number of workshops/schools that will be held in 2007 and 2008. These include:

New Instruments and Methods for Electron Crystallography, Aachen, Germany, 16–20 September 2007, <http://www.elcryst2007.de/>;

Electron Microscopy and Multiscale Modelling, Moscow, Russia, 3–7 September, 2007, <http://ns.crys.ras.ru/EMMM07/>;

Microscopy Society of America Annual Meeting, August 2007, which will have many sessions involving electron crystallography, including one on precession electron diffraction and other advanced crystallographic techniques, <http://www.microscopy.org/MMMeetings/MM07/HomePage.html>;

Electron Microscopy in Materials Science, Oxford, UK, December 2007;

Electron and X-ray Crystallography, Taipei, 3–4 November 2007, a satellite of the 2007 meeting of the Asian Crystallographic Association.

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

**L. D. Marks**, Chair

#### 4.11. Commission on High Pressure

Crystallography at high pressure remains a technical and scientific challenge. Yet the demand of exploring structural properties of material at non-ambient pressure conditions is growing both in

quantity and quality. More groups across the full spectrum of physical-chemical and material sciences (including Earth materials) try to obtain crystallographic data at more and more extreme conditions of pressure and often also temperature.

The task of the Commission is to provide platforms that help in the dissemination and exchange of new techniques, ideas and scientific achievements in this field. The main tool for this goal is annual workshops, which are organized in different places across the world.

The International Workshop on Crystallography at High Pressure – 2006 followed the sequence of workshops organized on behalf of the Commission (ESRF, Grenoble, France, 1997; Argonne, USA, 1998; SPring-8, Japan, 2000; Orsay, France, 2001; Berkeley, USA, 2003; Saskatoon, Canada, 2004) and also the sequence of meetings on Neutron Scattering at High Pressure (NSHP) organized by the Frank Laboratory of Neutron Physics Joint Institute for Nuclear Research (FLNP JINR) (NSHP-I in 1994 and NSHP-II in 1999, Dubna, Russia). This was organized at FLNP JINR, Dubna, Russia, 28 September–1 October 2006. The organization was coordinated by D. P. Kozlenko. I. Goncharenko served as the liaison to the Commission.

The Workshop attracted nearly 80 scientists from 10 countries. Its scientific programme contained 10 oral sessions and 2 poster sessions, covering the full range of scientific activities of the Commission. During three and half days, 30 oral and 35 poster presentations (including 9 poster orals) were made. A number of invited oral talks and poster orals were given by young scientists. The sessions covered the topics: Simple Elements; Molecular Solids; Physical Properties and Magnetic Structures; Materials Science and High Pressure Synthesis; Mineral Physics and Geophysics; Technical Developments; Organic Materials; Liquids and Amorphous Materials; and Carbon and Nano Materials. During the guided excursion to the IBR-2 high-flux pulsed reactor facility, participants were able to familiarize themselves with capabilities for neutron scattering investigations under high pressure, available at FLNP JINR.

The 2007 Workshop is currently planned and will be held in the vicinity of the new UK synchrotron source Diamond. Commission member J. S. Loveday acts as the Commission link to the local organizers.

For the Osaka Congress, Commission member N. Hamaya has been selected to represent the Commission on the Programme Committee. The Commission is currently working on putting together a coherent and interesting high-pressure crystallography programme. In 2009, Commission consultant P. Dera will be organizing a summer school on high-pressure crystallography in Erice, Italy. The school is scheduled to take place 4–14 June 2009. This is a follow-up to the very successful summer school organized in 2003.

The Commission's home page is maintained by Commission member J. S. Loveday and continues to update the high-pressure community with information with respect to software, future and past meetings, software specific for high-pressure crystallography, central facilities, scientists and publications in the high-pressure field. The homepage can be accessed at <http://www.iucr.org/iucr-top/comm/chp/index.html>.

**M. Kunz**, Chair

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

Contacts among the members and consultants of the Commission (CIMS) have been maintained mainly *via* email and the web site at <http://www.lcm3b.uhp-nancy.fr/cims/> administered by consultant member M. Nespolo. Some members had the opportunity of meeting

and discussing CIMS activity on the occasion of the following events: 19th Meeting of the International Mineralogical Association (IMA), Kobe, Japan, 23–28 July 2006; ECM-23, Leuven, Belgium, 6–11 August 2006; AsCA '06/Crystallographic Society of Japan (CrSJ) satellite meeting on Theoretical Crystallography and Materials Science, Tsukuba, Japan, 18–19 November 2006, co-organized by CIMS and the Commission on Mathematical and Theoretical Crystallography (MaThCryst).

The main activity of CIMS in 2006 has been the organization of the following events.

(1) A satellite of ECM-23 on Mathematical and Theoretical Crystallography, Leuven, Belgium, 4–6 August 2006 (<http://www.lcm3b.uhp-nancy.fr/mathcryst/leuven2006.htm>), co-organized by CIMS and MaThCryst. G. Ferraris lectured on Symmetry Constraints and Modularity: Tools to Model Inorganic Crystal Structures. The satellite had 46 registered participants from 15 countries.

(2) A satellite meeting of AsCA '06/CrSJ on Theoretical Crystallography and Materials Science, Tsukuba, Japan, 18–19 November 2006 (<http://www.lcm3b.uhp-nancy.fr/mathcryst/asca2006.htm>), co-organized by CIMS and MaThCryst. The satellite was attended by 31 participants from 9 countries. The following lectures were delivered by members of CIMS: G. Ferraris, Symmetry Constraints on the Physical Properties of an Anisotropic Material; M. Matsui, Computer Simulation of Temperature–Pressure–Volume Equations of State of Melts in the System CaO–MgO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub>; D. Pandey, Phase Transitions in Mixed Perovskites.

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

W. Depmeier: Chair of the ECA Special Interest Group SIG5 on Mineralogical Crystallography; member of the Programme Committee for ECM-23.

G. Ferraris: member of the Programme Committee and Convener of IMA-19; Vice-Chair of the Commission on New Minerals and Mineral Names (CNMMN) of IMA; member of the Organizing and Programme Committees of the above-mentioned satellite meeting of AsCA '06/CrSJ.

M. Matsui: Chair of the Meeting Secretariat for IMA-2006; principal Convener of the Scientific Session on Computational Study of Mineral Structures and Properties at the same meeting; Editor of *Physics and Chemistry of Minerals*.

L. B. McCusker: invited lectures at Heyrovsky Institute (Prague, Czech Republic), School on Structure Determination by the Combination of X-ray Powder Diffraction and Electron Crystallography (Antwerp, Belgium, satellite to ECM-23), ECM-23 and EPDIC-10; member of the Organizing Committee for EPDIC-10 and the Programme Committee for IZC-15; co-maintainer of the International Zeolite Association web sites <http://www.iza-online.org/> and <http://www.iza-structure.org/>.

M. Nespolo: Chair of MaThCryst; Associate Editor of *European Journal of Mineralogy*; Secretary of the Special Interest Group SIG5 on Mineralogical Crystallography of the ECA; Chair of the Organizing and Programme Committees of the above-mentioned satellite meetings of ECM-23 and AsCA '06/CrSJ; Chair of MS19 Phase Transitions in Inorganic and Mineralogical Materials at ECM-23; Co-Convener of MS8 Crystal Structure, Topology and Crystal Chemistry at IMA-2006; Guest Editor of *Acta Crystallographica* Section A [(2006), Volume 62, Part 3].

D. Pushcharovsky: invited lecturer at ECM-23; Associate Editor of *European Journal of Mineralogy*.

P. Thomas: member of the Programme Committee for ECM-23.

E. Tillmanns: Chief Editor of *European Journal of Mineralogy*: Chair of the Organizing Committee of the 20th General Meeting of the IMA (Budapest, Hungary, 2010).

G. Ferraris, Chair

## 4.13. Commission on Mathematical and Theoretical Crystallography

M. Hosoya, a consultant of our Commission, retired from his position in the University of the Ryukyus, Japan; he has been replaced as consultant by U. Müller, University of Marburg, Germany.

During 2006, the Commission on Mathematical and Theoretical Crystallography (MaThCryst) has organized the following activities.

(1) A satellite meeting of ECM-23, Leuven, Belgium, 4–6 August 2006. The satellite had 46 registered participants from 15 countries, although in the end a few registrants were not able to attend. The programme, the abstracts and the slides of several lectures are available from the satellite meeting web site (<http://www.lcm3b.uhp-nancy.fr/mathcryst/leuven2006.htm>).

(2) A satellite meeting on Theoretical Crystallography and Materials Science of the AsCA '06/CrSJ joint meeting, Tsukuba, Japan, 18–19 November 2006. The satellite had 31 participants from 9 countries. The programme, abstracts and slides of several lectures are available from the satellite meeting web site (<http://www.lcm3b.uhp-nancy.fr/mathcryst/asca2006.htm>).

(3) A Special Issue of *Acta Crystallographica* Section A [(2006), Volume 62, Part 3], Guest Editor M. Nespolo, containing articles contributed by lecturers and participants of the School held in Nancy, France, 20–24 June 2005 (<http://www.lcm3b.uhp-nancy.fr/mathcryst/nancy2005.htm>) (see <http://journals.iucr.org/a/issues/2006/02/00/issconts.html>).

M. Nespolo represents MaThCryst in the IUCr working group on an Online Dictionary of Crystallography ([http://reference.iucr.org/dictionary/Main\\_Page](http://reference.iucr.org/dictionary/Main_Page)), a Wiki-based online dictionary with free reading access but with editing limited to selected authors.

Forthcoming activities include the following.

A summer school in Havana, Cuba, 15–20 July 2007 (see <http://www.lcm3b.uhp-nancy.fr/mathcryst/havana2007.htm>), in cooperation with the Commission on Inorganic and Mineral Structures and the Commission on Crystallographic Teaching; the school, initially scheduled for January 2007, had to be postponed because of local organizing problems.

A conference on Art and Crystallography with the title *The Enchanting Crystallography of Moroccan Ornaments*, as a satellite of ECM-24, Marrakech, Morocco, 20–22 August 2007 (see <http://www.lcm3b.uhp-nancy.fr/mathcryst/marrakech2007.htm>); the conference will include presentations of traditional craftsmanship and an excursion to the Kasbah de Telouet – a site renowned for the richness of its ornaments; the conference director is E. Makovicky, University of Copenhagen, Denmark.

A summer school at Gargnano, Lake Garda, Italy, 27 April–3 May 2008 (see <http://www.lcm3b.uhp-nancy.fr/mathcryst/gargnano2008.htm>), in cooperation with the Commission on Crystallographic Teaching.

The proposal for a book on *Graph Theory in Crystallography and Crystal Chemistry* (authors J. Rutherford, J.-G. Eon and W. Klee), discussed in the 2005 Report, has now been approved. It will appear in the series IUCr/OUP *Monographs on Crystallography*. We plan a thematic school based on the content of the book, which should be used as a textbook and be distributed to the participants. The first

possible date for the school, given that it must be held after the publication of the book, is late 2008 or early 2009. The site of Nancy, France, which previously hosted the Summer School in 2005, is currently the most likely venue, although a final decision has not yet been made.

We have made some inquiries about possible venues for the thematic school on Irreducible Representations of Space Groups considered in the 2005 Report. One offer from CIASU Bari, Italy (<http://www.ciasu.it/>), has been withdrawn because the new site, currently under construction, will not be completed within the original schedule. Various sites have been investigated with local contacts but at the moment progress is slow.

M. Nespolo, Chair

## 4.14. Commission on Neutron Scattering

Increasing efforts were put into training by the neutron scattering community. In 2006, a series of neutron-scattering-relevant training courses addressed young researchers – for example, the ISIS Neutron Training Course held in February and December 2006 at the Rutherford Appleton Laboratory (UK). Further events were organized for PhD and post-doctoral researchers, such as the HMI Tutorial Session on Neutron Scattering held at the Hahn-Meitner-Institut Berlin (Germany) in February/March and the LANSCE Joint Neutron Scattering School in Soft Condensed Matter and Structural Biology, held at the Los Alamos National Laboratory (USA) in May. These schools and tutorial sessions are very important for training and education of young scientists to broaden their knowledge in these scientific methods.

In addition, various workshops and conferences on neutron scattering were held all over the world. These include the Workshop on Polarized Inelastic Neutron Scattering (PINS) at Brookhaven National Laboratory, USA, 6–7 April, and the American Conference on Neutron Scattering (ACNS), St Charles, USA, 18–22 June.

The 1st International Symposium of the Quantum Beam Science Directorate of the Japan Atomic Energy Agency (QuBS2006) entitled *Advances in Neutron, Synchrotron Radiation,  $\mu$ SR and NMR* Researches was held in Tokyo, Japan, 28–30 August. This symposium was one of the satellite meetings of the 17th International Conference on Magnetism (ICM2006, Kyoto, Japan, 20–25 August). About 160 researchers from all over the world participated in QuBS2006, which was focused on magnetism, superconductivity and related materials studied with four complementary probes, namely neutrons, synchrotron-radiation X-rays,  $\mu$ SR and NMR.

More than 500 scientists attended the German Conference for Research with Synchrotron Radiation, Neutrons and Ion Beams at Large Facilities (SNI2006) in Hamburg, Germany, 4–6 October. During SNI2006, the Wolfram Prandl Prize for young scientists in neutron research was awarded to O. Stockert and T. Keller by the Committee on Research with Neutrons (KFN). They received the prize for their excellent work in the areas of correlated electron systems and high-resolution spectroscopy, respectively.

Concerning neutron sources worldwide, several changes occurred in 2006. A special highlight took place in April: The accelerator-based Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, USA, produced its first neutrons. This marks a great step for the neutron community in realizing the first accelerator-based neutron source that uses a liquid target to generate neutrons. As the first instrument at this neutron source the SNS Backscattering Spectrometer was commissioned and went into user operation in May

2006. By 2011, approximately 15 neutron beam instruments will have been installed and made available to scientists.

At ISIS Rutherford Appleton Laboratory (UK), up to now the world's leading pulsed neutron and muon source, the construction of a second target station is ongoing and first neutron production is scheduled for June 2007. The experimental programme will start in 2008, and seven state-of-the-art neutron instruments will make use of the high flux for long wavelength neutrons. The ISIS Second Target Station Project will expand the ISIS science programme especially in the fields of soft matter, advanced materials and bioscience.

Australia's new research reactor OPAL (Open Pool Australian Light-Water) went critical in August and reached its full power of 20 MW for the first time in November 2006. Official inauguration was scheduled for April 2007.

The Japan Proton Accelerator Research Complex (J-PARC) is currently under construction and its completion is scheduled for 2008. In February 2006, the J-PARC Center was established by its first Director, S. Nagamiya, to operate J-PARC jointly by the Japan Atomic Energy Research Institute (JAERI) and KEK (The High Energy Accelerator Research Organization). J-PARC is a three-stage accelerator complex with a 200 MeV Linac, a 3 GeV Rapid Cycling Synchrotron and a 50 GeV proton synchrotron, located near the upgraded research reactor JRR-3. One of the central facilities of J-PARC is the 1 MW Japanese Spallation Neutron Source (JSNS). The FRM II, a high-flux reactor source in Munich, Germany, which came into operation in 2004, reached its nominal power of 20 MW in May 2006 when the first neutrons were delivered to users. In a new, nearly finished, experiment hall at FRM II, the Forschungszentrum Jülich (FZJ) will operate eight scattering instruments (formerly located at FRJ-2) with its own team of scientists, engineers and technicians. FZJ inaugurated the Jülich Centre for Neutron Science (JCNS) at FRM II in February 2006 and herewith strengthens its activities at external neutron sources after the shut-down of their own research reactor FRJ-2 in May 2006, after 44 years of successful operation.

After several shut-downs between July 2005 and June 2006, the ILL (Institute Laue-Langevin) in Grenoble (France), the world's most intense neutron source, is running successfully and provides the best opportunities for fruitful experiments. At ILL, about 2,000 visiting scientists from 45 countries carry out 750 experimental investigations per year on the microscopic structure and dynamics of materials.

After the completion of a new second Neutron Guide Hall at the neutron source BER II of the Hahn-Meitner-Institut, Berlin (Germany) a number of instruments are being brought into operation. Besides the spin-echo spectrometer SPAN, a new diffractometer EXED (for extreme sample environments) and a new high-resolution small-angle scattering instrument (VSANS) will be located in the new Neutron Guide Hall. In addition, the world's strongest magnet for neutron experiments (between 25 and 30 Tesla), the so-called High Field Magnet Project, will also be installed there. This new magnet will be built in cooperation with the National High Magnetic Field Laboratory (NHMFL) at Florida State University, Tallahassee, USA, and is planned to be completed by 2011.

In 2006, after several years of standstill, the European Spallation Source (ESS) project has regained momentum by the announcement of a number of European regions ready for financial commitments for hosting this project. This is very important for the future of neutron science in Europe and for the whole neutron community.

**M. Steiner**, Chair

#### 4.15. Commission on Powder Diffraction

**4.15.1. Newsletters.** Issues 33 and 34 of the CPD Newsletter were expected to be produced in 2006. These, however, have been delayed although Issue 34 is near completion. The CPD has taken the decision that all future Newsletters will only be available electronically from the CPD web site. Various members of the Commission have agreed to produce Newsletters on a twice-yearly basis. The computer software pages are produced by L. M. D. Cranswick and are very much appreciated by readers for their informative content and their effective presentation. News from ICDD and from IXAS is also present in all issues, together with news on forthcoming events.

**4.15.2. Projects.** *Organic Structures from Powders.* One ongoing CPD initiative is the project on best practice for the analysis and deposition of organic structures from powder diffraction data. There have also been discussions about a 'Blind Test' Round Robin on structure determination from powder diffraction data.

**4.15.3. Meetings/Workshops/Schools.** The 2006 CPD meeting was held at EPDIC, Geneva, Switzerland, 6 September 2006. Future regional meetings in Indonesia and Brazil and two workshops at the ESRF, Grenoble, France, have been supported by the Commission, which continues to encourage crystallographers around the world to promote powder diffraction research and education. The fifth Size-Strain Conference 'Diffraction Analysis of the Microstructure of Materials', 2–9 October 2007 in Garmisch-Partenkirchen, Germany, has also been endorsed by the Commission (see <http://www.mf.mpg.de/en/abteilungen/mittemeijer/ss-v/welcome.htm>).

**4.15.4. Web site.** The CPD web site (<http://www.iucr-cpd.org>) continues to be developed and is being refurbished by the current CPD Chair. The web site gives free access to the CPD Newsletter archive, from which recent and past issues can be downloaded in pdf (Acrobat) format. On a long-term scale, the CPD is involved in a project for a basic textbook on powder diffraction that will be published by the Royal Society of Chemistry.

**W. I. F. David**, Chair

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

**4.16.1. Commission meetings and communication.** The members of the Commission discussed the work of the Commission at meetings and conferences around the world. The most important meeting of the Commission took place during the XIII International Conference on Small-Angle Scattering (SAS2006), Kyoto, Japan, 8–13 July, 2006, which was attended by most Commission members. Routine communications were accomplished by e-mail.

**4.16.2. Activities.** The most prominent event of 2006 was SAS2006. Most of the Commission members served on the International Advisory Committee. N. Yagi was a Vice-Chair of the Organizing Committee and Y. Amemiya was Chair of the Programme Committee. The conference was attended by 548 participants from 33 countries and 5 continents. There were 538 presentations including 125 oral presentations and 413 poster presentations; the number of presentations exceeded that at the previous SAS2002 in Venice, Italy, by about 150.

The scientific programme of the conference contained seven plenary lectures on hot topics covering various scientific fields, nineteen general sessions and five special sessions. The general sessions included Polymer, Instrumentation, Biological Solution Scattering, Colloids, Surfactants and Lipids, Alloys and Ceramics, Magnetic Materials, Non-Crystalline Materials, Surface and Interface, GI-SAS, Theory and Modeling, and Fiber Diffraction, while special sessions were devoted to the topics of an interdisciplinary

nature on (1) dynamics and kinetics, (2) hierarchical structures studied with a wide range of momentum transfer, (3) new methods concerning contrast variations *etc.* and (4) open-non-equilibrium systems under various external fields. In some special sessions, a concerted use was considered of combined SAS methods, *e.g.* SAS and Ultra-SAS of X-rays, and neutrons and SAS of light, applied to given systems in order to explore systematically their mesoscopic scale structures and dynamics.

Young researchers from 14 countries were financially supported by the IUCr. The proceedings will be published in a Special Issue of *Journal of Applied Crystallography* (April 2007).

SAS2006 also provided a good opportunity to increase the visibility of the Commission and to receive feedback from the scientific community. On the last day of the meeting, the Chair of the Commission, D. Svergun, presented the scope of the work of the Commission to the participants of the Conference and highlighted the plans for future activity. Among the topics discussed were a possible textbook on SAS, the use of the SAS listserver, standard samples and standard data formats.

In coordination with the organizers of SAS2006, the Commission made a call to the SAS community to prepare applications from scientific institutions willing to host the XIV SAS Conference in 2009. The applications from Oxford, Hamburg and Argonne were received and presented at SAS2006 as posters and oral talks. After a ballot by the participants, Oxford, UK, was selected as the venue of SAS2009.

**4.16.3. Educational activities.** A discussion on writing a textbook on small-angle scattering initiated in 2005 by the members of the Commission was continued in 2006. The most frequent opinion was that one should aim rather for an entry-level textbook written by a few authors and not for a more advanced book written by a larger group of authors and also covering cutting-edge applications. The current problem is that it is difficult to find people who would take responsibility for writing the first type of book. Many scientists would be prepared to contribute a chapter to a larger volume, but not to write a full textbook. Members of the Commission (A. Allen, P. Thiyagarajan, D. Svergun) approached some prominent representatives of the SAS community who might be prepared to act as contributors, and this issue was also publicly raised and discussed at the SAS2006 conference. Currently, the format of the book and its possible authors are still under discussion.

As before, the members of the Commission were actively involved in giving seminars and tutorial lectures explaining SAS methods to young researchers/students in the entire world. Below are some examples.

Members of the Commission (D. Svergun, J. Trehella, J. S. Pedersen) were lecturers and tutors at the EMBO Practical Course on Solution Scattering from Biological Macromolecules, EMBL Hamburg Outstation, Germany, 23–30 October, 2006.

D. Svergun gave the tutorial lectures Small-Angle Scattering from Biological Macromolecules (5th Summer School on Condensed Matter Research, Zuzo, Switzerland, August 2006) and Analysis of Small-Angle Scattering from Solutions of Biological Macromolecules (SSRL BioSAXS Workshop, Stanford, USA, July 2006).

P. Thiyagarajan provided hands-on training on SANS of block copolymer micellar solutions (on the SAND instrument) for 20 National School students at the 8th National School on Neutron and X-ray Scattering, Argonne National Laboratory, August 2006. He gave lectures entitled Some Applications of SANS in Soft Condensed Matter Science (LANSCE Neutron School, May 2006), and Small-Angle X-ray and Neutron Scattering: Fundamentals and Applications (National School on Neutron and X-ray Scattering, Argonne National Laboratory, August, 2006).

J. Trehella promoted educational activities on the Pacific Rim. Interest in small-angle scattering in the Pacific Rim Countries continues to grow, especially as a complement to crystallographic and NMR studies of proteins and protein complexes. The technique and its practitioners have increased visibility at meetings. Small-angle scattering will feature strongly at Crystal XXV, the 25th Meeting of the Society of Crystallographers in Australia and New Zealand (SCANZ), in the Hunter Valley, NSW, Australia, 10–13 April 2007. There are 125 registrants for the Conference to date, and the themes of the Conference feature small-angle scattering in a number of sessions: New Facilities and Crystallography at the Beamline; Allied Methods: SAX, WAX, XAFS and Imaging; Materials Science and Nanotechnology.

I. Torriani offered a short course in Argentina on SAXS theory and applications including a description of SAXS–WAXS *in situ* experiments during the Annual Meeting of the Argentinian Crystallographic Association in Puerto Madryn, Patagonia.

P. Fratzl represents the Commission on the working group on the Online Dictionary of Crystallography.

**4.16.4. Community building activities.** As in the previous year, numerous scientific presentations were given by the members of the Commission at conferences, workshops and round-table meetings devoted to the future development of SAS and also to interactions with related scientific methods. The members of the Commission further contributed to the widening of the user community of the SAS instruments in their laboratories and large-scale facilities.

J. S. Pedersen contributed to the round-table discussion on the future of the SANS activities at the Frank Laboratory of Neutron Physics in connection with the International Small-Angle Scattering Workshop, Frank Laboratory of Neutron Physics Joint Institute for Nuclear Research, Dubna, Russia, 5–8 October 2006. J. S. Pedersen also continued to support new users at his laboratory's SAXS facility at the University of Aarhus, Denmark. The facility is used by a large number of researchers from the University of Aarhus, mainly from the iNANO Interdisciplinary Nanoscience Center and from the Department of Structural Molecular Biology. The instruments also attract a large number of collaborators from other Universities and Research Institutes in Denmark, Scandinavia and the rest of Europe. Many students and post-docs have been trained in the SAS technique in Aarhus.

D. Svergun promoted biological solution scattering in Europe. The beamline X33 run at EMBL Hamburg has displayed a steady increase in the number of users by about 20–30% per year since 2000 and this increase continued in 2006 with the number of registered user groups exceeding 80 from 22 countries. The users are trained and they further disseminate knowledge about SAXS in their institutions. To establish links with other experimental methods, D. Svergun participated in the Workshop on Complementary Techniques with NMR for Structure Determination of Biological Macromolecular Complexes (Florence, May 2006) and presented the talk Joint Use of NMR and SAXS for Structure Analysis of Biological Macromolecules in Solution.

A. Allen promoted the use of the NIST USANS instrument, which, including two recent innovations (suppression of back crystal reflections to reduce background and a focused pre-monochromator to increase the flux), is the only dedicated USANS beamline in the world with a regular external user programme.

P. Thiyagarajan trained a number of young graduate students from various US universities and abroad in the SANS and reflectivity experiments at IPNS and SAXS at APS. He continued to provide a SAS analysis software package to the students and faculty who visit IPNS and APS for experiments.

I. Torriani offered support to the users at the Brazilian Synchrotron Facility (LNLS), contributing significantly to community building in South America. She received a group from Spain who stayed three weeks for general training and performed several types of SAXS–WAXS experiments. Lectures were given at the annual meeting of the Brazilian Materials Research Society (BMRS) and the Brazilian Crystal Growth Society on SAXS characterization of materials.

Support was given by the Commission for the funding applications to the IUCr from the organizers of the International Conference on Neutron and X-ray Scattering (Indonesia, 2007) and of the 9th International Conference on Biology and Synchrotron Radiation (UK, 2007).

**4.16.5. Consultant activities.** D. Svergun and J. S. Pedersen served as members of the Scientific Committee at Geestacht Neutron Scattering Facility (GeNF) at GKSS Research Centre, Geestacht, Germany.

D. Svergun was a member of proposal review Committees of the European Synchrotron Radiation Facility (ESRF, Grenoble, France) and of the synchrotron Elettra (Trieste, Italy) (evaluation of beam-time applications).

P. Thiyagarajan was a Chair of the Cross-Cutting SAC review in Polymer Science, Argonne National Laboratory, USA (January 2006), a member of the ACNS Programme Committee, Biological Sciences (June 2006), a Chair of the EQSANS IAT meeting, SHUG Meeting, Oak Ridge National Laboratory, USA (October 2006), and a Chair of the SAXS Proposal Review Panel for APS (the panel convenes three times a year). He was also a member of the BioCAT Advisory Committee, APS, and served as a reviewer for the beam-time proposals for NIST and SSRL (Stanford, USA). He was a Selection Committee Member, SAS's Guinier Prize Committee, of NSSA's Shull Prize, and of Pittsburgh Diffraction Community Sidhu Prize, 2006.

**4.16.6. Organizational activities.** J. S. Pedersen was a member of the Organizing Committee of the European Summer School Scattering Applied to Soft Condensed Matter that took place in Bombannes, Gironde, France, 10–17 June 2006, and he was also among the teachers at the School.

The Commission together with the Organizing Committee of SAS2006 in Kyoto organized the applications, selection and award of the IUCr-sponsored prizes at the Conference. These were a Guinier Prize for outstanding contributions to the field of SAS, and three Prizes to young scientists who have made distinguished presentations at SAS2006. The Commission called for applications, evaluated them together with the Conference Organizers (members from the Commission served on the Selection Committees) and organized the award ceremony. The Guinier Prize was awarded to H. Sturhmann for his seminal contribution and life achievements in the development of contrast variation methods in SAS.

J. Trehella is a Programme Chair for the Annual Meeting of the American Crystallographic Association in Salt Lake City, USA, 2007. Small-angle scattering will feature prominently with five sessions focusing on techniques and applications.

D. Svergun was a co-organizer of the EMBO Practical Course on Solution Scattering from Biological Macromolecules (Hamburg, Germany, October 2006) and of the first EMBL Beamline Workshop 'BIOSAXS @ PETRA-III' (Hamburg, Germany, November 2006).

**4.16.7. Technical activities.** P. Thiyagarajan continued to be active in an advisory role for the developments of new capabilities for SAXS, GISAXS, ASAXS and area detector development at 12-ID (Argonne National Laboratory, USA).

The group of D. Svergun further developed the program suite *ATSAS 2.1* for the analysis of small-angle scattering data, which is freely available from the EMBL web site to academic users and since 2003 has received more than 10,000 downloads from more than 400 laboratories worldwide. Methods are being developed for automated data processing and model building and for web-based access to the programs.

The work on the NIST Standard Reference Material (SRM) on a diffraction-based standard for wavelength for SAXD and SAXS is still in progress (A. Allen). The demand for this is driven primarily by the SAXD needs in the pharmaceutical industry; however, the work on this SRM will only start once other present diffraction-based SRM work is completed.

I. Torriani finished the commissioning of the second (D02-SAXS2) beamline at the LNLS source (Campinas, Brazil). This instrument is now open to external users from Brazil and other South American countries.

**D. I. Svergun, Chair**

#### 4.17. Commission on Structural Chemistry

According to the guidelines expressed by the Executive Committee, the Commission has established a list of responsibilities for members and consultants for the year 2006: *IUCr Newsletter* reporter: D. C. Levendis, A. Beatty, A. Bacchi (consultant: J. L. Flippen-Anderson); *World Directory of Crystallographers*: P. Bombicz, O. Piro, M. Hong (consultant: E. Gutiérrez-Puebla); teaching and schools: M. T. Duarte, P. Raithby (consultants: F. Lahoz, J.-C. Daran); nomenclature: P. Raithby, M. Hong; journals: H. Uekusa, L. Brammer (consultants: F. Lahoz, J.-C. Daran); *International Tables*: O. Piro, M. T. Duarte; IUCr/OUP: A. Beatty, P. Bombicz (consultant: J. L. Flippen-Anderson); web master: A. Bacchi, H. Uekusa (consultant: E. Gutierrez-Puebla); *Acta* 60th Anniversary: L. Brammer, D. C. Levendis. Other active consultant: D. Braga.

During 2006, the following tasks have been addressed under the responsibilities of different members:

the web site has been restyled and updated (A. Bacchi); suggestions have been sent for the 60th Anniversary Special Issue of *Acta A* (L. Brammer);

lists of those attending crystallographic schools and meetings are being collected for entry into the *World Directory of Crystallographers* (P. Bombicz);

suggestions for implementing crystallographic nomenclature are being collected and forwarded to the Working Group designated by the Commission on Crystallographic Nomenclature to implement a pilot project for an Online Dictionary of Crystallography (P. Raithby);

reports on events endorsed by the Commission during 2005 [Russian Fourth National Crystal Chemical Conference, French Crystallographic School, Indaba 5 (South Africa)] have been collected (A. Bacchi);

the report on the meeting Indaba 5 has been sent to the *IUCr Newsletter* (D. C. Levendis).

The Commission met in 2006 at the Kruger National Park (South Africa), during Indaba 5. Current and future activities have been discussed, in particular regarding the programme for structural chemistry for the Osaka Congress. A. Bacchi (Italy) and A. Nangia (India) have been suggested to represent the Commission on the International Programme Committee for the Osaka Congress. During 2006, the Commission has endorsed the following events:

American Crystallographic Association Annual Meeting (Salt Lake City, 21–26 July 2007);

First School on Materials Applications of the Organic Solid State (SMAOSS) and the XVIII International Conference on the Chemistry of the Organic Solid State (XVIII ICCOSS) (Merida, Venezuela, 1–6 and 8–13 July 2007).

**A. Bacchi**, Chair

#### 4.18. Commission on Synchrotron Radiation

The main event for the Commission was the Ninth International Conference on Synchrotron Radiation Instrumentation (SRI-2006) held in the EXCO Center Daegu, Korea, 28 May–2 June. This meeting was jointly organized by the Pohang Accelerator Laboratory and the Japan Synchrotron Radiation Research Institute. There were more than 750 participants from 25 countries. In addition to the classical synchrotron-radiation instrumentation topics special emphasis was given to the linac-based, or fourth-generation, sources indicating the importance and potential of these sources for the future of photon science. Of particular interest and strongly endorsed by the Commission was a session on Light Sources in Developing countries. A subset of the Commission held an informal meeting during the conference.

The Commission also endorsed the establishment of the Asia Oceania Forum for Synchrotron Radiation Research (AOFSSR). The AOFSSR had their first and very successful meeting in Tsukuba, Japan, 24–25 November 2006. The 2nd meeting of AOFSSR is planned for Hsinchu, 1–2 November 2007, as a satellite conference of AsCA '07. In addition to these meetings dedicated to synchrotron-radiation sources and science, the Commission has also endorsed a number of other meetings, in particular: the 5th Sesame Users Meeting and associated school, 27 November–2 December 2006; the 6th International Conference on X-ray Scattering (IXS2007), Hyogo, Japan, 7–11 May 2007; the RapiData course, in particular for financing the participation of students from Latin America; the Erice Summer School (June 2007) on X-ray Micro- and Nanoprobes: Instruments, Methodologies and Applications; and the 9th International Biology and Synchrotron Radiation Conference, Manchester, UK, August 2007. In addition, members of the Commission were involved in many other meetings and collaborations (covering detectors, coherence, optics *etc.*) that are relevant to the technical and scientific remit of the Commission. For example: the XVI International Synchrotron Radiation Conference (SR-2006) held at the Budker INP, Novosibirsk, Russia, July 2006; and the NATO Advanced Research Workshop on Brilliant Light Facilities and Research in Life and Material Sciences, Yerevan, Armenia, 17–21 July 2006.

Finally, members of the Commission are involved with the planning of the Osaka Congress.

**H. Graafsma**, Chair

#### 4.19. Commission on XAFS

The goal for the Commission continues to be to promote XAFS in the crystallographic community and to drive new developments.

The Commission web site, directly linked from the IUCr web page (<http://www.iucr.org/iucr-top/iucr/cxafs.html>), was developed further during the last year. It is hosted by the Physics Department of the University of Bologna, Italy, and maintained by F. Boscherini. XAFS-related events (conferences, workshops, schools), a compendium of XAFS beamlines at synchrotron facilities all over the world and a list

with names and e-mail addresses of the members of the Commission can be found there.

An announcement on the new IUCr Commission on XAFS was published in the *IUCr Newsletter* [A. Molenbroek and I. Ascone (2006). *IUCr Newsletter*, Volume 14, No. 4].

The Commission supports the 9th International Conference on Biology and Synchrotron Radiation (BSR2007), Manchester, UK, 13–17 August 2007 (<http://www.srs.ac.uk/bsr2007>). The Commission also supports the satellite meeting related to this conference, 10–11 August 2007: the 3rd BioXAS Study Weekend at SOLEIL (Saint-Aubin, France) that will be focused on Metalloproteomics (<http://www.synchrotron-soleil.fr/workshops/2007/BIOXAS-SWE>).

Many members of the Commission were present at the 13th International Conference on X-ray Absorption Fine Structure (XAFS-XIII) held at the Stanford Campus (<http://www-ssrl.slac.stanford.edu/xafs13>), 9–14 July 2006. This triennial conference was organized by the International XAFS Society (IXS; see <http://www.i-x-s.org>). The Commission members held some good meetings and also some fruitful discussions with the new IXS Executive Committee. We jointly decided to appoint a small Committee to take care of improvement of mutual relations for the benefit of the XAFS and the crystallographic communities. A short presentation on the IUCr and the Commission on XAFS was given at this conference.

Finally, we started to work on the organization of two Microsymposia, one on Combined XAFS and Diffraction of Inorganic Structures and one on XAFS in Biocrystallography, to be held at the Osaka Congress, and a workshop on XAFS, to be held at Photon Factory, Tsukuba, Japan, in relation to the Congress.

**A. Molenbroek**, Chair

#### 5. Sub-committee on the Union Calendar

The Sub-committee receives and considers requests for IUCr sponsorship and nominal financial support and makes recommendations to the Executive Committee. Acting on the recommendations made by the Sub-committee, during 2006 the Executive Committee approved sponsorship of various schools and meetings, mostly with financial support. Those held in 2006 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 2007, but approved in 2006, are listed below.

BCA Intensive Course in X-ray Structure Analysis, Durham, UK, 4 March–2 April, 2007.

Latin-American Workshop on Applications of Powder Diffraction and School on Methods of Powder Diffraction, Campinas, Brazil, 16–20 April 2007.

RapiData 2007, Brookhaven, USA, 22–27 April 2007.

6th International Conference on Inelastic X-ray Scattering, (IXS2007), Hyogo, Japan, 7–11 May 2007.

Fifth International Conference on Solid State Crystals and Eighth Polish Conference on Crystal Growth (ICSSC-5 and PCCG-8), Zakopane, Poland, 20–24 May 2007.

Engineering of Crystalline Materials Properties: State-of-the-Art in Modeling, Design, Applications, Erice, Italy, 7–17 June 2007.

School and Workshop on X-ray Micro- and Nanoprobes: Instruments, Methodologies and Applications, Erice, Italy, 11–17 June 2007.

Gordon Research Conference on Electron Distribution and Chemical Bonding Dynamics and Densities, South Hadley, USA, 1–6 July 2007.

First School on Materials Applications of the Organic Solid State (SMAOSS) and XVIII International Conference on the Chemistry of

the Organic Solid State (XVIII ICCOSS), Merida, Venezuela, 1–6 and 8–13 July 2007.

XVI International Conference on Crystal Chemistry and Diffraction Studies of Minerals; Workshop Minerals as Advanced Materials, Miass, Russia, 2–6 and 8–12 July 2007.

International School on Mathematical and Theoretical Crystallography, Havana, Cuba, 15–20 July 2007.

ACA Annual Meeting, Salt Lake City, USA, 21–26 July 2007.

International Conference on Neutron and X-ray Scattering 2007, Serpong and Bandung, Indonesia, 23–31 July 2007.

VIII Latin-American Workshop on Magnetism and Magnetic Materials and Their Applications (LAW3M), Rio de Janeiro, Brazil, 12–16 August 2007.

24th European Crystallographic Meeting (ECM-24), Marrakech, Morocco, 22–27 August 2007.

Advanced Methods in X-ray Charge Density Analysis: Extracting Properties from a Multipolar Refinement, Martina Franca, Italy, 3–6 September 2007.

MSA-GS-ANL Short Course on Amphiboles, Rome, Italy, 29–31 October 2007.

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 D. Viterbo. For up-to-date contact information, application procedures and rules, see <http://www.iucr.org/iucr-top/iucr/calendar.html>.

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

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

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

B. McMahon attended the CODATA International Conference and General Assembly in Beijing, People's Republic of China, 22–27 October 2006 (see the report of the CODATA Representative).

B. McMahon attended a Consultation Workshop exploring the roles and responsibilities of data centres and institutions in curating research data, sponsored by the Joint Information Systems Committee (JISC), at CCLRC, Didcot, UK, 10 October 2006. The IUCr was able to provide substantial input to the resultant report entitled *Dealing with Data: Roles, Rights, Responsibilities*

and Relationships (<http://www.ukoln.ac.uk/ukoln/staff/e.j.lyon/publications.html#2007-06-19>).

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

Since 2005 was the year of the Florence Congress at which the future of CIF was examined in some detail, our report for that year looked back on the 15 years of CIF development and usage, presenting the perspective of what COMCIFS had achieved and where it was going in the future. 2006 has been mostly a year of consolidation of these decisions.

The most far-reaching project that COMCIFS is currently pursuing is the development of the new Dictionary Definition Language with Methods, DDLm (previously referred to as DDL3). Its adoption in principle by COMCIFS during the Florence Congress opened the way for the development of a DDLm dictionary which will shortly be presented to COMCIFS for adoption. On adoption, it will be used to develop a new suite of CIFm dictionaries that incorporate innovative features such as methods (computer-readable algebraic algorithms). It is also designed to simplify dictionary maintenance and management. Most importantly, programs written to exploit the new features of these dictionaries will be able to read all previously written CIFs, both those using coreCIF and mmCIF that are currently mutually incompatible. The detailed work on DDLm has been undertaken by N. Spadaccini, S. R. Hall and J. D. Westbrook, assisted by the visit of J. D. Westbrook to Perth, Australia, and a three-day workshop involving B. McMahon, S. R. Hall and I. D. Brown held in Chester, UK, during the year, with financial support from the IUCr. Following the expected adoption of DDLm to complement the current DDL1 and DDL2, work will begin on preparing CIFm dictionaries. The approval of a coreCIFm dictionary will provide the materials essential for those interested in developing software for the new standard. It is not the intention that DDLm will replace the existing dictionaries and software, but it will provide enhancements that are not currently available.

Work continues on the evolution of CIF dictionaries. The coreCIF Dictionary Maintenance Group continued working on the coreCIF dictionary revisions suggested by over a decade of extensive use, and it is coming within sight of the end of this project. I. Guzei and I. D. Brown started developing a component of the coreCIF dictionary describing the constraints and restraints used in structure refinement, and A. van der Lee and his colleagues have started work on a new CIF dictionary for reflectivity measurements.

2006 and early 2007 have been a time of renewed activity for imgCIF. H. J. Bernstein and R. Sweet organized a successful workshop in conjunction with the 2006 American Crystallographic Association Annual Meeting in Hawaii to promote the implementation of the imgCIF dictionary in capturing images of diffraction patterns, primarily at synchrotron sources. They have obtained funding for two more imgCIF workshops, one in the USA at Brookhaven National Laboratory immediately after the NSLS/CFN meeting in May 2007 and one in the UK in conjunction with the 9th International Biology and Synchrotron Radiation Conference in August 2007. There has been significant progress in the use of imgCIF both at SLS and at Diamond. Changes to the imgCIF dictionary to support uses of imgCIF at SLS, Diamond and ESRF will be proposed on the imgCIF list shortly and will be discussed at the upcoming workshops.

H. M. Einspahr worked closely with J. D. Westbrook, of the PDB, and the IUCr editorial staff to develop streamlined procedures for incorporating structural data from PDB deposits in associated

publications. This work has involved identifying mmCIF data items relevant to a full literature description, and the development of a tool for authors that will create experimental tables for inclusion in manuscripts from mmCIF files.

The IUCr editorial office has released a public version of its *publCIF* software. This software may be used to edit CIFs for publication. It combines dictionary-based CIF validation with a sophisticated collection of utilities that will assist prospective authors. These include active links to the checkCIF service, the ability to incorporate validation report forms (VRFs) generated by checkCIF, data-entry wizards, table editors, previews of articles formatted in the styles of the different IUCr structural journals, citation sorting and checking, private databases of authors and citations, and dictionary browsing facilities. The software is being further developed to support publication of biological macromolecular structures.

With financial help from the IUCr, H. J. Bernstein and students have produced updated versions of standard software libraries and tools (the *CIFTEST* parser test and validation suite, *CIFtbx3*, *cyclops*, *vcif2*, and a new utility to fold and unfold long-line CIFs) that are compliant with the version 1.1 CIF specification.

The CIF-developers list continues to act as a discussion list and opportunity for software developers to advertise their new software. The Python package *PyCIFRW* was described in a CIF applications paper in *J. Appl. Cryst.* [Hester (2006). *J. Appl. Cryst.* **39**, 621–625].

Finally, but by no means least, the IUCr won the 2006 Award for Publishing Innovation of the Association of Learned and Professional Society Publishers (ALPSP) for its development of the Crystallographic Information Framework and the use of checkCIF in data exchange, quality assurance and integrated data publication.

**I. D. Brown**, Chair

## 8. Committee on Crystallographic Databases

The Committee discussed modalities for possible collaborations between the IUCr and existing and upcoming databases. It was noted that at present the IUCr has a collaboration with the ICSD that is jointly produced by NIST and FIZ. Other proposals have been declined in the past by the IUCr, while yet others are under consideration at the present time. There was a general consensus that the IUCr should act so as to judiciously support such activities, but that it should be consistent in providing this support and encouragement. It was recognized that it is costly to assemble data properly and very costly to maintain a software arm and support/marketing presence for specialized crystallographic databases especially in smaller organizations. The IUCr could play a facilitating role to the data provider wherever there is an overall benefit to the scientific community, and especially if IUCr support would make a key difference to such database generation activity, keeping in mind overall financial viability.

**G. R. Desiraju**, Chair

## 9. IUCr Newsletter

Four issues of the *IUCr Newsletter* were distributed in 2006 (Volume 13, No. 4, Volume 14, Nos. 1, 2 and 3). By the end of the year, Volume 14, No. 4 was nearly complete and material for Volume 15, No. 1 was in hand. This report will cover all four issues of Volume 14. Volume 14, No. 1 contained 40 pages and the remaining issues were 24 pages in length. Coverage of the Florence Congress that began in Volume 13, No. 4 was completed in the first issue of Volume 14. 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, future meeting announcements and a general meeting calendar.

Each issue carried a President's column written by Y. Ohashi. Issue 2 included a guest editorial written by the newly elected President of the ECA, J. R. Helliwell, and Issue 4 carried a guest editorial written by M. Yousef to accompany articles on the SESAME project (the synchrotron that will be constructed in the Middle East). Editorial responsibilities for the *Newsletter* were shared by W. L. Duax and J. L. Flippin-Anderson.

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 continued with *Crystallography* in Australia and New Zealand, edited by J. L. Martin (Volume 14, No. 1), in Portugal, edited by M. Figueiredo, M. Costa, A. Damas, M. Duarte and M. A. Carrondo (Volume 14, No. 2), and Singapore, edited by K. Swaminathan and J. J. Vittal (Volume 14, No. 3). Material on crystallography in Poland is on hand and being edited for publication in 2007.

Reports were published covering meetings in Egypt, Italy, Russia, Spain, Slovenia, the USA and South Africa. A book review described Volume G of *International Tables* and there was an article featuring the IUCr's publication award.

The mailing list was 11% larger than in 2005 with an average distribution of 18,637. Twenty-one countries assist in the effective and economic distribution of the *Newsletter*. (Distributors: H. Fodil, Algeria; G. Jameson, Australia; J. Valderrama, Colombia; B. Kojic-Prodic, Croatia; J. Hasek, Czech Republic; C. Lecomte and Å. Kvik, France; A. Nangia and Executive Secretary, India; Ismunanda, Indonesia; P. Spadon, Italy; A. Satomi, Japan; A. Hamid Othman, Malaysia; R. Rendle, New Zealand; J. Lipkowski, Poland; M. Costa, Portugal; J. J. Vittal, Singapore; L. R. Nassimbeni, South Africa; H. Grimmer, Switzerland; Yu Wang, Taiwan; K. Haller, Thailand; H. Kooijman, The Netherlands; G. Diaz De Delgado, Venezuela.) Individual distribution was sent to 100 additional countries.

**W. L. Duax**, Co-Editor

**J. L. Flippin-Anderson**, Co-Editor

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

In 2006, the cooperation between Oxford University Press (OUP) and the IUCr/OUP Book Series Selection Committee has been very productive.

A new volume in the series *IUCr Monographs on Crystallography* was published: No. 19, *Molecular Aggregation Structure Analysis and Molecular Simulation of Crystals and Liquids*, by A. Gavezzotti (publication date 30 November 2006).

A new volume in the series *IUCr Texts on Crystallography* was published: No. 8, *Crystal Structure Refinement: a Crystallographer's Guide to SHELXL*, by P. Müller, R. Herbst-Irmer, A. L. Spek, T. Schneider and M. Sawaya (publication date 13 July 2006).

In the case that a book has proven to be successful, a paperback edition may be published. Two volumes in the series *IUCr Monographs on Crystallography* appeared in 2006 in paperback editions: No. 12, *The Chemical Bond in Inorganic Chemistry. The Bond Valence Model*, by I. D. Brown (publication date 4 May 2006); No. 13, *Structure Determination from Powder Diffraction Data*, by W. I. F. David, K. Shankland, L. B. McCusker and Ch. Baerlocher (publication date 3 August 2006).

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.

In one case, where there was competition with other publishers, it appeared to be feasible to prepare a balanced judgement in about five weeks. Mostly such time pressure is not present as authors appreciate the fact that our series is well established and gives as such added value. OUP is present at major crystallographic conferences and their crystallography editor, S. Adlung, is then also available for discussions with potential authors for new proposals.

The Committee is very interested in proposals for new volumes and encourages prospective authors to contact the Chair of the Committee (schenk@science.uva.nl). 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.

**H. Schenk**, Chair of Book Series Committee

## 11. Regional Associates and Scientific Associates

### 11.1. American Crystallographic Association (ACA)

The most important activities of the ACA for this year are represented in the programme and organization of the 2006 Annual Meeting. Taking place in Honolulu, Hawaii, 22–27 July 2006, the event was organized with the expectation of attracting crystallographers from other Pacific Rim countries, adding the beauty of the environment to the excellent scientific agenda of the meeting. The results were up to the expectations: as reported by the ACA Secretary, L. Keefe, the meeting had one of the largest attendances of all times (963 participants) and 688 scientific contributions. On this occasion, R. Bau, ACA President, and the local organizers of the meeting made special efforts to obtain reduced accommodation rates and to obtain travel grants for students and young scientists. A donation campaign among ACA members to gather student travel funds was also organized by W. L. Duax. As in previous years, the meeting was preceded by one-day workshops on 22 July: (Wk.1) Methods in Neutron Protein Crystallography; (Wk.2) Management of Synchrotron Image Data: imgCIF File Systems and Beyond; and (Wk.3) An Introduction to Grazing Incidence Small-Angle Scattering with X-rays and Neutrons.

The awards and related symposia for this year were as follows.

The Martin Buerger Award, granted to H. D. Berman (Rutgers University) for her pioneering work in the establishment of the Protein Data Bank and the creation of the Nucleic Acid Database.

The B. E. Warren Award, whose recipient was C. Majkrzak (NIST), for his contributions to neutron reflectivity and development of related methods.

The Margaret C. Etter Early Career Award, presented to C. Wilmot (University of Minnesota), for her outstanding work in the study of fundamental enzymatic processes.

The subject of the Transactions Symposium was Smaller Crystals and Larger Molecules with Neutron Diffraction.

The 2006 ACA Summer School on Macromolecular Crystallography was held at the Illinois Institute of Technology (Chicago, Illinois) and the Advanced Photon Source (Argonne, Illinois), 1–22 July 2006. The school was designed for graduate students and post-doctoral researchers, and lectures, laboratory exercises, including hands-on data collection were offered to the participants. Several scholarships were awarded to candidates from the USA and Latin-

American countries to enable them to attend these courses, mainly financed by the ACA, the US National Committee for Crystallography and some commercial firms. The ACA summer courses represent a remarkable educational effort on the part of the ACA.

The ACA Newsletter under the new name *ACA Reflexions* published four times per year is fundamental in keeping the membership informed and promoting active participation in the activities of the Association. Information on the latest developments in database access and distribution, diffraction and computer technology, listings of national and international meetings, reviews of meetings, notes on the activities of the International Union of Crystallography, and programme and registration materials for the ACA meetings are very welcome by the community. Its editing staff is doing a remarkable job that is certainly very much appreciated by the community.

The 2007 ACA Annual Meeting will take place in Salt Lake City, Utah.

**I. L. Torriani**, IUCr Representative

### 11.2. Asian Crystallographic Association (AsCA)

The main activities centred on the joint AsCA '06/CrSJ meeting which was successfully conducted in Tsukuba, Japan, 20–23 November 2006 (Programme Chair, S. Wakatsuki). Keynote Lectures by S. Kitagawa (Crystal and Functional Engineering for Unique Microporous Materials), Z. Rao (Structural Insights into SARS Coronavirus Proteins), S. Iwata (Towards Structure Determination of Human Membrane Proteins) and C. Howard (Structures and Phase Transitions in Perovskites) were the meeting highlights. A total of 18 Microsymposia in 21 sessions were presented in three parallel sessions. Including the Keynote Lectures, 115 speakers gave oral presentations at the conference and 331 posters were displayed and presented. Approximately 450 registered participants were involved in the academic programme.

The current status and activities of AsCA were presented at a council meeting held during AsCA '06. The minutes are available at the AsCA web site, which is now fully operational and maintained by J. M. Guss (<http://www.asiancrystassn.org>). Y. Ohashi (IUCr President) discussed some of the IUCr policies affecting AsCA and the region. One goal of the IUCr was to increase the number of adhering countries. Only 7 of the 17 AsCA countries are associated with the IUCr. A subscription fee has to be paid for the Adhering Body to be a member of the IUCr. Since this fee might be too high for small developing nations, Professor Ohashi suggested that several such countries could apply jointly and pay a single shared fee. The smaller countries would pay subscriptions to AsCA and AsCA would then pay one fee to the IUCr on behalf of the group of countries. In return, the block of countries would be allowed to have a representative with voting rights at the IUCr General Assembly. It was decided to formalize this at the next council meeting to be held during AsCA '07.

It is noted that the financial position of AsCA has improved to just over AUD 100,000. However, support is still required from IUCr for young scientists. Such support has been received for AsCA '07 which will be held in Taipei, 4–7 November 2007 (Chair, International Organizing Committee, S.-L. Chang, Program Chair, Se Won Suh). 300 abstracts have already been received.

AsCA has continued to prosper and strives to foster international links between crystallographers in the region. AsCA welcomes increased participation by crystallographers from the People's Republic of China, Korea and Malaysia, countries where significant scientific activity is now seen. The increasing prosperity through

much of Asia, especially China and India, as well as improved communication conduits through available web sites and e-mail, should help maintain prospects for continued growth and success. Economic disparities and geographical challenges in the region are unique problems and mean that IUCr assistance to AsCA will remain an important foundation in its efforts to further the crystallographic sciences throughout the Asian region.

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

## 11.3. European Crystallographic Association (ECA)

The present membership of the ECA Executive Committee was appointed in 2006 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 (*ex-officio*).

### Meetings

The ECA has supported the following meetings between August 2006 and August 2007:

ECM-23 + satellites (Leuven, Belgium);

HEC-9 (BioCrystallography, Göttingen, Germany);

First Joint Italian-Spanish Meeting of Crystallography MISCA2007 (Calabria, Italy);

The Zürich Crystallography School 2007 (Zürich, Switzerland);

ECM-24 + satellite (Marrakech, Morocco).

Future meetings will be held as follows: 2008 is an IUCr Congress year; ECM-25, Istanbul, Turkey, August 2009; ECM-26, Darmstadt, Germany, August 2010 (this will be held along with EPDIC XII); 2011 is an IUCr Congress year; the location of ECM-27 to be held in 2012 is to be discussed in Marrakech in August 2007.

ECM-24 is to be held in Marrakech, Morocco, 22–27 August 2007, and is preceded by satellite meetings on (i) Mathematical and Theoretical Crystallography: The Enchanting Crystallography of Moroccan Ornaments and (ii) Science Meets Industry, as well as an Advanced Training Workshop on Development Training in Computational Methods and Synchrotron Facilities for Crystallography.

### Prizes

The first prize awardee for the new ENSA/ECA Prize for young scientists, named after E. L. Bertaut, is H. M. Rønnow of the Laboratory of Quantum Magnetism, Ecole Polytechnique Fédérale de Lausanne, Switzerland, whose work has concentrated on experimental and theoretical aspects of quantum magnetism; he has also been involved in development of neutron instrumentation as well as simulation and data analysis software.

The ECA Perutz Prize awardee for 2007 is D. Stuart of The Wellcome Trust Centre for Human Genetics in Oxford, UK, who is one of the pioneers of virus crystallography and his award is in recognition of his impact in this field, and his contributions to the structural chemistry of disease at the atomic level.

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

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

No formal meeting of the International Organization for Crystal Growth (IOCG) was organized in 2006. The updated information about the IOCG can be found at <http://www.iocg.org/>.

The main IOCG activity was focused on preparation for the International Conference on Crystal Growth ICCG-15, Salt Lake

City, Utah, USA, 12–17 August 2007 (Co-Chairs R. Feigelson and G. Stringfellow), and for the International Summer School on Crystal Growth ISSCG-13, Park City, Utah, USA, 5–10 August 2007 (Co-Chairs J. DeYoreo and C. Wang). Detailed information about both venues can be found at <http://www.crystalgrowth.us/iccg15/index.php> and <http://www.crystalgrowth.us/isscg13/index.php>, respectively.

The next General Assembly of IOCG will take place in Salt Lake City during ICCG-15. During this meeting, the new President and Officers will be confirmed following the election in early 2007.

The IOCG Executive Committee collected suggestions for candidates for the Frank, Laudise and Schieber Prizes. These prizes will be awarded during ICCG-12 in Salt Lake City. The IOCG Frank Prize is awarded for significant fundamental contributions to the field of crystal growth, the IOCG Laudise Prize is presented for significant technological contributions to the field of crystal growth and the Schieber award has been established with the purpose of recognizing a young author for his or her outstanding scientific publications in the field of crystal growth.

National Associations for Crystal Growth are active in promoting crystal growth science in their own countries as well as in collaborating in the organization of international events.

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

## 11.5. International Centre for Diffraction Data

J. A. Kaduk has played a full role as the ICDD representative to the Commission on Powder Diffraction (CPD). The CPD maintains close links with the ICCD and also with IXAS (<http://www.ixas.org/>); IXAS information is available via the ICDD web site at <http://www.icdd.com/> and the IXAS web site at <http://www.ixas.org/>.

**W. I. F. David**, IUCr Representative

## 12. Representatives on Other Bodies

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

There was no meeting of the ICTNS in 2006.

Of interest is the updating of IUPAC publications on nomenclature:

*Nomenclature of Inorganic Chemistry* (Red Book) (2005), RSC Publishing, prepared by N. G. Connelly, T. Darnhus, R. M. Hartshorn, A. T. Hutton;

*IUPAC Handbook* (<http://www.iupac.org/handbook.html>);

*The IUPAC Compendium of Chemical Terminology* (Gold Book) (<http://gold.zvon.org>).

A new edition of the Purple Book, *Compendium of Macromolecular Terminology & Nomenclature* is in preparation.

The following recommendations have been submitted for approval in 2006:

IUPAC Explanatory Dictionary of Key Terms in Toxicology;

Definitions of terms relating to the structure and processing of inorganic and polymeric gels and networks, and inorganic-polymeric materials;

Atomic Weights of the Elements 2005;

International Vocabulary of Basic and General Terms in Metrology (VIM);

Structure-Based Nomenclature for Cyclic Macromolecules.

**A. Authier**, IUCr Representative

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

ICSTI offers a unique forum for interaction among organizations that create, disseminate and use scientific and technical information. ICSTI is a scientific associate of ICSU, the International Council for Science. ICSTI's mission cuts across scientific and technical disciplines as well as international borders, to give member organizations the benefit of a truly global community.

In February 2006, ICSTI organized a workshop on Information and Data in e-Science: Making Access to Data a Seamless Reality, held in Paris, France, at the French Ministry of Research, INIST-CNRS and INSERM. This was a timely discussion spanning the fields of the physical sciences, the social sciences and the biological sciences. The workshop brought together scientists, publishers, library managers and information scientists. There were 12 talks; a detailed report is available at [http://www.icsti.org/winter\\_mtg\\_2006/index.html](http://www.icsti.org/winter_mtg_2006/index.html). On behalf of the IUCr, J. R. Helliwell spoke on The Role of Quality and emphasized that the crystallographic community is energetic in its efforts to uphold quality standards in a diverse scientific environment. The development of a crystallographic information file (CIF) and associated data dictionaries has allowed the seamless transfer of information for deposition and publication. It also allows the definition of formal publication data quality standards, and the deployment of mechanisms for checking compliance with such standards, such as the IUCr checkCIF service. The role of IUCr journals in maintaining quality and the possibilities provided by the CIF dictionaries for semantic web applications were also discussed.

In June 2006, ICSTI organized a public conference on the theme of Partnering in Science Information: Necessities of Change. This event was held at the National Library of Medicine in Bethesda, Maryland, at the USA National Institutes of Health. A report can be found at <http://www.warr.com/pisi.html>. On behalf of the IUCr, J. R. Helliwell presented a talk on Experience of Global Responsibilities in Science Publishing: Examples from an Editor-in-Chief for ICSU International Union of Crystallography. A key aspect emerged within the ICSTI context, namely concerning the Global Information Commons Initiative (<http://www.codata.org/wsis/GlobalInfoCommonsInitiative.html>). It was emphasized that the IUCr already makes globally available as much of its data and material as possible within the basic constraint of retaining the sustainability of the IUCr journals. However, it was stressed that the IUCr is discussing how to enhance further its efforts in the global information supply for the good of science.

The UK-based Research Information Network organized a conference in June 2006 held at Imperial College, London, on the theme of Data Webs: New Visions for Research Data on the Web (<http://www.rin.ac.uk/data-webs>). On behalf of the IUCr, J. R. Helliwell presented a talk entitled Changing Methods of Data Sharing in Crystallography. In addition, a session was devoted to The Future of Scientific Publications. Within this session, two lectures were presented: the first was given by P. Bourne, Editor-in-Chief of the Public Library of Science – *Computational Biology*, and entitled The Convergence Between Scientific Papers and Scientific Databases, and the second was given by A. de Waard of Elsevier Advanced Technology Group, Amsterdam, and Centre for Content and Knowledge Engineering, University of Utrecht, and entitled Separating Fact from Fiction: a Rhetorical Structure for Scientific Publications. Publications as a hot topic also featured in the closing Panel Discussion with criticism of peer review being evident from several speakers. Instead, J. R. Helliwell spoke up in defence of the good value and important role of peer review in maintaining the security

and quality of research information accessed by readers of all levels of experience.

Within the business meetings of ICSTI, held in Paris, France, in February 2006, and in Washington DC, USA, in June 2006, many topics were discussed. These included a general review of ICSTI's role, including its links with CODATA within the ICSU framework, whereby the rapid changes that are occurring in science publishing and information provision generally obviously mean that such regular review is important. In addition, J. R. Helliwell, on behalf of the IUCr, was able to keep close contact with the IUPAC and IUPAP science delegates, namely W. Warr and Sir Roger Elliott FRS, respectively, as well as library managers and information scientists across the world.

J. R. Helliwell acknowledges with gratitude the close collaboration with the IUCr journals Managing Editor, Peter Strickland, and with IUCr's Representative to CODATA, Brian McMahon, with whom each of the talks presented by J. R. Helliwell, described above, were prepared.

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

## 12.3. International Council for Science (ICSU)

The 94th Meeting of the Executive Board took place in Paris, France, 25–26 October. The Board was happy to note that the Deputy Minister for Higher Education and Research, François Goulard, had affirmed France's commitment to providing permanent annual support to ICSU of EUR 500,000. This announcement was first made at ICSU's 75th Anniversary Symposium on 4 July 2006.

As part of the 75th anniversary celebrations, planning is under way for an international conference for young scientists on Global Scientific Challenges to be held in Lindau, Germany, 4–6 April 2007.

**12.3.1. Regional offices.** In 2006, the Regional Office for Africa set up four important scoping groups on sustainable energy, health and human well-being, natural and human-induced hazards and disasters, and global change. These groups prepared draft science plans that were debated and approved by a broader scientific community at a Second Regional Consultative Forum in Boksburg, South Africa, 25–27 September 2006.

The ICSU Regional Office for Asia and the Pacific is located at the Academy of Sciences Malaysia. The inauguration took place 18–19 September 2006 in conjunction with a regional symposium on Natural and Human-Induced Hazards and Disasters. Professor Mohd Nordin Hasan has been appointed as Director.

The Regional Committee for Latin America and the Caribbean had its first meeting in Panama on 15 October. Professor José Antonio de la Peña from Mexico was elected Chair of the Regional Committee. The meeting was followed by the First ICSU Regional Meeting for Latin America and the Caribbean, hosted by the University of Panama and organized in collaboration with the UNESCO Regional Office for Science in Latin America and the Caribbean. Four initial priorities were identified: sustainable energy, biodiversity, hazards and natural disasters, and education in mathematics.

**12.3.2. Freedom and responsibility.** The new Committee on Freedom and Responsibility in the Conduct of Science (CFRS) held its first meeting in Paris in November. Several important issues were addressed, including challenges to the universality of science in the USA and the Middle East. The Committee also began to define its future *modus operandi* and priorities and, in doing so, emphasized the critical importance of linking with the ICSU Members, Interdisciplinary Bodies and other key international partners.

All Member organizations that are organizing international meetings are reminded of the ICSU guidelines and procedures to be followed to minimize any likely problems with visas. For meetings in the USA, in particular, it is advisable to register all meetings with the International Visitors Office at the US Academy of Sciences.

**12.3.3. Data and information.** The 12th meeting of the Committee on Scientific Planning and Review (CSPR) was held 1–2 September 2006 at the ICSU Secretariat. Terms of Reference for an *ad hoc* Strategic Committee on Information and Data were approved and Roberta Balstad was appointed as CSPR liaison for this Committee. The importance of the Global Information Commons for Science Initiative was noted and it was agreed that CODATA should be strongly encouraged to develop a strategic plan for this initiative. It was also decided to recommend that the Secretariat take steps to pursue the establishment of an Observatory on Science and Intellectual Property Rights issues.

**W. L. Duax**, IUCr Representative

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

The major event for CODATA during 2006 was the biennial conference and General Assembly held in Beijing, People's Republic of China, 22–27 October.

### *CODATA Conference*

The 20th International CODATA Conference had the title Scientific Data and Knowledge Within the Information Society, to emphasize CODATA's role within society as shaped by information technology, and its involvement over the past few years in the UN/ITU World Summit on the Information Society and related activities. Also running through the programme were a number of sessions in which CODATA continued to evaluate its own purpose, through a retrospective view of its first 40 years of existence, and a session looking to its future directions.

Presentations of interest to the IUCr were delivered in the Keynote sessions and lectures covering CODATA's history and future directions, e-Science and Cyberinfrastructure, and the Global Information Commons for Science Initiative; and in the meeting sessions on: Data archiving; Electronic journal production and metadata; Primary biological databases; e-Science; Data access policy, at which the IUCr representative gave a presentation on the impact of publishing policy on data quality.

A full meeting report is available at <http://www.iucr.org/iucr-top/data/docs/>.

### *General Assembly*

Consideration was given to the evolving draft of a CODATA Strategic Plan, arising from the ICSU Priority Area Assessment review on Scientific Data and Information discussed at the preceding General Assembly. The General Assembly passed resolutions confirming adoption of specific initiatives proposed in the draft [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]. Resolutions were also passed recommending an Associates Member programme (to encourage individual scientists and data professionals to become active long-term contributors to CODATA activities) and an Endowment and Gift Fund; and recommending various advisory committees to the Executive to assist in the development of the Strategic Plan.

The 2006 CODATA Prize for outstanding achievement in scientific and technical data was awarded to J. Rumble, Information Interna-

tional Associates (formerly Director of the Standard Reference Data Program at the National Institute of Standards and Technology). The citation stated 'Dr Rumble was honored for being an innovator in the world of scientific and technical data. He has been instrumental in extending data evaluation techniques in new disciplines, including engineering, materials, and biotechnology. Rumble has long been a leader in using advanced information technology for developing computerized databases, online data networks, and data exchange standards'.

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 25th General Assembly for 2006–2008 are as follows (those marked with an asterisk are continuations of existing Task Groups):

Access to Biological Collection Data;\*

Anthropometric Data and Engineering;\*

Comprehensive Information System on Natural Disaster Mitigation;

Data on Natural Gas Hydrates;\*

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

Data Sources in Asian–Oceanic Countries;\*

Exchangeable Materials Data Representation to Support Scientific Research and Education;

Fundamental Constants;\*

Global Species Data Networks;\*

International Polar Year Data Policy and Management Subcommittee;

Preservation and Archiving of Scientific and Technical Data in Developing Countries.\*

Ireland and Georgia were formally welcomed as National Members of CODATA. Germany and France became Associate National Members.

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; 2004–2008); Treasurer: J.-J. Royer (France; 2004–2008). Ordinary Members of the Executive Board are listed on the CODATA web site <http://www.codata.org>.

### *Other activities*

Important meetings during 2006 involving CODATA included: a CODATA Meeting at the Royal Irish Academy (12 April) focusing largely on the Global Information Commons for Science Initiative; a WEAR panel session at the International Ergonomics Association Congress (Maastricht, The Netherlands, 10–14 July); a EUCHEM conference on molten salts and ionic liquids (Hammamet, Tunisia, 16–22 September) and a UNESCO consultation meeting on WSIS action line C7 on e-Science (Beijing, People's Republic of China, 22 October).

The *Data Science Journal* is now disseminated from the J-Stage platform of the Japan Science and Technology Agency, with J. Rumble as Editor. During 2006 the journal published an article by I. D. Brown and B. McMahon on the Crystallographic Information File (DOI: 10.2481/dsj.5.174).

Agreement for a 10 year implementation plan for a Global Earth Observation System of Systems, known as GEOSS, was reached by member countries of the Group on Earth Observations (GEO) at the Third Observation Summit. CODATA and GEO organized a meeting in Beijing during October, focused specifically on Task DA-06-01: Furthering the practical application of the agreed GEOSS data sharing principles. CODATA is now taking the lead on furthering the application of these data sharing principles.

The IUCr CODATA Representative continues to work closely with the ICSTI Representative, J. R. Helliwell, on matters of common interest. Results of this collaboration during 2006 included: an article entitled *The Role of Quality in Providing Seamless Access to Information and Data in e-Science; the Experience Gained in Crystallography* (with P. R. Strickland) in *Information Services and Use*, [(2006), 26, pp. 45–55]; a formal response to the Global Information Commons for Science Initiative, submitted to the CODATA General Assembly; and consultations on the development of crystallographic data repositories.

**B. McMahon**, IUCr Representative

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

COSPAR's main objectives (to promote international level scientific research in space, with an emphasis on the exchange of results, information and opinions) did not change, but – as the Organization approaches its 50th anniversary in 2008 some become re-defined. More emphasis is now placed on international cooperation and 'cross-disciplinarity', including developing a scientific and ethical framework for major space research and exploration programmes. Developing world standards for the space environment and its protection requires creation of national and international organizations and specialist working groups.

COSPAR acts mainly as a body responsible for organizing biennial Scientific Assemblies, with strong contributions from most countries engaged in space research. These meetings allow the presentation of the latest scientific results, the exchange of knowledge and also the discussion of space research problems. Several decades of providing this service have brought recognition to the COSPAR Scientific Assembly as the premier forum for presenting the most important results in space research in all disciplines and as the focal point for truly international space science. In this regard, it should be observed that COSPAR has played a central role in the development of new space disciplines such as life sciences or fundamental physics, by facilitating the interaction between scientists in emergent space fields and senior space researchers.

The 36th COSPAR Scientific Assembly was held in Beijing, People's Republic of China, 16–23 July 2006.

The General Assembly provided a forum, open to all scientists, for the discussion of problems that may affect scientific space research. More than 2,000 scientists from around the world participated in this meeting (1,499 full participants, 399 students and 27 press representatives). A total of 228 full day sessions accommodated 80 scientific events.

The COSPAR Awards recognizing outstanding contribution to space science were accepted by A. Nishida (Japan) for his pioneering work in nearly every field of space physics and by E. Grun (Germany) for shaping the concept of dust astronomy. More information about the 2006 Assembly and its Programme can be found at <http://www.cosparhq.org/>.

The 37th COSPAR Assembly will be held in Montreal, Canada, 13–20 July, 2008.

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

### 13. Finances

Extracts from the full financial statements, namely the Income and Expenditure account, Balance Sheet and Summary of Fund Accounts, are given in Tables 2, 3 and 4, respectively. The full audited

accounts are available from the IUCr electronic archives (Reference ES0360). For comparison, the figures for 2005 are provided in italics. The accounts are presented in CHF.<sup>1</sup>

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 2006 have been translated into CHF in the balance sheet at the rate operative at that date. For the income and expenditure accounts, transactions have been translated into CHF by applying the rates appropriate to the individual dates of these transactions. As a consequence of the fluctuation in exchange rates, overall an apparent gain has arisen on the assets of the Union, in terms of CHF, amounting to CHF 11,790. The gain 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 2006. It should be noted that this overall gain in CHF is not a real gain of money, but rather a gain on paper resulting from the accounts being expressed in CHF.

Investments are noted in the balance sheet at their market value at 31 December 2006.

The balance sheet shows that the assets of the Union, including the gain of CHF 11,790 resulting from fluctuations in rates of exchange, have increased during the year, from CHF 4,710,914 to CHF 5,104,584. The movement in market value of the investments was CHF 406,310 in 2006 (CHF 235,005 in 2005).

A transfer of CHF 120,000 was made to the Publications and Journals Development Fund from the *Acta Crystallographica* Fund. A transfer of CHF 165,000 was made to the Research and Education Fund from the *Acta Crystallographica* Fund. A transfer of CHF 75,000 was made to the *Journal of Synchrotron Radiation* Fund from the *Acta Crystallographica* Fund. A transfer of CHF 50,000 was made to the *Newsletter* Fund from the *Journal of Applied Crystallography* Fund. A transfer of CHF 5,000 was made to the President's Fund from the *Journal of Applied Crystallography* Fund.

The following comments refer to figures in the full accounts.

The General Fund account shows a deficit of CHF 229,913, as compared with a deficit in 2005 of CHF 336,530. The administrative expenses were CHF 486,057 in 2006 as compared with CHF 501,140 in 2005. Of this amount, CHF 218,544 was charged to the publications of the Union.

The expenses of the Union Representatives on other bodies were CHF 8,829. The cost of the Finance Committee meetings held in 2006 was CHF 15,470, while the Executive Committee meeting cost CHF 49,717. The income from the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 19,030. The subscriptions from Adhering Bodies were CHF 153,000. Interest on bank accounts and investments credited to the General Fund was CHF 112,026.

The President's Fund, the Publication and Journals Development Fund, the Research and Education Fund and the Ewald Fund received interest, at a nominal rate of 2.5% per annum, on the balances in the funds.

The President's Fund therefore received interest of CHF 2,196. Grants totalling CHF 3,953 were paid from the fund in 2006.

The *Acta Crystallographica* account for 2006 shows a surplus of CHF 555,402 before the transfer of CHF 360,000 to the other fund

<sup>1</sup> Services for accessing these data are described at the back of the journal.

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**Table 2**  
Income and Expenditure Account for the year ended 31 December 2005.

	2006	Swiss Francs	2005
<b>Income</b>			
Membership subscriptions		153,000	153,000
Sales			
Journals, back numbers and single issues	4,226,721	3,850,828	
Books	112,602	387,435	
Open Access Grant	85,922	72,475	4,310,738
Investment income			
Income from investments	146,333	153,116	
Bank interest	18,263	14,942	
Profit on sale of investments	10,270	27,886	195,944
Other income			
Royalties and copyright fees	12,139	8,648	
Advertising income	238,659	240,022	248,670
<b>TOTAL INCOME</b>	<b>5,043,909</b>		<b>4,908,352</b>
<b>Expenditure</b>			
Journals			
Publication costs	960,362	878,389	
Editorial expenses	340,726	363,937	
Technical editing	1,528,058	1,507,842	
Subscription administration	59,946	54,303	2,804,471
Books			
Publication costs	29,733	37,316	
Editorial expenses	25,441	100,350	
Technical editing	273,038	142,682	280,348
Newsletter			
Publication costs	125,424	93,268	
Editorial expenses	132,427	123,573	216,841
President's Fund Grants and Young Scientists' support		150,185	113,172
General Assembly costs		3,892	76,189
Ewald Prize		–	40,110
Committee meetings and expenses		65,188	123,345
Publications and journals development			
General	636,639	586,402	
Electronic Publishing Committee/Section			
Editors meeting expenses	2,292	1,997	
STAR/CIF	37,350	40,375	
Promotion	174,884	173,082	801,856
Subscriptions paid		9,709	7,382
Visiting Professorship Programme		1,165	1,750
Administration expenses:			
General Secretary and Treasurer:			
Honorarium to Treasurer	10,216	11,377	
Audit and accountancy charges	84,971	72,169	
Legal and professional fees	16,741	14,549	
Travelling expenses	18,584	21,811	
Bank charges	2,307	2,423	122,329
Executive Secretary's office:			
Salaries and expenses	348,306	358,564	
Travel expenses of IUCr Representatives on other bodies	8,829	2,459	
Sponsorship of meetings	5,148	(17,282)	
President's secretary	–	6,780	
IUCr/FIZ agreement	(19,030)	(17,061)	
Bad debts	7,601	23,894	357,354
Depreciation		28,207	53,211
<b>TOTAL EXPENDITURE</b>	<b>5,068,339</b>		<b>4,998,358</b>

**Table 2 (continued)**

	2006	Swiss Francs	2005
<i>Deficit of income over expenditure</i>		(24,430)	(90,006)
Movement in market value of investments in year		<u>406,310</u>	<u>235,005</u>
Fluctuation in rates of exchange		381,880	144,999
Trading activities	(17,223)		12,659
Investment activities	<u>29,013</u>	11,790	<u>301,432</u>
Total recognized gains and losses relating to the year		393,670	459,090
Opening fund accounts at 1 January		<u>4,710,914</u>	<u>4,251,824</u>
Closing fund accounts at 31 December		<u>5,104,584</u>	<u>4,710,914</u>

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 Fund Account are not given, as the information is incorporated in the above.

**Table 3**

Balance sheet as at 31 December 2006.

	2006	Swiss Francs	2005
<b>FIXED ASSETS</b>			
Tangible fixed assets		<u>52,119</u>	<u>27,077</u>
<b>CURRENT ASSETS</b>			
Stock		270,364	350,917
Cash at bank and in hand			
Current accounts	15,437		50,213
Deposit and savings accounts	1,503,441		215,339
Cash with Union officials	<u>17,575</u>	1,536,453	<u>21,290</u>
Investments at market value		4,236,550	3,867,338
Debtors, accrued income and payments in advance		684,040	611,534
Subscriptions due from Adhering Bodies		<u>57,000</u>	<u>26,500</u>
<b>TOTAL CURRENT ASSETS</b>		6,784,407	5,143,131
<i>Creditors: amounts falling due within one year</i>		<u>(1,731,942)</u>	<u>(459,294)</u>
<b>NET CURRENT ASSETS</b>		<u>5,052,465</u>	<u>4,683,837</u>
<b>TOTAL FUNDS</b>		<u>5,104,584</u>	<u>4,710,914</u>

accounts, as compared with a surplus of CHF 402,141 in 2005 before the transfer of CHF 340,000 to the other fund accounts.

The subscription rates were increased for 2006. In 2006, the number of paid subscriptions to *Acta Crystallographica* were as follows: Section A 664 (685) including 57 (67) personal subscriptions (values for 2005 are given in parentheses); Section B 631 (664) including 31 (35) personal subscriptions; Section C 600 (626) including 34 (38) personal subscriptions; Section D 647 (671) including 97 (115) personal subscriptions. The cost of the technical editing office has been divided between the *Acta Crystallographica*, the *Journal of Applied Crystallography*, the *Journal of Synchrotron Radiation* and the *International Tables* accounts in percentages based on the staff time spent on each publication. The technical editing costs (comprising salaries and expenses, computer expenses and depreciation of office equipment) for *Acta Crystallographica* were

CHF 1,336,642 (for 15,830 published pages) as compared with CHF 1,243,677 in 2005 (12,986 published pages). The journal's accounts have also been charged with administration expenses as in previous years as shown in the General Fund.

The *Journal of Applied Crystallography* account shows a surplus of CHF 271,903, as compared with a surplus of CHF 144,262 in 2005. In 2006, the number of paid subscriptions, including 77 (86 in 2005) personal subscriptions, was 588 (608 in 2005).

The *Journal of Synchrotron Radiation* account shows a surplus of CHF 3,378, as compared with a deficit of CHF 81,791 in 2005. In 2006, the number of paid subscriptions, including 48 (59 in 2005) personal subscriptions, was 202 (213 in 2005).

The *International Tables* account shows a deficit of CHF 300,781, as compared with a surplus of CHF 28,025 in 2005. The net sales income was CHF 85,539 in 2006 as compared with CHF 287,893 in

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**Table 4**

Summary of Fund Accounts as at 31 December 2006.

	Swiss Francs						Balance at 31 December 2006
	As at 1 January 2006	Transfers between funds	(Deficit)/ excess of income over expenditure for the year	Increase in market value of investments	Fluctuations in exchange rates		
					Trading	Investments	
FUND ACCOUNTS							
General Fund	551,135	13,549	(229,913)	406,310	(2,488)	29,013	767,606
President's Fund	91,785	5,000	(1,757)	–	(322)	–	94,706
<i>Acta Crystallographica</i>	1,037,617	(360,000)	555,402	–	(4,133)	–	1,228,886
<i>Journal of Applied Crystallography</i>	447,926	(55,000)	271,903	–	(2,255)	–	662,574
<i>International Tables</i>	136,211	–	(300,781)	–	543	–	(164,027)
Book Fund	12,535	(13,549)	1,014	–	–	–	–
Publications and Journals Development Fund	832,350	120,000	(122,971)	–	(2,816)	–	826,563
Research and Education Fund	961,172	165,000	(131,104)	–	(3,375)	–	991,693
Ewald Fund	512,124	–	12,803	–	(1,780)	–	523,147
<i>Newsletter</i> Fund	135,451	50,000	(82,404)	–	(349)	–	102,698
<i>Journal of Synchrotron Radiation</i>	(7,392)	75,000	3,378	–	(248)	–	70,738
	<u>4,710,914</u>	<u>–</u>	<u>(24,430)</u>	<u>406,310</u>	<u>(17,223)</u>	<u>29,013</u>	<u>5,104,584</u>

2005. The significant difference is largely attributable to the fact that the income for 2006 includes an adjustment for sales for Volume G in 2005 (an internal transfer of 500 copies was wrongly attributed to sales in 2005).

The Book Fund is credited with the sales of the remaining publications of the Union. Because there is little activity in this Fund it has been closed and the balance of CHF 13,549 transferred to the General Fund.

The *Newsletter* Fund account received a transfer of CHF 50,000 from the *Journal of Applied Crystallography* Fund in 2006 (CHF 45,000 from the *Journal of Applied Crystallography* Fund in 2005). The cost to the Union of producing the *Newsletter* in 2006 was CHF 82,404 (CHF 28,273 in 2005).

As mentioned earlier, the income for the President's Fund account, the Publications and Journals Development Fund account, the Research and Education Fund account and the Ewald Fund account includes interest as well as transfers from

other fund accounts. In the Publications and Journals Development Fund account, the computing and promotion expenses are divided between the General Fund, the *Acta Crystallographica* Fund, the *Journal of Applied Crystallography* Fund, the *Journal of Synchrotron Radiation* 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 2006, CHF 62,430 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 143,272 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.