international union of crystallography

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Report of the Executive Committee for 2005

1. Twentieth General Assembly and International Congress of Crystallography

The Twentieth General Assembly and International Congress of Crystallography were held at the Fortezza da Basso Conference Centre, Florence, Italy, 23–31 August 2005, by invitation of the National Research Council and the Italian National Committee for Crystallography. A report, including a detailed report of the General Assembly, has been published [*Acta Cryst.* (2006), A**62**, 465–526].

The General Assembly and Congress were attended by about 2,800 scientists, 200 accompanying members and 52 exhibitors from 62 countries. The Seventh Ewald Medal and Prize were accepted by Professor P. Coppens at the Opening Ceremony. There were 36 Keynote Lectures, 98 Microsymposia and 8 Open Commission Meetings. The early afternoon sessions were reserved for poster sessions. The abstracts in the published book of Collected Abstracts were prepared from electronic submissions and were also provided on a CD-ROM. A commercial exhibition comprising 52 companies and booksellers was organized. Computer terminals and a designated area with wireless hotpoint were provided to enable e-mail access for all attendees.

The General Assembly met on the evenings of Wednesday 24 August, Thursday 25 August and Sunday 28 August. An application for membership from the Adhering Body for Greece (the Hellenic Crystallographic Association) in Category I was accepted. The withdrawals of the Adhering Bodies for Bulgaria and Ukraine were confirmed. The changes in the names of the Adhering Bodies for Brazil and Spain were accepted. Changes in Category of Adherence of the Adhering Bodies for Brazil (from Category III to Category I) and Russia (from Category IV to Category V) were accepted. The Minutes of the Nineteenth General Assembly in 2002 were approved. It received the triennial financial report and the reports of the Executive Committee, the Commissions, the Scientific Associates and Regional Associates and the Union Representatives on Other Bodies since the Nineteenth General Assembly in 2002. New officers of the Union, Chairs and members of Commissions and Union Representatives were elected; the full list of these people is given as an Annex to the report of the Twentieth General Assembly and Congress. The formation of a new Commission on Mathematical and Theoretical Crystallography was approved. Reports of the Chair of the Sub-committee on the Union calendar, of the Chair of the Committee on Electronic Publishing, Dissemination and Storage of Information, of the Chair of the Committee for the Maintenance of the CIF Standard, of the Chair of the Committee on Crystallographic Databases and of the Editor of the *IUCr Newsletter* were received. The good progress of the IUCr/Oxford University Press Book Series was noted. The General Assembly approved the recommendation that the unit contribution should remain unchanged at CHF 1,000 for the years 2006–2008 inclusive. It reaffirmed its decision to hold the Twenty-First General Assembly and Congress in Osaka, Japan, in 2008. It also provisionally accepted an invitation from the Spanish Committee for Crystallography on behalf of the Subdirección General de Programas y Organismos Internacionales, Ministerio Educación y Ciencia to hold the Twenty-Second General Assembly and Congress in Madrid, Spain, in 2011.

The Executive Committee met for several days before, and most days during, the Congress, mainly to deal with matters directly related to the business of the General Assembly and the work of the Commissions.

2. Other meetings

Other meetings held in 2005 and sponsored by the Union were:

International School on Crystal Growth: Fundamentals, Methods and Applications to Biological Nano Crystals, Puebla, Mexico, 7–11 March.

BCA/CCG 10th Intensive Course in X-ray Structure Analysis, Durham, UK, 4–11 April.

RapiData 2005, Brookhaven, USA, 10–15 April.

Evolving Methods for Macromolecular Crystallography, Erice, Italy, 19–29 May.

Nancy 2005 International School on Mathematical and Theoretical Crystallography, Nancy, France, 20–24 June.

XVIIth International School on Physics and Chemistry of Condensed Matter and Vth International Symposium on Physics in Material Science: Materials in Transition, Bialowieza, Poland, 21–29 June.

Crystallographic Computing School (Congress satellite), Siena, Italy, 18–23 August.

ElCryst2005 – new Frontiers in Electron Crystallography (Congress satellite), Brussels, Belgium, 2–8 September.

VII Latin-American Workshop on Magnetism, Magnetic Materials and their Applications, Refiaca, Chile, 11–15 December.

3. Executive Committee

The membership of the Executive Committee, including new members elected at the General Assembly in 2005, is as follows:

President: Professor Y. Ohashi (Japan); Vice-President: Professor I. Torriani (Brazil); General Secretary and Treasurer: Professor S. Lidin (Sweden); Immediate Past President: W. L. Duax (USA); Ordinary members: Professor P. M. Colman (Australia), Professor G. R. Desiraju (India), Professor C. J. Gilmore (UK), Professor G. Heger (Germany), Professor C. Lecomte (France), Professor D. Viterbo (Italy).

4. Publications

Volume 61 of *Acta Crystallographica*, Volume 38 of *Journal of Applied Crystallography*, Volume 12 of *Journal of Synchrotron Radiation*, a corrected reprint of the Fifth Edition of Volume A and the First Edition of Volume G of *International Tables for Crystallography* were published.

5. Adhering Bodies

A list of Adhering Bodies of the Union, with names and addresses of the Secretaries of the National Committees for Crystallography, was published as Annex IV to the Report of the Twentieth General Assembly and International Congress of Crystallography [*Acta Cryst.* (2006), A**62**, 465–526].

6. Work of the Commissions

6.1. Commission on Journals

6.1.1. Overview. Comparing 2005 with 2004, the increase in the number of published pages has continued. This increase has been largely driven by the expansion of Section. E and the launch of *Acta Cryst*. Section F: *Structural Biology and Crystallization Communications* in January 2005, as well as by an expanded number of pages for *Journal of Synchrotron Radiation* (*JSR*). The citation impact of IUCr journals continued to be high, occupying three of the top six ranking positions in crystallography. The overall withdrawal plus rejection rate for the journals was 25% in 2005 compared with 26% in 2004.

The first issue of Section F was published in January 2005, the major IUCr journals event of 2005. The new journal is edited by H. M. Einspahr and J. M. Guss, and publishes protein structure, structural genomics and crystallization communications. Section F had a successful first year with over 300 articles and 1,100 pages published. Extensive work has been done jointly with the Protein Data Bank by H. M. Einspahr concerning streamlined deposition-to-publication methodologies for Section F.

The Florence Congress proved to be one of the largest ever Congresses in terms of numbers of attendees. It also proved an outstanding opportunity for the Commission on Journals and for the promotion of the journals. A joint launch party for Section F and **International Tables Online** proved to be a very popular event with approximately 500 guests.

Before the Congress, the Journals Commission met in Montecatini Terme, Italy, and held a very intensive programme of discussions and various decisions were taken. Notable amongst these decisions was the policy to allow Co-editors to return manuscripts with language problems to authors before refereeing. This policy is intended to help the streamlining of handling of papers, particularly for Sections C and E.

At the IUCr General Assembly, J. R. Helliwell delivered his third and final report as Editor-in-Chief. He emphasized the general health and vitality of the journals, made possible by enthusiastic cohorts of editors and referees gladly serving the wider crystallographic community. He noted the apparent challenge from the open publishing drive of research funding agencies (*e.g.* those in the USA and UK) whose view was that publicly funded research should be freely available to the public. He also stressed his view that the IUCr's policies and pricing structures were open and transparent, as well as good value, and thus these would compete well in the new 'golden open access' era that these research agencies wished to see established, and which would now pay for such open access fees in research grant awards. Members of the General Assembly, he argued, should be very vigilant on this matter. The General Assembly confirmed the appointment of Gernot Kostorz as the next Editor-in-Chief of IUCr journals and Chair of the Commission on Journals.

J. R. Helliwell, Chair August 1996–August 2005
G. Kostorz, Chair August 2005 onwards

6.1.2. *Acta Crystallographica* Section A. Section A published 622 pages in 2005, down from 644 in 2004. In addition, the Abstracts of the Florence Congress comprise 498 pages. 5.2 issues were regular while 80% of the January issue, *i.e.* 121 pages, was a Special Issue on Phase Transitions edited by Guest Editor D. Pandey. The number of pages devoted to Research Papers and Short Communications also decreased from 619 to 531; without Special Issues, the decrease is from 459 to 410 pages. The average publication time for regular papers decreased from 6.2 to 5.1 months; the average review time was 3.3 months.

There were 55 full research papers, including 10 in the Special Issue, giving an average of 9.2 pages per article. This is somewhat more than in the past years (7.8 pages). These numbers include two Topical Reviews, on time-resolved X-ray diffraction by Coppens *et al.*, and on 'forbidden' resonant reflections by Dmitriev *et al.* There were 5 Short Communications. The portions of 19% of withdrawn and 19% of rejected manuscripts remain high and are slightly increasing. The numbers of submitted and of accepted papers in 2005 show an important decrease: Section A shrinks alarmingly. The report for 2006 will have to mention the thinnest issue ever. There is no backlog in the editorial offices. One of the reasons may be a trend to mathematically difficult papers for which *Foundations of Crystallography* certainly is the preferred platform, but which are outside the scope of many crystallographers. Topics such as aperiodic crystals or electron densities tend to move to Section B.

Section A is a high-level journal with a very diverse range of topics, including geometry, topology, twinning, growth models; anomalous scattering; perfect, distorted, faulted crystals in diverse environments; theories and methods of structure determination and the phase problem; electron diffraction, convergent-beam method, diffraction theory; phase transitions. Single-particle imaging has all but vanished. The geographical distribution of the origins of the articles (counted as integral or half-integral numbers) remains nearly unchanged with Europe 60%, the Americas 23% and Asia+Australia 17%. The Co-editors perform well, but the work is very unequally distributed: 46% of the submissions are handled by two Co-editors, a third Co-editor adds 10%. But even with few papers, some Co-editors face a considerable workload since many papers are difficult to handle.

In the pipeline for 2006 are two Special Issues, the second part of Phase Transitions, and the Proceedings of the 2005 MaThCryst Summer School in Nancy, France [this appeared in March 2006]. I have good hopes that at least one commissioned Lead Article will be submitted in 2006, but commissioning of Lead Articles remains difficult. In addition, there is a Special 60th Anniversary Issue planned for January 2008.

D. Schwarzenbach, Editor of Section A

6.1.3. *Acta Crystallographica* Section B. The 2005 statistics for Section B show that the number of articles has been essentially constant for three years (88, 87, 87 for 2003–2005). The number of pages, however, was down again in 2005 (821, 763, 730) because papers were slightly shorter. The average length of a full paper has

varied since 2002 between 8.5 and 10 pages; the average for articles published in 2005 was at the low end of that range.

There is no question that competition from *CrystEngComm* (started in 1999 by the Royal Society of Chemistry) and *Cryst. Growth Des.* (started in 2001 by the American Chemical Society) has been important. An analysis over five years shows that most of the decline in Section B pages is in the categories of metal-organic and organic papers, which are the categories most likely to be affected by the two competing journals. The inorganic category of papers remains strong. Section B is attracting a good share of the papers that report determinations of modulated and incommensurate structures, and activity in this area is expanding. The number of papers reporting diffraction from polycrystalline samples is also increasing.

Concern about the decreased number of Section B pages printed in 2005 is mitigated by the very significant increase in pages printed in the first two issues of 2006.

The impact factor continued to rise in 2005. An important factor in the very strong trend (values 2.0, 3.6, 5.4 announced in 2003–2005 for articles published in the previous year) is almost certainly a consequence of the 2002 Special Issue on databases. Since impact factors are calculated for articles published in the three most recent years the database issue of 2002 will not contribute to impact factors in the future.

The time to publication has been essentially steady since 2002 (5.4, 4.8, 5.8 months in 2003–2005). It seems unlikely that those times can be reduced significantly without putting undue pressure on referees and authors.

The decision was made in 2005 to limit the number of figures printed in colour to those for which colour was judged to be very important to the information content of the drawing. Figures can always appear in colour in the online version of the journal.

The Chester staff, and especially Jill Bradshaw, continues to do a wonderful job in arranging the components of the papers (text, figures, tables, schemes, and footnotes) to produce pages that are attractively balanced and papers that are easy for readers to follow. An additional constraint has been the attempt to reduce printing costs by placing colour figures so that the number of pages printed in colour is minimized. Mention must also be made of the significant help provided by the Chester office in making the English usage as standard as possible. This assistance is very much appreciated by all.

During 2005, Co-Editors P. G. Jones, L. R. Nassimbeni, and M. R. Taylor retired, each having completed three full terms of fine service to the journal. We welcomed to the Board new Co-Editors C. H. Görbitz, J. A. Kaduk, F. K. Larsen, L. B. McCusker, U. Rychlewska and M. A. Spackman.

C. P. Brock, Editor of Section B

6.1.4. 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. Publication times are now steady with the majority of technically correct and well written papers appearing on line (http://journals.iucr.org/c) within two months of submission. In 2005, Section C published 437 papers (41 inorganic, 134 metal-organic, 262 organic) in a total of 1,412 pages – an 18% decrease in papers over 2004. This decrease almost certainly arises from changes which were made to the 2005 Notes for Authors in an attempt to improve the quality of initial submissions. After review 58% of submissions to Section C in the past year were either subsequently withdrawn by the authors or rejected – a 9% increase over 2004. As noted in previous years, the principal reasons for this withdrawal/rejection rate were that either the text in the Comment section of the CIF was deemed not to provide the 'significant added value to the numerical data freely available in the CIF' as detailed in Notes for Authors or the text in the Comment section was very poorly crafted and difficult to understand.

I must also acknowledge and warmly thank J. R. Helliwell who retired as Editor-in-Chief for his support and advice over the last six years, and also F. R. Fronczek, W. C. Stallings and M. R. Taylor, 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

6.1.5. Acta Crystallographica Section D. The past year has been one of significant change for Section D, following the creation of its all-electronic sister journal, Section F. The first immediate consequence was that Crystallization Papers, which had begun to dominate Section D, in number if not in pages, would be moved to Section F. Since these generally receive few citations, it was expected that the impact factor of Section D would increase, leading to an ability to attract more high-profile structural papers. A second consequence was the need to develop clear roles and identities for these two journals, an issue which is still evolving.

With the removal of Crystallization Papers, which represented a significant part of its previous content (about 40% of pages in 2004), it was unclear to what extent Section D would diminish in size. In the event, the flow of Research Papers in both structural biology and crystallographic methods has increased by just over 20% (from 165 in 2004 to 200 in 2005). When added to 24 Short Communications, this increase in structural and methodological papers is a good sign for the future. Other contributions to the journal included a Topical Review on post-crystallization treatments for improving crystal quality by B. Heras and J. L. Martin and a historical essay by C. Abad-Zapatero. We are keen further to diversify the journal through such articles. Sadly, the journal also noted, with an affectionate obituary by N. Yathindra, the death of another pioneering crystallographer, M. Sundaralingam, who died, with his wife, in the Asian tsunami of December 2004.

Twelve issues of Section D were published in 2005, with a total number of pages of 1,681, a decrease from the 2004 number. Among these, the June issue was a Special Issue, covering the Proceedings of the 10th International Conference on the Crystallization of Biological Macromolecules, held in Beijing, People's Republic of China, in 2004. Guest Editors for this issue were J. D. Ng and M. Bartlam. Protein crystallization methods are enjoying a resurgence of activity, which is reflected in the wide range of articles. In a departure from previous years, a decision was made to delay publication of the Special Issue dedicated to the annual CCP4 study weekend until the first issue of 2006. Papers from these issues are highly cited, and publication in January each year will mean that the impact factor of the journal will benefit from their citation over the whole of that year.

One issue to arise in relation to Special Issues is that of refereeing. The standards of the journal require that articles submitted for Special Issues should be refereed. This can conflict with the expectation of authors who anticipate that their conference presentation will be published, as of right. We hold firmly to the view that all articles must be refereed, and will not be published if they do not meet the standards of peer review.

One clear trend that has emerged during 2005 is for many structural papers to be shorter, less discursive and with less descriptive

Table 1
Survey of the contents of IUCr journals.

Acta Crystallographica

Vol.	Year	Number of pages§		Number of papers		Full Articles† Number		Full Articles† Average length		Short Communications‡ Number		Short Communications‡ Average length	
A57	2001	803		103		78		8.9		25		5.6	
B57		877		110		100		8.6		10		1.6	
C57		1504	7162	545	1948	541	527	2.7	6.4	4	85	2.8	3.6
D57		1980		390		349		5.2		41		3.3	
E57		1998		800		795		2.5		5		1.7	
A58	2002	630		102		65		8.0		37		2.8	
B58		1088		132		115		8.9		17		1.1	
C58		1570	7905	535	2148	531	605	2.6	6.1	4	94	1.8	2.2
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	8735	482	2424	478	568	2.8	6.1	4	81	2.2	4.7
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	10183	556	3061	554	624	3.0	5.8	2	80	4.0	2.7
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		79		76		8.6		3		3.0	
C61		1412	12986	439	4023	437	640	3.2	6.0	2	66	4.0	4.1
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	

Journal of Applied Crystallography

Vol.	Year	Number of pages§	Number of papers	Full Articles†† Number	Full Articles†† Average length	Short Communications‡‡ Number	Short Communications‡‡ Average length	Short items§§ Number	Short items§§ Average length
34	2001	798	140	93	7.1	21	3.5	26	1.5
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

Journal of Synchrotron Radiation

Vol.	Year	Number of pages§	Number of papers	Full Articles Number	Full Articles Average length	Short Communications Number	Short Communications Average length	Short items§§ Number	Short items§§ Average length
7	2000	419	65	58	6.6	4	2.8	3	1.3
8	2001	1255	376	70	5.4	280	2.9	26	1.1
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

§ Numbered pages excluding contents pages. † 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. †† 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.

detail. This is a trend in all journals that publish structural biology papers, in part driven by space and cost considerations, but also by the increasing accessibility of structural information from resources such as the Protein Data Bank. In some cases, papers have been submitted that are effectively structure reports. Some are from structural genomics projects, but others are mutants, ligand complexes or new crystal forms which bring little new information and may be driven by pressures on authors to publish. The slightly

increased number of papers that were rejected (10%) or withdrawn (13%) in 2005 reflects this trend.

In this context, an important discussion took place between the Editors and Co-Editors of Sections D and F at the meeting of the Commission on Journals in Montecatini Terme, Italy, in August 2005. This related to the differentiation of the two journals, and led to a decision that structural papers published in Section D should contain 'new insights into chemistry, biology or structure'. This has been added to the Notes for Authors for 2006. Structural papers that do not meet these criteria are transferred to Section F for consideration, with the authors' agreement. This is a somewhat subjective judgement, and may sometimes be uneven in its application, but it should raise the profile of Section D. What is important for both journals is that we continue to insist on the publication of full experimental details so that results are validated and can be replicated.

All submissions to Section D are now electronic and the on-line system is working extremely well. For that, special thanks are due to the staff taking care of Section D at the Chester Office, especially Louise Jones, who also makes a remarkable contribution to the beautiful finished quality of the journal.

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

6.1.6. Acta Crystallographica Section E. The year 2005 has seen another sustained period of growth for Section E. The proportions of papers published in each category were: inorganic 3%, metal-organic 29%, organic 68%; there was a total of 2,996 papers, in 7,439 pages, compared with 4,676 pages in 2004. The average length of papers remained the same, at 2.6 pages. The average publication time remained the same at 0.8 month.

During the year, 342 papers were rejected and 256 withdrawn. This represents a total rejection and withdrawal rate of 16% of papers received. The distribution of papers by country of principal author saw increases for People's Republic of China and India, and decreases for the USA and Turkey.

The journal's impact factor has risen from 0.453 to 0.491.

For authors, the most important development has been the introduction of a new system for the submission, handling and tracking of papers. This new procedure, which was developed and tested in 2005 and made standard for 2006, is designed to be easier to use at all stages, for authors, for Co-editors, and for the Editorial Office staff. The submission of a new paper now involves uploading all relevant files in a single operation, the online selection of a Co-editor, and the author's declaration regarding copyright and ethical issues. Any CIF generating a level A alert will not pass the submission stage unless an author response to such alerts is included; this response is assessed by the Co-editor as part of the review process. Revisions to submitted papers are also made through the web interface, at the Co-editor's invitation, and the status of the paper can be checked at any time. The introduction of this new system has been a major development task for the Chester staff, and is a very welcome step forward in streamlining our operations.

The Notes for Authors have been extensively revised to take account of the various changes; they are available, together with much other important and useful material, in the Author Services section of the journal web site at http://journals.iucr.org/e/services/authorservices.html.

In order to apply some restraint to the journal's growth, there is now a limit of 400 words on the Comment section; papers longer than this, which must be justified in the submission process as a response to a level A alert, will be accepted only at the discretion of the Co-editors and Section Editors, and such exceptions are intended to be rare.

The task of reviewing and editing papers is undertaken by our team of expert Co-editors, whose time is valuable and must not be wasted on dealing with poorly prepared submissions. Papers which are difficult to understand, which fall well short of the requirements of the Notes for Authors, or which require extensive text correction and editing will be returned to the author for revision without a detailed review; it is the responsibility of authors, not of Co-editors, to generate an acceptable text for the Abstract, Comment and Experimental sections and to ensure that other CIF items are correct and complete. Co-editors and the Section Editors make moderate changes where required so that papers conform to the journal's standards and style. Authors can save the Co-editors considerable effort and time by checking their own papers before submission for errors, unacceptable and undesirable features; a list of common problems, which corresponds to guidelines provided to the Co-editors, is given in the Author checklist at http://journals.iucr.org/e/services/authorchecklist.html.

To cope with the increasing number of papers submitted to the journal we appointed a number of new Co-editors (in two batches) during 2005: M. Akkurt (Erciyes University, Turkey), L. Barbour (University of Stellenbosch, South Africa), S. Bernès (Universidad Autonoma de Puebla, Mexico), A. Bond (University of Southern Denmark, Odense, Denmark), I. Brito (Universidad de Antofagasto, Chile), M. Czugler (Hungarian Academy of Sciences, Budapest, Hungary), C. Esterhuysen (University of Stellenbosch, South Africa), J. Fabry (Academy of Sciences of the Czech Republic, Prague, Czech Republic), A. Fischer (Royal Institute of Technology, Stockholm, Sweden), M. Gdaniec (A. Mickiewicz University, Poznan, Poland), T. Hokelek (Hacettepe University, Turkey), Ning-Hai Hu (Chinese Academy of Sciences, Changchun, People's Republic of China), H. Kooijman (Utrecht University, The Netherlands), R. Rajaram (Madurai Kamaraj University, Madurai, India), M. da Silva (Universidade de Coimbra, Portugal), A. Slawin (University of St Andrew's, Scotland), Duan-Jun Xu (Zhejiang University, People's Republic of China), B. Yamin (Universiti Kebangsaan Malaysia, Malaysia). This brings the total number of Co-editors to 48, or 50 including the two Section Editors.

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 and Sean Conway who look after Section E on a daily basis.

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

6.1.7. Acta Crystallographica Section F. Section F: *Structural Biology and Crystallization Communications* was launched by the International Union of Crystallography with the January issue in 2005. This purely electronic journal for biological crystallography is now more than a year old, and its first year has been a good one; the 12 issues published included over 300 articles and 1,100 pages.

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 and, in its first year, the journal has worked very hard to ensure rapid publication. The result: average publication time from submission to publication including peer review was just 2.2 months. The journal has also been working during the year on a streamlined route from database deposition to publication. Volunteers are now testing a version of the RCSB program *PDB_EXTRACT* that has been adapted to harvest data identified as required or recommended

for publication by consensus of the editorial boards of Sections F and D.

In January we were gratified to learn that Section. F had been approved for inclusion in Medline. In February, the entire first volume was sent to the National Library of Medicine so that Section F will be accessible *via* PubMed from the first issue on and we have begun to hear from interested authors what we have learned ourselves, namely that attempts at PubMed access to Section F now meet with success.

In addition to indexing by Medline, the journal has been accredited by the Institute for Scientific Information, leading to inclusion of articles in the Science Citation Index. The journal is also covered by other major databases such as Chemical Abstracts, and, as part of **Crystallography Journals Online**, benefits from indexing by search engines such as Google and Scirus.

We are proud of the success of Section F in its first year of publication. It 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. To cope with the high flow of articles and the retirements of two of our founding Co-editors, A. Vrielink and A. Zagari, we have had to expand the Editorial Board. We now welcome T. Bergfors (Uppsala University, Sweden), J. García-Ruiz (University of Granada, Spain) and B. Hazes (University of Alberta, Canada) as new members.

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

6.1.8. Journal of Applied Crystallography. *JAC* published 1,045 pages in 2005 (1,049 in 2004). The number of full articles was 111 in 2005 (110 in 2004). Shorter items like Short Communications, Laboratory Notes, Letters to the Editor *etc*. remained at the same level (about 25) during the last three years. The number of manuscripts submitted was 196, compared with 226 in 2004 and 216 in 2003. The impact factor was 3.53 in 2005 (2.21 in 2004).

Efforts are continuing to make *JAC* an even more attractive medium for crystallography-based work in all fields, *e.g*. by appropriate pamphlets distributed at relevant conferences, or the choice of new Co-editors in promising fields. In 2005, S. Ciccariello, W. I. F. David, P. F. Fewster and K. A. Kantardjieff were appointed as Co-editors with this idea in mind, but also to maintain certain areas of competence as S. S. Hasnain, A. M. Moore, Å. Oskarsson, D. Pandey and H. Zimmermann finished their nine-year terms.

On-line submission is now almost exclusively used and works well. The publication time fell slightly to 6.4 months (4.3 months for editors/reviewers and 2.1 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

6.1.9. Journal of Synchrotron Radiation. For the 2005 calendar year, *JSR* published 121 articles and a total of 838 pages in the six issues. This was a sizable increase in the number of articles (>40%) and the number of pages (>60%) as compared with 2004. This is due in large part to six Special Issues that were published in 2005: BioXAS and Metallogenomics (I. Ascone, Guest Editor, January 2005), Applications of Synchrotron Radiation to Materials Research (G. Shenoy and P. James Viccaro, Guest Editors, March 2005), Radiation Damage in Macromolecules (E. Garman and C. Nave, Guest Editors, May 2005), Softer X-rays in Structural Studies (R. J. Cernik, J. R. Helliwell and M. Helliwell, Guest Editors, July 2005), Structure Determination by Single-Crystal X-ray Diffraction at Megabar Pressures (P. Dera, C. T. Prewitt and S. D. Jacobsen, Guest Editors, September 2005) and Synchrotron Radiation and Nanobioscience (E. Pechkova and C. Nicolini, Guest Editors, November 2005). We 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 continued in 2005. These pages provide an opportunity for these facilities to communicate important news and updates to the international community of synchrotron radiation users.

In 2005, the terms expired for several Co-editors including J. R. Helliwell, J. Kirz and J. Penner-Hahn. We would like to take this opportunity to express our thanks for their contributions to *JSR* and to welcome two new Co-editors, S. McSweeny and S. Wakatsuki.

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

6.2. Commission on International Tables

The main activities of the Commission centred around the Florence Congress, at which the Commission held both an Open and a Closed Meeting. The Open Meeting served as a platform for presenting the online version of *International Tables* to delegates. The full series of all eight volumes will be available online through Springer in 2007 as html and pdf. Users will be able to choose to view a chapter, a section or a subsection, or even just a single table or figure, and will be able to search through the full text of the series. Links are provided from each chapter to related chapters in the series and there are also links between each space group and its sub- and supergroups. **International Tables Online** has been designed to be quick and easy to use, so users will not need to know the printed volumes in great detail in order to find what they need online. In addition to all the information in the printed volumes, **International Tables Online** includes supplementary information, databases and programs. All Congress delegates were also invited to a wine and cheese party to celebrate the launch of **International Tables Online**.

The future of *International Tables* was discussed in the Closed Meeting. The most important question was the role of the printed volumes in the future. The Commission decided that printed volumes are still needed, but that **International Tables Online** may eventually become a new and distinct product. There were detailed discussions about the content of some of the volumes. The question of whether the extensive tables of form factors should still be part of Volume C was discussed, and the fact that some topics are covered in more than one volume was also considered.

6.2.1. Volume A. Space-Group Symmetry; Editor Th. Hahn. Corrected reprints of the Fifth Editions of both Volume A and the Brief Teaching Edition appeared in the summer of 2005. A brief report on the status of Volume A was presented during the Open Meeting of the Commission at the Florence Congress.

6.2.2. Volume A1. Symmetry Relations between Space Groups; Editors H. Wondratschek and U. Müller. Part 1 of Volume A1 deals with group-theoretical aspects of space groups, group–group relations and their underlying background. Part 2 contains listings of all maximal subgroups and Part 3 lists the relations between the Wyckoff positions.

6.2.3. Volume B. Reciprocal Space; Editor U. Shmueli. Significant progress was achieved with the preparation of the third edition of Volume B. Most major revisions, announced in the 2004 report, are in the hands of the Technical Editor in Chester, and it is expected that all the revised and new material to be incorporated in the third edition of Volume B will be submitted by October 2006. A detailed list of revised and new contributions, and their status, can be found at

the home page of the Commission at the URL: http://crystal.tau.ac.il/xtal/comit/index.html or at the IUCr home page. In brief, the topics more extensively treated are direct methods, Patterson techniques, convergent-beam electron diffraction, three-dimensional (image) reconstruction, single-particle reconstruction, molecular modelling, an extension of the Ewald method, and thermal and disorder diffuse scattering of X-rays and neutrons. Several minor revisions or corrections have also been submitted.

6.2.4. Volume C. Mathematical, Physical and Chemical Tables; Editor H. Fuess. The fourth edition is being planned and many chapters will be revised. The extensive tables on form factors are to be reduced and recent progress in methods will be taken into account.

6.2.5. Volume D. Physical Properties of Crystals; Editor A. Authier. Volume D is selling well, with about half the stock sold so far. It 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: *Ten*χ*ar* (calculations with tensors and characters) and GI$\star$KoBo-1 supporting Part 3 on structural phase transitions.

A number of minor errors and misprints have been found and Volume D going online is a good opportunity for correcting them. A number of chapters need updating and this will be done progressively. The updates of two chapters, 1.1 and 1.3, have already been sent to the Technical Editor, and more are in preparation.

One planned chapter did not materialize because its potential author failed to deliver his manuscript on time, that on the tensorial aspects of dielectric properties. 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; this should be done well in advance of the time of the eventual planned second edition.

6.2.6. Volume E. Subperiodic Groups; Editors V. Kopsky and D. B. Litvin. A list of corrections to Volume E was presented at the Open Commission meeting at the Florence Congress. Suggestions for additions and changes to the presentation of specific material in future editions of Volume E were discussed. These include: additional headings in multi-column tables, re-ordering sequences of symmetry operations and generators, including explanations of subperiodic group symbols used by other authors, and including the explicit tables of monoclinic/inclined scanning for groups of orthorhombic and higher symmetries [Litvin & Kopsky (2004). *Acta Cryst*. A**60**, 637] in the web-based and/or future edition of Volume E.

6.2.7. Volume F. Macromolecular Crystallography; Editors M. G. Rossmann and E. A. Arnold. Recent work on Volume F has been devoted to making the volume available online and to preparing a second edition of the volume.

6.2.8. Volume G. Definition and Exchange of Crystallographic Data; Editors B. McMahon and S. R. Hall. Volume G was published just in advance of its official launch at the Florence Congress. The volume and its accompanying CD-ROM provide a comprehensive survey of the Crystallographic Information File and related standards. The Editors are grateful to the authors and reviewers for their unstinting efforts, to COMCIFS for cooperation in updating and rationalizing many aspects of the CIF dictionaries in time for publication, and to the many software authors who contributed content to the CD-ROM.

H. Fuess, Chair

6.3. Commission on Aperiodic Crystals

The Commission has continued to be active in the promotion of aperiodic crystallography as well as in 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 2005, the triennial Congress of the IUCr was held in Florence and aperiodic crystallography was again strongly represented. Prior to the opening of the Conference itself, a full day preconference Workshop (WK04) on the Structural Analysis of Aperiodic Crystals was held. The workshop was organized under the auspices of the Commission by S. van Smaalen and R. Withers. During the Congress itself, two Keynote Lectures on Aperiodic Crystallography (Structure Analysis of Modulated Crystals: Trends and Tendencies by V. Petricek and Quasicrystal Structure Analysis: The State of the Art by A. Yamamoto) were presented in well attended sessions. In addition, three separate Microsymposia (MS19, News from Incommensurate Crystals; MS26, Recent Advances in Quasicrystal Research; and MS 83, Computational Solutions for Aperiodic Crystals) were also held and, again, were well supported.

In addition to the activities associated with the Florence Congress, a well attended Microsymposium on Crystal Chemistry and Complex Superstructures co-organized by S. van Smaalen was held during the German Crystallographic Association meeting held in Cologne, Germany, 28 February–4 March, 2005, while a Microsymposium on Disordered and Modulated Materials was held during Crystal 24, the 24th meeting of the Society of Crystallographers in Australia and New Zealand (SCANZ), held at Marysville near Melbourne, Australia, 29 March–1 April 2005.

The most important upcoming meeting for the Commission is Aperiodic 2006 to be held in Zao (near Sendai), Japan, 17–22 September 2006. The meeting is organized by A. Yamamoto (Chair), An Pang Tsai (Vice-Chair), Y. Gotoh, Y. Michiue, Y. Miyazaki and K. Saitoh and is shaping up to be a very exciting meeting. Other upcoming activities include the 5th Workshop on the Structural Analysis of Aperiodic Crystals organized by S. van Smaalen to be held in March 2007 at the University of Bayreuth in Germany. A meeting on Quasicrystals to be organized by R. Lifshitz is also planned for Israel in 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 (SIG) on aperiodic crystals of the European Crystallographic Association. It is maintained by M. Dusek (Prague, Czech Republic), and it can be found at http://www-xray.fzu.cz/sgip/aphome.html.

R. Withers, Chair

6.4. Commission on Biological Macromolecules

The Commission has continued to support the vitality of the biological crystallography community, particularly through recommending and supporting IUCr proposals to hold meetings, workshops and schools. Several meetings of this type will be held in Europe, Northern Africa and Southeast Asia in 2006.

A key event in 2005 was the Florence Congress. Structural biology was represented at all levels, with spectacular macromolecular structures and evolving methods described in plenary talks, invited presentations, topical sessions and posters. A large number of students from all corners of the world attended and participated and the travel costs of many young scientists were sponsored by the IUCr.

Regional meetings with biologically relevant content sponsored by the IUCr in 2005 included an International School on Crystal Growth (Puebla, Mexico) in March, the BCA/CCG 10th Intensive Course in X-ray Structure Analysis (Durham, UK), the RapiData course (Brookhaven, USA) in April, an Erice (Italy) School on Evolving Methods for Macromolecular Crystallography in May, and the Nancy 2005 International School on Mathematical and Theoretical Crystallography (Nancy, France). The Annual American Crystallographic Association (Orlando, USA) was also a central forum for the biological crystallography community. These meetings, schools and workshops provide tremendous value in training in and dissemination of novel scientific methods.

E. Arnold, Chair

6.5. Commission on Charge, Spin and Momentum Densities

The most important event of the Commission was at the time of the Florence Congress. A Keynote Lecture was given by M. Spackman, former Commission Chair, on the electrostatic properties that can be derived from high-resolution X-ray diffraction, where he nicely showed the successes but also the problems and pitfalls of the method. Four Microsymposia were also devoted to our field (MS34, MS49, MS63, MS89) as well as common sessions with computing crystallography and diffraction physics and time-resolved crystallography. As, at least for charge-density studies, the method begins to be easier to apply, a large audience attended these sessions.

The Commission met during the Congress and selected its nominations for new members; Professor Yu Wang, Taiwan, accepted to Chair the Committee and was elected. During the Commission meeting the next Sagamore meeting to be held in the UK in August 2006 was presented by M. J. Cooper, Chair, and discussed; the decision to include in the community research dealing with photo-excited-state crystallography (which was proposed by P. Coppens and C. Lecomte) was taken.

6.5.1. Sagamore Project: D. Jayatilaka. *Progress of the Constrained Experimental Wavefunction Project*. A number of groups were approached personally by D. Jayatilaka in January and February 2005 during his sabbatical stay at C. Lecomte's laboratory, to help them to initiate the project. A personal visit was found to be much more useful.

Essentially, the project consists of an application of the *Tonto* program to extract an experimental wavefunction, using the data of Birkedal *et al*. on urea crystals. Different groups will try to analyse the data on this system and the results will be collated. The second part of the project will involve various groups trying the program on their own data, with an understanding to publish the results within the year. This part of the project is proving very popular.

The groups which are actively using the program now are as follows:

Lecomte group (Nancy, France). Here there are two systems being studied with S. Pillet, a ligand 'btr' for a LIESST spin crossover system, and a more ambitious study with Jayatilaka involving joint refinement of X-ray and polarized neutron diffraction data. The former project has encountered problems because of slow evaluation of certain integrals, while the latter has encountered problems because of slow convergence and incorrect symmetry. Both problems are being slowly rectified.

Iversen group (Aarhus, Denmark) with P. Macchi (Milan, Italy). Here a study is being commenced on an oxalic acid/water co-crystal. Initial problems because of incorrect treatment of symmetry have been solved. The data were collected on a point detector by P. Macchi at Aarhus and are of excellent quality. No problems are anticipated and the group has agreed that a paper will be produced by August.

Howard group (Durham, UK). Here there are about 10 different systems that are able to be investigated! The data have been collected on a CCD and it appears there are large discrepancies between the wavefunction model and observed data. Although no problems were observed in fitting the data, such a situation is unacceptable and further investigations were pursued. A new merging program was written and it was observed that there were serious discrepancies between the standard deviations.

Spackman group (University of Western Australia). B. Dittrich will use the program to produce a constrained wavefunction for a small dipeptide. I have had no contact for several months on this project.

D. Jayatilaka (University of Western Australia). The study on urea has commenced, using the Birkedal data and theoretical data calculated from the *Crystal* program, in collaboration with the Torino group (B. Civallerri). The purpose of the study is to introduce controlled errors into theoretical data to see if the original electron densities can be recovered. These results will benchmark the method against refinements against the real data of Birkedal. This work should be complete by August.

Capelli and Bürgi (ESRF, France, and Berne, Switzerland). A study has commenced on a dipeptide system. Experimental data will be taken in March at the ESRF, including neutron data, and multi-temperature X-ray diffraction. The purpose will be to try and develop force constants and nuclear vibration wavefunctions from X-ray data. These studies will not be completed by the next report in August.

Kozisek group (Bratislava). A study has commenced on a transition-metal system, but there are unspecified problems concerning the quality of the data. A student, M. Hudak, will visit at the end of April to try to resolve the problems.

Other groups have indicated a desire to participate but the start has been delayed to try and resolve some annoying problems. The problems of solution convergence, generation of plotting images using *XDGraph* and parallelization (for speed) have been solved. The only remaining problem is the use of efficient numerical integration for DFT calculations. This is important for realistic results on transition metal systems.

C. Lecomte, Chair 2002–2005
Yu Wang, Chair 2005–

6.6. Commission on Crystal Growth and Characterization of Materials

In 2005, the responsibility for the Commission passed smoothly from R. Fornari to H. Dabkowska. It is appropriate here to thank Dr Fornari again for the many years of excellent direction he has given the Commission. In the future he will continue his work in the Commission, helping us all to develop and implement new ideas.

Following the Florence Congress, five more consultants were added, representing Brazil, Japan, Mexico, Poland and Russia. They replaced three consultants who have stepped down, from the Czech Republic, Sweden and Germany.

The Commission started its 2005 activities on a positive note, with an International School on Crystal Growth: Fundamentals, Methods and Applications to Biological and Nano Crystals [http://www.ifuap.buap.mx/ISCG05/school.html], which took place in Puebla de Los Angeles, Mexico, 7–11 March 2005. The main objective of this meeting was to provide basic crystal growth concepts along with an overview of growth technologies. There were about 45 participants, mostly from Mexico, but with significant representation from other

Latin-American countries. Sixteen lecturers from Canada, France, Germany, Mexico, Spain, Switzerland, Uruguay and the USA gave tutorial lectures on specific subjects, such as computer modelling of growth processes, epitaxy of semiconductors, bulk growth of oxides and semiconductors, organic materials for NLO, ferroelectrics, solution growth of biocrystals, and structural studies and defects in real crystals. Four members of our Commission were enrolled as lecturers at this school.

No more schools or conferences were proposed for 2005, as no sponsorship could be granted for events falling in the months preceding or following the Congress.

During the Florence Congress, eight members and observers met to discuss further activities.

The three symposia organized at the Congress directly by the members of the Commission (by Drs Vlieg, Garcia-Ruiz and Ohachi, respectively) were well received and well attended.

The Commission supported the application of Dr Garcia-Ruiz for IUCr sponsorship of the International School on Biological Crystallization (ISBC) (http://isbcgranada.org), which will be organized in 2006 in Granada, Spain. This school has a high profile and is very much needed in this area.

Another meeting supported by the IUCr, the International Workshop on Crystal Growth and Characterization of Advanced Materials, is planned to be held in 2006 in Chennai, India.

The application from the IOCG for support of the International Summer School on Crystal Growth in Salt Lake City, USA, in 2007 was also encouraged.

H. A. Dabkowska, Chair

6.7. Commission on Crystallographic Computing

A successful IUCr Crystallographic Computing School was organized at the Certosa di Pontignano, Siena, Tuscany, Italy, 18–23 August 2005, prior to the Florence Congress. The latter featured nine crystallographic computing related sessions and a Keynote Lecture. The former brought together a 'next generation' of young crystallographers interested in the development of crystallographic software with the 'current generation' of crystallographic software developers. Several of the last category are due to reach retirement age in the near future.

The course material can be downloaded from: http://www.iucr.org/iucr-top/comm/ccom/newsletters/2005sep/index.html. Details on the programme can be found at http://www.iucr.org/iucr-top/comm/ccom/siena2005/index.html.

The Commission brings out a Newsletter (edited by L. M. D. Cranswick). There were two issues in 2005; see http://www.iucr.org/iucr-top/comm/ccom/newsletters/index.html.

A. L. Spek, Chair

6.8. Commission on Crystallographic Nomenclature

The Commission met in closed session in Florence, on 28 August 2005. Its activities are pursued essentially through its working groups.

(1) Working Group on Phase Identifiers [I. D. Brown (Chair), S. C. Abrahams, M. Berndt, J. Faber, V. Karen, W. D. S. Motherwell, J.-C. Toledano, P. Villars, J. Westbrook, B. McMahon (consultant)]: its work has now been completed and its report was adopted in May 2005 and published in *Acta Cryst*. (2005). A**61**, 575–580.

(2) Working Group on Synchrotron Radiation Nomenclature [D. M. Mills (Chair), Å. Kvick, T. Ohta, I. A. Robinson, A. Authier]: its report on brilliance/brightness was adopted in February 2005 and published in *J. Synchrotron Rad*. (2005), **12**, 385. A discussion on the usage of the word 'emittance' concluded that the present acceptance of the word within the synchrotron-radiation community, for which the best beam is the one with the smallest emittance, is so well established that it cannot be changed, although in visible optics emittance is, on the contrary, considered as a measure of the flux of electromagnetic radiation emitted by an area of the source, the best source having an emittance as large as possible.

(3) Working Group on the Online Dictionary of Crystallography [A. Authier (Chair), I. D. Brown, W. Clegg, J. R. Helliwell, B. McMahon, P. Spadon]: following a suggestion by A. Authier about the need for a dictionary of crystallographic terms and the encouragement of the Executive Committee to pursue this idea, a working group was designated to implement a pilot project. This pilot project, which has been set up thanks to the unceasing efforts of the Research & Development Officer, B. McMahon, is based on the principle of Wikipedia and uses *Mediawiki* software. It can be seen at the web page http://reference.iucr.org/dictionary/Main_Page.

The details of the project and the report of the working group are given at http://reference.iucr.org/dictionary/Report_of_Working_Group.

The members of the Finance Committee, which met at the end of March 2006, were enthusiastic about progress so far, and are happy that the project should continue along the lines indicated in the report.

A. Authier, Chair

6.9. Commission on Crystallographic Teaching

Commission members present at the Florence Congress met three times to plan future activity. The general demand for basic crystallographic courses because basic crystallographic curricula are regressing in the academic bachelors and masters field, was widely discussed and led to the decision to organize an International School on Basic Crystallography. The aim of the Commission is to fill this gap by organizing an intensive one week course, possibly on a periodic basis. The organization of the school was decided to be close to the successful model adopted by the British Crystallographic Association (BCA), which has acquired an excellent popularity since its formation. In addition the Commission would like to set a minimum standard on the teaching schools it supports, in terms of concentrating on the fundamentals that are no longer being taught in most universities; the Commission wishes to see this done in a quality manner.

The result of this decision was the proposal for a Basic Crystallographic School to be held in August 2006 in Pontignano, near Siena, Italy, with G. Chapuis (coordinator, EPFL, Lausanne, Switzerland, gervais.chapuis@epfl.ch), A. J. Blake (Nottingham, UK), A. Gavezzotti (Milan, Italy) and R. Neder (Wuerzburg, Germany) as Programme Committee and M. Mellini (University of Siena, mellini@unisi.it), P. Spadon (University of Padova, paola.spadon@unipd.it) as Local Organizers. The following scientists agreed to act as lecturers in the school: P. Main (York, UK), D. J. Watkin (Oxford, UK), R. O. Gould (Edinburgh, UK), J. Cole (Cambridge, UK), A. J. Blake (Nottingham, UK), G. Chapuis (EPFL, Switzerland), G. Ferraris (Torino, Italy), G. Cruciani (Ferrara, Italy) and C. Giacovazzo (Bari, Italy).

In addition, the Commission decided to collaborate in the organization of a school in Cuba with the Commission on Mathematical and Theoretical Crystallography chaired by M. Nespolo. This school is planned for Janaury 2007 [subsequently postponed to July 2007].

The Commission also agreed on the need to reformat and update its web site and edit an online Commission Newsletter that tentatively could be a regular 12 monthly Newsletter; L. M. D. Cranswick volunteered to coordinate this work.

G. Chapuis and P. Spadon are also involved in the organization of MS45: Communicating and Educating Crystallography, planned for ECM-23 in Leuven, August 2006.

P. Spadon, Chair

6.10. Commission on Electron Diffraction

The year 2005 was significant for the relatively large number of sessions and workshops with a significant electron crystallography session. The Florence Congress had two, one on Electron Crystallography of Organic Crystals and Biomolecules organized by H. Hebert and U. Kolb, the other on Electron Crystallography of Inorganic Crystals organized by J. Jansen and V. Kletschkovskaia. Immediately following the Congress, a satellite conference, ElCryst2005 – New Frontiers in Electron Crystallography, was held in Brussels, Belgium, 2–8 September 2005, for which the web site is http://www.gfe.rwth-aachen.de/sig-ec/ElCryst2005/ElCryst2005.htm. This was attended by about 70 students and teachers, and had a strong focus on new developments in the area of precession electron diffraction. Lecture notes for the presentations are available for download, and a Special Issue of *Ultramicroscopy* focusing on electron crystallography and precession electron diffraction edited by T. Weirich and S. Nicolopoulos will appear in 2006.

There was also a significant session at the American Crystallographic Association meeting in Florida, with two sessions on Electron Nanocrystallography organized by J.-M. Zuo and L. D. Marks, one with a focus on Techniques and Time-Resolved Diffraction, the other on Applications to Materials Science. The area of time-resolved electron diffraction is continuing to make rapid advances.

In addition to the major sessions at the IUCr and ACA meetings, there was also significant discussion of aspects of electron crystallography at the Microscopy Society of America meeting in Hawaii, the Midwest Conference on Electron Microscopy at the University of Illinois and the International Workshop on Phase Retrieval and Coherent Scattering in Porquerolles among others.

Looking towards the future, the Commission is interested in expanding its activities. The membership of the Commission has been increased with the inclusion of new consultants to provide additional expertise in both established areas such as surface electron crystallography, as well as newly developing areas such as ultrafast electron diffraction. The web site for the Commission has also been redesigned, and additional links including a general electron crystallography software search interface are in the process of being constructed.

The Commission is also active in trying to increase the number of workshops/schools on electron crystallography beyond the traditional ones in the developed nations. Three workshop are planned in 2006, one in Munich Gauting, Germany, in May (http://www.tvips.com/Workshop.html), a second in Antwerp, Belgium (http://www.emat.ua.ac.be/XEl2006/XElhome.htm) as a satellite of the European Crystallography Meeting, and the last is planned to occur in Bangalore, India [subsequently cancelled]. Three workshops/schools are currently in the planning stages for 2007, in Hong Kong, Moscow and Oxford, and a session on electron crystallography at the 2007 meeting of the American Crystallographic Association.

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

L. D. Marks, Chair

6.11. Commission on High Pressure

Combining high pressure with crystallography remains a very challenging and growing field with a large variety of technical developments and scientific applications. The stated goal of the Commission is to facilitate the exchange of new ideas, development and know-how. The main way this is achieved is through special workshops in each of the two years between the triennial IUCr Congresses. In the years of the triennial Congress and General Assembly, the Commission tries to integrate this workshop into the Congress by organizing Microsymposia specifically targeted to high-pressure crystallography.

Therefore, the Commission organized six Microsymposia within the Florence Congress. The topics covered were: biological and organic soft condensed material under pressure; computational crystallography applied to extreme conditions; novel materials under high pressure; structural phase transitions and properties at high pressure; crystallography at conditions of earth and planetary interiors; and liquids and amorphous systems at high pressure. In addition, Commission members J. S. Loveday and I. Goncharenko organized two Open Commission Meetings on the topics 'Technical Development in High-Pressure Crystallography' on the one hand and 'Advances in High-Pressure Single-Crystal Diffraction' on the other. Both, Microsymposia and Open Commission Meetings (OCMs) were very well received with attendances between 60 (OCMs) and 100 (Microsymposia).

The Commission was also happy to see two of the Keynote Lectures given by high-pressure scientists, namely J. Tse (Canadian Light Source, Commission member) and M. McMahon (University of Edinburgh, UK).

The Florence Congress was also used for a closed Commission meeting. The most important topic of this meeting was a major reshuffling of Commission members. Four very active members (J. B. Parise, R. J. Hemley, W. F. Kuhs, I. N. Goncharenko) reached the limit of their terms and were replaced by V. Soloshenko, S. A. T. Redfern, A. Katrusiak and G. Galli. When replacing the departing members, the Commission tried to take into consideration geographical and gender balance, as well as scientific expertise. It is the stated goal of the Commission to cover the whole breadth of high-pressure crystallography. This is also the reason that the Commission insists on its rather unusually large number of members. As well as the new members, four new consultants have been appointed: R. Angel, P. Dera, G. Shen and I. N. Goncharenko. They were selected in view of their specific expertise (Shen, Angel), and/or active role in organizing future workshops (Dera, Goncharenko).

Further topics discussed were the Commission's involvement in establishing a high-pressure specific CIF code (Angel, Katrusiak) as well as upcoming workshops and summer schools. In 2006, the Commission is planning for a workshop hosted in Dubna, Russia. A. Balagurov is the head of the local organizing committee; Commission consultant I. N. Goncharenko will be the link to the Commission.

In 2007, another workshop is planned, this time at the new UK synchrotron source Diamond. Commission member J. S. Loveday will be the Commission link to the local organizers. For the Osaka Congress in 2008, Commission member N. Hamaya is proposed to act as member of the Programme Committee representing this

Commission. In 2009, Commission consultant P. Dera is organizing a summer school on high-pressure crystallography in Erice, Italy. 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 on information with respect to software, future and past meetings, central facilities, scientists and publications in the high-pressure field. The home page can be accessed *via* http://www.iucr.org/iucr-top/comm/chp/index.html.

M. Kunz, Chair

6.12. Commission on Inorganic and Mineral Structures

The contacts among the members and consultants of CIMS have been maintained mainly *via* e-mail and the web site http://www.lcm3b.uhp-nancy.fr/cims/ administered by consultant M. Nespolo. Most of the members who served the Commission in the triennium 2002–2005 and/or are serving for the triennium 2005–2008 attended the Florence Congress, so there it was possible to meet and discuss the activity and programmes of CIMS live.

The main activity of CIMS in 2005 has been the organization of the following events proposed by the Commission at the Congress (members of CIMS who acted as Conveners are indicated in parentheses): OCM05 – Open Commission Meeting of CIMS (G. Ferraris); MS7 – Crystal Chemistry of Inorganic and Mineral Compounds (W. Depmeier); MS35 – Polytypism and Twinning (G. Ferraris); MS79 – Inorganic and Mineral Structures Solved and Refined by Powder Diffraction Data (J. Rius); MS14 – Modularity and Modulation in Inorganic and Mineral Structures; MS28 – Structure/Properties Relationships of Technologically Relevant Inorganic and Mineral Compounds (J. Rocha); Keynote Lecture: L. B. McCusker. Unfortunately, a second Keynote Lecturer, T. White, could not attend the meeting.

In general, an increase in the number of participants, Microsymposia and contributions in the field of inorganic and mineral structure, in comparison with previous IUCr Congresses, has been noted in Florence. The following oral contributions were presented by members of CIMS at the shown Microsymposia/OCM: G. Ferraris: MS14; D. Yu. Pushcharovsky: OCM05; I. D. Brown: OCM05; M. Matsui: OCM05; M. Nespolo: MS35; D. Pandey: MS05; J. Rocha: MS18.

Following the meeting Micro- and Mesoporous Mineral Phases (Rome, Italy, 6–7 December 2004) organized by CIMS, the twelve invited lectures have been published as Volume 57 of the series *Reviews in Mineralogy and Geochemistry* of the Mineralogical Society of America (same title as the meeting; editors: G. Ferraris and S. Merlino; CIMS contributors: L. B. McCusker, W. Depmeier, G. Ferraris and J. Rocha). A further ten contributions have been published in a dedicated issue of the *European Journal of Mineralogy* (issue 2005/6).

CIMS co-sponsored the International School on Mathematical and Theoretical Crystallography organized by M. Nespolo (Nancy, France, 20–24 June 2005). The school was attended by 61 participants from 20 countries of 4 continents. A Special Issue of *Acta Crystallographica* Section A (issue 2006/2), Guest Editor M. Nespolo, containing articles contributed by lecturers and participants to the Nancy school has been published.

The ECM-22 satellite meeting Crystallography at the Start of the 21st Century: Mathematical and Symmetry Aspects (Budapest, Hungary 24–26 August 2004) was organized by M. Nespolo and supported by CIMS. A Special Issue of *Zeitschrift für Kristallographie* (issue 2006/1) containing articles contributed by lecturers and participants of the satellite has been published.

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

G. Ferraris is member of the Programme Committee and convener of the 19th Meeting of the International Mineralogical Association (IMA) (Kobe, Japan, 23–28 July 2006); Vice-Chair of the Commission on New Minerals and Mineral Names (CNMMN) of IMA; member of the Organizing and Programme Committees of the satellite meeting of the Asian Crystallographic Association (AsCA): Theoretical Crystallography and Materials (Tsukuba, Japan, 18–19 November 2006).

D. Pushcharovsky represented CIMS on the Programme Committee of the Florence Congress.

W. Depmeier has been co-organizer of the meeting Mineralogical Museums (St Petersburg, Russia, 14–17 June 2005); a volume with the same title was edited by V. G. Krivovichev and W. Depmeier (St Petersburg, 2005). He is Chair of the ECA Special Interest Group SIG5 Mineralogical Crystallography and member of the Programme Committee for ECM-23 (Leuven, Belgium, 6–11 August 2006).

M. Jansen co-organized an international workshop on *in situ* powder diffraction (Stuttgart, October 2005). The workshop manual and some impressions are available at http://www.fkf.mpg.de/xray.

M. Matsui is Chair of the Meeting Secretariat for IMA-2006 (Kobe, Japan, 23–28 July 2006) and principal Convener of the Scientific Session Computational Study of Mineral Structures and Properties at the same meeting; he is Editor of *Physics and Chemistry of Minerals*; he was an invited speaker at the 15th Annual Goldschmidt Conference (Moscow, Idaho, USA, 20–25 May 2005).

L. B. McCusker besides the Keynote Lecture at the Florence Congress delivered invited lectures at Jilin University (People's Republic of China) and Kiel University (Germany). She is a member of the Organizing/Programme Committees for ZMPC2006 (Yonago, Tottori, Japan, 2006), EPDIC-10 (Geneva, Switzerland, 2006) and the 15th IZC (Beijing, People's Republic of China, 2007). She co-maintains the IZA web sites http://www.iza-online.org/ and http://www.iza-structure.org/ (database of zeolite structures).

M. Nespolo is Chair of the Commission on Mathematical and Theoretical Crystallography, Associate Editor of the *European Journal of Mineralogy*, and Secretary of the Special Interest Group SIG5 Mineralogical Crystallography of the ECA. He is Chair of the Organizing and Programme Committees of the Satellite Meetings of the European Crystallographic Association (ECM-23): Mathematical and Theoretical Crystallography (Leuven, Belgium, 4–6 August 2006), and of the Asian Crystallographic Association (AsCA): Theoretical Crystallography and Materials (Tsukuba, Japan, 18–19 November 2006), Chair of the MS19 Phase Transitions in Inorganic and Mineralogical Materials at ECM-23 (Leuven, Belgium, 6–11 August 2006), and co-Convener of the MS8 Crystal Structure, Topology and Crystal Chemistry at IMA-2006 (Kobe, Japan, 23–28 July 2006).

J. Rius was Chair of the Special Interest Group SIG8 of the ECA and Associate Editor of the *European Journal of Mineralogy*.

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

G. Ferraris, Chair

6.13. Commission on Mathematical and Theroetical Crystallography

The Commission (MaThCryst) was formally approved by the IUCr General Assembly at the Florence Congress. However, as the informal MaThCryst working group had already been active prior to its official IUCr inception, activities for the whole of 2005 are reported.

A Special Issue of *Z. Kristallogr.* (issue 2006/1, published in November 2005), Guest Editor H. Grimmer, containing articles contributed by lecturers and participants of the satellite meeting Crystallography at the Start of the 21st Century: Mathematical and Symmetry Aspects held in conjunction with ECM-22, Budapest, Hungary, 24–26 August 2004 (see http://www.extenza-eps.com/OLD/toc/zkri/221/1_2006;jsessionid=oKNiA6GZLBTaH5H3pN).

An International Summer School on Mathematical and Theoretical Crystallography, Nancy, France, 20–24 June 2005, attended by 61 participants from 22 countries (see http://www.lcm3b.uhp-nancy.fr/mathcryst/nancy2005.htm).

A Special Issue of *Acta Crystallographica* Section A (issue 2006/2), Guest Editor M. Nespolo, containing articles contributed by lecturers and participants to the Nancy school (see http://journals.iucr.org/a/issues/2006/02/00/issconts.html).

A web site (http://www.lcm3b.uhp-nancy.fr/mathcryst/) with several didactic pages (either directly hosted on our server or linked from external resources related to MaThCryst).

A book entitled *Graph Theory in Crystallography and Crystal Chemistry* (authors J. Rutherford, J.-G. Eon and W. Klee) is under consideration by Oxford University Press for inclusion in the IUCr/OUP series Monographs on Crystallography. Currently, the referees' reports have been received and the proposed plan for the book has received positive reviews.

Our future activities will be divided into three types: (1) satellite conferences on the occasion of large crystallographic meetings, to be held essentially in the form of workshops; (2) general schools, to give an introduction to basic or advanced topics in mathematical and theoretical crystallography; (3) thematic schools, where we plan to analyze some specific topics from the introductory steps to the working practice.

Our planned activities to be held in 2006 and in the following years are listed below.

A satellite meeting of ECM-23, Leuven, Belgium, 4–6 August 2006 (see http://www.lcm3b.uhp-nancy.fr/mathcryst/leuven2006.htm), in cooperation with the Commission on Inorganic and Mineral Structures;

A satellite meeting Theoretical Crystallography and Materials Science, on the occasion of the Asian Crystallographic Association meeting (AsCA '06, Tsukuba, Japan, 18–19 November 2006 (see http://www.lcm3b.uhp-nancy.fr/mathcryst/asca2006.htm) in cooperation with the Commission on Inorganic and Mineral Structures;

A winter school in Havana, Cuba, 14–19 January 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;

A satellite meeting of ECM-24, Marrakech, Morocco, 20–22 August 2007 (see http://www.lcm3b.uhp-nancy.fr/mathcryst/marrakech2007.htm);

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

We also plan two thematic schools, whose details have yet to be fixed:

a thematic school on graph theory, to be held after the publication of the above-mentioned monograph with the authors of the monograph as lecturers;

a thematic school on irreducible representations of space groups, with main lecturers M. I. Aroyo and B. Souvignier.

M. Nespolo, Chair

6.14. Commission on Neutron Scattering

An important event for the neutron scattering community in 2005 was the International Conference on Neutron Scattering (ICNS), held in Sydney, Australia, 27 November – 2 December. The conference served as an international forum for scientists using neutrons and instrumentation specialists in order to present and discuss new developments in the fields of physics, chemistry, biology, materials science and industry. The topics covered the whole field of neutron scattering and included Condensed Matter Physics, Condensed Matter Chemistry, Structure and Dynamics, Magnetism, Materials Science, Soft Condensed Matter, Life and Biological Sciences, Industrial and Medical Applications, Earth Sciences, Advanced Neutron Sources and Neutron Instrumentation and Techniques.

At a special session of the ICNS the prestigious Walter Hälg Prize was awarded to A. Furrer (ETH Zürich and Paul-Scherrer-Institute) and H. U. Güdel (University of Bern). The Prize is awarded biennially by the European Neutron Scattering Association (ENSA) to European scientists for outstanding, coherent work in neutron scattering with long-term impact on scientific and/or technical neutron scattering applications.

A particular highlight during the ICNS was the tour to the nearly completed ANSTO reactor OPAL. Many of the ICNS attendees took the opportunity to visit this new 20 MW research reactor which will be fully operational in 2006. It will feature a large state-of-the-art cold neutron source, supermirror guides and a large guide hall with support laboratories. OPAL will initially have eight neutron scattering instruments.

During the ICNS, the Commission held a meeting where most of the new members had the opportunity to introduce themselves. Additionally, tasks of the Commission were discussed and arranged.

In 2005, as existing neutron sources showed smooth operations, the neutron scattering community had a sufficient and broad neutron supply at its disposal.

The new reactor FRM-II in Munich (Germany) has been fully operational since spring 2005. The first evaluation of instruments took place in February 2006. At the research reactor BER-II, operated by Hahn-Meitner-Institut Berlin (Germany), a new second Neutron Guide Hall was completed in January 2005. In the coming years, new advanced instruments will be installed in this hall in order to comply with the users' needs. The operation of the reactor FRG-1 in Geesthacht (Germany) is secured until the end of 2009.

At ISIS, the world's leading spallation neutron source at the Rutherford Appleton Laboratory (UK), the construction of a second target station which began in July 2003 is ongoing and first neutron production is scheduled for June 2007. The construction of the frame of the experimental hall building was finished in the middle of June 2005. This is a significant step in the improvement of the neutron source at ISIS. In October 2005, a meeting of the Scientific Advisory Committee was organized to identify further areas of instrumentation to be developed. The experimental programme will begin in October 2008. Seven state-of-the-art neutron instruments will then be available to users. With the new target station, the ISIS science

programme will be able to expand into the research areas of soft matter, advanced materials and bio-science.

The ILL in Grenoble (France), the most powerful neutron source, in 2000 launched the so-called Millennium Programme, a modernization programme, with the aim to renew the instrumentation. More than 10 Millennium projects have already been successfully completed for the users' benefit. Additionally, a refit programme with the aim of increasing the safety of the reactor is running until 2006.

The discussions concerning the ESS project (European Spallation Source) are still ongoing. In April 2005, an initiative for the European Spallation source, ESS-I, was created. The aims of this initiative are, amongst others, to act as a contact for the decision makers and to stimulate the technical development in fields such as accelerator and target technology. The community hopes that a positive decision will be taken in a couple of years.

At J-PARC, the Japan Proton Accelerator Research Complex, the commissioning of the equipment was started in the linac and the 3 GeV synchrotron building. Two parts of the accelerator tunnel have been completed and the equipment is now being installed. The test of the first stage of the J-PARC accelerators has been completed. Parallel to this development, the JAERI reactor JRR-3 is running smoothly and serving a very lively community.

The new accelerator-based Spallation Neutron Source SNS, which is being built at Oak Ridge National Laboratory (USA), will provide up to ten times more intensity than any other such source in the world. The construction of conventional facilities was completed in 2004. One important step was the commissioning of the cold linac in August 2005. In January 2005, the commissioning of the warm linac was completed. This is the world's first high-energy and high-power linac that applies superconducting technology. The equipment installation and the commissioning will be completed in 2006.

As the SNS project is close to the first delivery of neutrons, the community is looking forward to this exciting event in early 2006.

M. Steiner, Chair

6.15. Commission on Powder Diffraction

6.15.1. Newsletters. Two issues of the CPD *Newsletter* were produced in 2005. Issue No. 30 entitled Powder Diffraction on Mars, the Red Planet was edited by R. Delhez. True to its title, the *Newsletter* did focus on the challenges of performing X-ray diffraction on Mars as part of a series of rock and soil analysis measurements planned for 2011. The issue also highlighted the importance of powder diffraction in the area of pharmaceutical science with practical discussions of how to measure real systems such as off-the-shelf pharmaceuticals. Issue No. 32 focused on 2D Powder Diffraction and was produced and edited by the outgoing chair of the Commission, R. E. Dinnebier. Two-dimensional detectors are finding increasing use in the area of powder diffraction and can offer significantly higher count-rate capabilities over conventional detectors. *In situ* diffraction measurements can be rapidly performed to allow kinetic and parametric measurements to be undertaken. The massive data volumes that are produced present significant data analysis and visualization challenges. The CPD-sponsored workshop Watching the Action: Powder Diffraction at Non-Ambient Conditions addressed many of these challenges; this workshop was run by R. E. Dinnebier and held in Stuttgart, Germany, 6–7 October 2005. Although these *Newsletters* are available in both hard-copy and electronic format, the CPD has taken the decision that future *Newsletters* will only be available electronically from the CPD web site. Again the popularity of the computer software pages in the CPD *Newsletter* is still very high. These 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.

6.15.2. New members and consultants. The Commission welcomes the new members elected at the Florence Congress: S. Billinge, D. Rafaja, R. Rizzi, P. Stephens and P. Whitfield. The Commission also has a number of consultants to advise across the breadth of powder diffraction; these are J. Cline, J. de Villiers, R. E. Dinnebier, J. A. Kaduk, Irene Margiolaki, P. Scardi and M. Yashima. The Commission also wishes to thank the outgoing members for their participation over their terms of office: they are R. Delhez, C. Hubbard, D. Balzar and G. J. Kruger. Special thanks are also due to the outgoing Chair, R. E. Dinnebier, for fulfilling the varied roles of *Newsletter* editor, workshop organizer, general CPD fund raiser and passionate advocate of powder diffraction.

6.15.3. 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.

6.15.4. Meetings/Workshops/Schools. Meetings of interest for the CPD in 2005 included the Florence Congress and the workshop entitled Watching the Action: Powder Diffraction at Non-Ambient Conditions, in Stuttgart, Germany 6–7 October 2005. The manual of this workshop is available at http://www.fkf.mpg.de/xray. The 2005 CPD meeting was held at the Florence Congress while the next meeting is planned at EPDIC, Geneva, Switzerland, 6 September 2006. Future meetings in Indonesia and Brazil have been supported by the Commission which continues to encourage crystallographers around the world to promote powder diffraction research and education.

6.15.5. Web site. The CPD web site 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 text book on powder diffraction which will be published by the Royal Society of Chemistry.

W. I. F. David, Chair

6.16. Commission on Small-Angle Scattering

6.16.1. Commission meetings and communication. Most of the Commission's communications were by e-mail, but various members of the Commission were able to meet at meetings and conferences around the world and had the opportunity to discuss the work of the Commission. In particular, a session of the Commission was held during the Florence Congress, where most of the Commission members were present.

6.16.2. Activities. The main activities that took place in 2005 were as folows.

(1) At the Commission meeting in Florence, a new Chair (D. I. Svergun) and new Commission members (J. Trewhella, A. Benedetti) were appointed. T. Sabine left the Commission and I. Torriani became a consultant.

(2) The Commission actively participated in providing visibility for SAXS during the Florence Congress. A Keynote Lecture in SAS from Biological Macromolecules was given (D. Svergun) and J. S. Pedersen organized a one-day satellite workshop on small-angle scattering. Several Commission members gave tutorial lectures at the workshop.

(3) The Commission became involved in the preparatory work for the International Conference on Small-Angle Scattering (SAS 2006,

Kyoto, Japan). N. Yagi from the Commission is a co-Chair of the Organizing Committee, Y. Amemiya is the Chair of the Programme Committee, and other members of the Commission are serving on the International Advisory Committee. The Conference with more than 500 participants expected will be by far the largest SAS event ever held.

(4) A discussion among the Commission members was initiated regarding preparation and publication of a text book on small-angle scattering. It was agreed that such a book would be very timely and of great help for the community, and that the Commission should take a lead in promoting/writing it. Two formats are currently under discussion: (i) an entry-level text book written by not more than three co-authors, and (ii) an advanced book covering cutting-edge applications written by a larger author group.

(5) The Commission took the lead in soliciting applications for the SAS 2009 conference. The venue of the conference is to be decided at SAS 2006 (July 2006, Kyoto) and the Commission made a call to the SAS community to prepare applications from scientific institutions willing to host the SAS Conference in 2009.

6.16.3. Educational activities. The members of the Commission were actively involved in giving seminars and tutorial lectures explaining SAS methods to young researchers/students. Below is a list of lectures illustrating the broad coverage provided.

I. Torriani gave lectures: Structure of Macromolecules in Solution using SAXS at the Annual Meeting of the Argentinian Crystallographic Association (La Plata, Argentina); and Dynamical Measurements in Soft Matter Research at the 2005 Users' Meeting of the Laboratorio Nacional de Luz Sincrotron, Campinas, Brazil.

I. Torriani, A. Allen and P. Thiyagarajan presented tutorial lectures: Small-Angle Scattering: Introduction and Basic Theory; Principles and Application of Ultra-Small-Angle Scattering (USAS); and Contrast Variation Techniques and Instrumentation for Small-Angle Neutron and X-ray Scattering at the Workshop on Introduction to Small-Angle Scattering at the Florence Congress.

J. S. Pedersen presented a lecture entitled Low-Resolution Structure Determination of Proteins in Solution by SAXS at Translation and Transport 2005, a symposium organized by the Centre for Structural Biology, University of Aarhus, Denmark, 24 January 2005.

J. S. Pedersen and D. I. Svergun were speakers at the BIOSAS Conference (Copenhagen Workshop on Bio-Macromolecules in Solution Studied with Small-Angle Scattering, Copenhagen, Denmark, 1–2 December 2005). The titles of their presentations were: Studying Bio-Macromolecules in Solution with Small-Angle Scattering and Computational Methods for Structure Determination from Small-Angle Scattering Data, respectively.

D. I. Svergun presented a lecture and tutorial on Solution Scattering Data Interpretation at the Workshop on Advances in Diffraction Studies on Non-Crystalline Biological Systems, Stanford, CA, USA, October 2005.

J. Trewhella gave several review and tutorial talks at Australian workshops and conferences about the use of small-angle X-ray and neutron scattering for studying biological macromolecular complexes (International Conference on Neutron Scattering, Sydney, November – December 2005, 30th Annual Lorne Conference on Protein Structure and Function, Phillip Island, February 2005, and the Small-Angle Scattering for Structure Determination of Macromolecules, Emerging Science Initiative for Synchrotron Science: Symposium and Workshop, Melbourne, April 2005).

6.16.4. Community building activities. The members of the Commission are often invited to present lectures and seminars on SAS methods and their use in various fields, also at conferences/workshops not specifically devoted to SAS. This gives them an excellent opportunity to promote SAS as a structural method, and in 2005 more than 30 such presentations were given (the complete list would have taken too much space to be presented here). Very important was the high visibility of SAS at the Florence Congress, which, the Commission hopes, should lead to much better interactions and collaborations between small-angle scatterers and crystallographers/powder diffractionists.

P. Thiyagarajan facilitated SANS experiments at IPNS and SAXS at APS for several groups, and trained several graduate students from the US universities to carry out SANS and SAXS at the user facilities at Argonne.

N. Yagi will give a talk about microdiffraction at the SPring-8 synchrotron at the CCP13 meeting in Cardiff, UK (June 2006).

A. Allen continued his work to determine the potential for a glassy carbon NIST Standard Reference Material (SRM) for SAXS absolute intensity calibration with round robin studies at the Advanced Photon Source. While development of a full SRM will require work with the manufacturer to control sample variability, the biggest hurdle to overcome remains the establishment of the market case. Progress was made in this regard during 2005 but much remains to be done.

D. I. Svergun, responsible for the Bio-SAXS facility at the EMBL Outstation in Hamburg, Germany, trained a number of students and post-docs from European research institutions to use SAS for biological solution scattering. He also promoted joint use of SAXS and SANS at a Neutrons in Biology conference in Grenoble, France, September 2005.

J. S. Pedersen 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. A large number of students and post-docs have been trained in the SAS technique in Aarhus.

J. Trewhella was actively involved in expanding the SAS Research Community in South East Asia. A major investment in small-angle scattering instrumentation is being made in Australia for materials, polymer and biological studies and these investments will all be aimed at increasing access to small-angle scattering for researchers in the region. The Australian Research Council has granted two awards for commercial SAXS instruments from their Large Equipment and Infra-Structure Fund for instruments at the University of Sydney and University of Queensland, while a state-of-the-art small-angle neutron scattering instrument is under construction at the new Open-Pool Australian Light Water Reactor (OPAL) and a small-angle X-ray instrument is being designed for the new Australian synchrotron. These latter two instruments are scheduled for commissioning at the beginning of 2007.

6.16.5. Consultant activities. D. I. Svergun and J. S. Pedersen served as members of the Scientific Committee at Geesthacht Neutron Scattering Facility (GeNF) at GKSS Research Centre, Geesthacht, Germany, and of the Soft Matter Committee at the European Synchrotron Radiation Facility (ESRF, Grenoble, France). D. I. Svergun was also a Review Committee Member of the synchrotron Elettra (Trieste, Italy) (evaluation of beam-time applications).

A. Allen serves as a member of the Programme Advisory Committee (PAC) at the NIST Center for Neutron Research (NCNR, Washington, USA), serving on the SANS proposal review panel and also providing input for the overall NCNR user programme. He was

also a member of the SAXS proposal review panel, Advanced Photon Source (APS), Argonne, IL, USA (term completed 1 September 2005). As a *J. Appl. Cryst.* Co-editor, A. Allen took part in the Journals Commission meeting, Montecatini, Italy, 2005.

P. Thiyagarajan has been Chair of the SAXS Proposal Review Panel for APS since April 2005 (the panel convenes three times a year). He is also a member of the BioCAT Advisory Committee, APS, and serves as a reviewer for the beam-time proposals for NIST and SSRL (Stanford, USA).

G. Kostorz was appointed Editor-in-Chief of IUCr journals at the General Assembly in Florence.

6.16.6. Organizational activities. I. Torriani organized a Workshop on The Use of Synchrotron Radiation for the Study of the Structure of Polymers as a satellite of the 17th Brazilian Crystallographic Association Meeting, Campinas, Brazil, 2005.

A. Benedetti served as a member of the Scientific Committee for the Florence Congress.

P. Thiyagarajan was a co-organizer of a workshop on SAS of Nanobiology and two scientific sessions at the ACA meeting, Orlando, FL, USA (27–31 May, 2005), and a Chair of the Extended Q SANS instrument at the Spallation Neutron Source Instrument Advisory Team meeting, SNS-HFIR User Group Meeting, ORNL, Oak Ridge (10–13 October 2005).

J. S. Pedersen was an organizer of the one-day workshop Introduction to Small-Angle Scattering in connection with the Florence Congress. He is also a co-organizer of the European School on Scattering Methods Applied to Soft Condensed Matter to be held in Bombannes, Gironde, France, 10–17 June 2006.

Y. Amemiya and N. Yagi are directly involved in the organization of the 13th International Conference on Small-Angle Scattering (SAS 2006, Kyoto, Japan, 9–13 July 2006; http://sas2006.scphys.kyoto-u.ac.jp/). With more than 500 registrations and more than 500 abstracts submitted, the Kyoto conference exceeds by a large margin all previous events on SAS (held since 1965) and vividly demonstrates the increasing popularity of the technique in different scientific fields.

6.16.7. Technical activities. I. Torriani coordinated the SAXS1 beamline at the Brazilian Synchrotron (LNLS) and was involved in commissioning a new beamline (SAXS2) at the LNLS, which will be opened to the community of users in Brazil and Latin America in June 2006.

D. I. Svergun coordinates a Design Study SAXIER funded by the European Commission under the Infrastructure Programme of the Sixth Framework Programme. The project includes Europe's main SAXS laboratories at synchrotrons in France, the UK, Germany and Italy involved in exploring novel scientific applications for the new generation of SAXS beamlines at high-brilliance synchrotron facilities. SAXIER started on 1 December 2005 and has a duration of 4 years.

N. Yagi was responsible for many on-going technical activities on SAXS experiments at SPring-8, especially on microbeam experiments, and in the development and evaluation of CMOS flat panel detectors for SAXS.

A. Allen published a feature article in the *Journal of the American Ceramic Society* in July 2005: *Characterization of Ceramics by X-ray and Neutron Small-Angle Scattering* [*J. Am. Ceram. Soc.* (2005), **88**, 1367–1381]. As of 20 March 2006, this article had been downloaded 856 times, the second highest of any article published in the 2005 volume of the journal.

P. Thiyagarajan played a leading role in the development of a GISAXS instrument at 12-ID (APS). He distributed the analysis package on Igor Pro platform to several users at IPNS and the SAXS instruments at 18-ID and 12-ID beam lines at APS.

J. S. Pedersen, Chair 2002–2005
D. I. Svergun, Chair 2005–

6.17. Commission on Structural Chemistry

The composition of the Commission for 2005–2008 was decided by the Florence General Assembly. New members are A. Beatty (USA), P. Bombicz (Hungary), M. T. L. Duarte (Portugal), Maochun Hong (People's Republic of China), O. Piro (Argentina) and P. R. Raithby (UK). The Commission also has a number of consultants who agreed to collaborate on specific subjects as well as on general issues. Following the suggestions of the IUCr Executive Committee, the Commission designated the distribution of responsibilities among members as follows: *IUCr Newsletter* reporter, D. C. Levendis; *World Directory* liaison, P. Bombicz; liaison with Commission on Crystallographic Teaching, M. T. Duarte; liaison with Commission on Crystallographic Nomenclature, P. R. Raithby; liaison with Commission on Journals, H. Uekusa; liaison with Commission on International Tables, O. Piro; liaison with the Chair of the IUCr/Oxford University Press Book Series Selection Committee, A. Beatty; webmaster, A. Bacchi; IUCr 60th Anniversary planning, L. Brammer.

The new Commission has started its activities by updating and restyling the web site. The Commission also endorsed the following events which will take place in 2006: Russian Fourth National Crystal Chemical Conference (Chernogolovka, Russia, 26–30 June 2006), French Crystallographic School (Nancy, France, 28 August–2 September 2006), Indaba 5 (Kruger National park, South Africa, 20–25 August 2006). Two Commission members are actively involved in the Organizing Committee (D. C. Levendis) and Programme Committee (T. Duarte) for the last meeting.

A. Bacchi, Chair

6.18. Commission on Synchrotron Radiation

The mission of the Commission is to promote the access of crystallographers worldwide to the world's synchrotron-radiation facilities. A subcharge is to promote the development of crystallographic instrumentation technology and standards, particularly in the direction of X-ray detectors. To foster communication, we endorse international meetings as the best means to achieve these goals.

Through the appointment of R. Felici to the Programme Committee for the Florence Congress, the Commission has been heavily involved in not only the planning of the meeting but also the meeting itself. The meeting has shown the continuously growing importance of synchrotron radiation in many fields of crystallography.

The construction of new synchrotron sources throughout the world, including those in developing countries, has increased the coordinating activities of the Commission. As an example, the Commission supported the establishment of the Asian–Oceanic Forum for Synchrotron Radiation Research (AOF). One of the goals of the AOF is the coordination of synchrotron related activities in Asia and Oceania, *via* joint user and scientific meetings. The first meeting of the AOF is planned for the fall of 2006. Various members of the Commission have been involved in the preparation and organization of Synchrotron Radiation Instrumentation 2006 (Deagu, Korea, May/June 2006), which is held every three years and is the main instrumentation conference in synchrotron research. The

rapid increase in size of this meeting reflects the growing number of sources world-wide.

A main activity in 2005 was the compilation of a Special Issue of *Journal of Synchrotron Radiation* on X-ray detectors (this appeared in March 2006). This was one of the activities to promote increased funding for detector developments at synchrotron sources.

In 2005, the Commission decided to pay special attention to the upcoming new generation sources, like Energy Recovering Linacs (ERLs) and Free Electron Lasers (FELs). These new sources are strictly speaking not synchrotron (or storage ring) sources, but Linac based sources. They will provide exciting new scientific opportunities, as well as exciting instrumental challenges. The Commission will try to stimulate the interplay between the 'classical' synchrotron sources and the new linac-based sources.

It is very encouraging to see that both the LCLS (Stanford) and the European XFEL (Hamburg, Germany) have decided to invest significant amounts of money in the development of proper X-ray area detectors. These new detectors will not only serve the science at these new facilities, but will certainly be used at the existing storage ring sources as well.

H. Graafsma, Chair

6.19. Commission on XAFS

The main goal for the Commission is to promote XAFS in the crystallographic community and to drive new developments. Members of the newly appointed Commission met in Florence. The Commission for this triennium contains nine members (including the Chair) and S. S. Hasnain continues as consultant. The increase in size of the Commission helped give rise to a higher level of activity during the last year.

At the Florence Congress a successful Microsymposium on Combined XAS and XRD techniques in Physics, Chemistry and Material Science was organized by S. Mobilio and J. Garcia-Ruiz.

A web site (www.df.unibo.it/iucr) has been developed with information on XAFS for crystallographers; this is linked to directly from the Commission's IUCr web page (http://www.iucr.org/iucr-top/iucr/cxafs.html) and is hosted by the Physics Department of the University of Bologna and maintained by F. Boscherini. At the moment it includes, for example, a list of XAFS-related events (conferences, workshops, schools), a compendium of XAFS beamlines at synchrotron facilities and a list with the names and e-mail addresses of the members of the Commission.

The contacts with the International XAFS Society (IXS) were strengthened. Some of the members of this Commission have dual membership and are eager to improve mutual relations for the benefit of both the XAFS and the crystallographic communities. Future activities might even include (re-)addressing the tough parts of XAFS (definitions, data collection and analysis procedures) and establishing a more direct link between the Commission and the IXS.

The Commission might be involved in the support of workshops and summer schools. The organization of the third BioXAS Study Weekend is already planned at the new synchrotron-radiation centre Soleil, in France, close to Paris (http://www.synchrotron-soleil.fr). This workshop will be held 10–12 August 2007 as a satellite meeting of the 9th International Conference on Biology and Synchrotron Radiation (BSR2007).

An important event, giving the Commission an opportunity to meet again, will be the 13th International Conference on X-ray Absorption Fine Structure (XAFS-XIII) to be held at the Stanford Campus (http://www-ssrl.slac.stanford.edu/xafs13), 9–14 July 2006. This triennial conference covers all fields and disciplines using XAFS and related techniques.

A. Molenbroek, Chair

7. Sub-committee on the Union Calendar

The Sub-committee receives and considers requests for IUCr sponsorship and nominal financial support and makes recommendations to the Executive Committee. Acting on the recommendations made by the Sub-committee, during 2005 the Executive Committee approved sponsorship of various schools and meetings, mostly with financial support. Those held in 2005 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 2006, but approved in 2005, are listed below.

International Workshop on Crystal Growth and Characterization of Advanced Materials, Chennai, India, 9–13 January 2006.

Fourth European Charge Density Meeting (ECDM-IV), Brandenburg, Germany, 25–29 January 2006.

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

Third Moroccan School of Crystallography, Agadir, Morocco, 8–12 May 2006.

Structure and Solution of Large Molecular Assemblies, Erice, Italy, 9–18 June 2006.

International School on Biological Crystallization, Granada, Spain, 18–24 June 2006.

Electron Crystallography School, Bangalore, India, 19–23 June 2006. [Subsequently cancelled.]

Fourth National Crystal Chemical Conference, Chernogolovka, Russia, 26–30 June 2006.

Thirteenth International Conference on Small-Angle Scattering, Kyoto, Japan, 9–13 July 2006.

ACA Annual Meeting, Hawaii, USA, 22–27 July 2006.

23rd European Crystallographic Meeting (ECM-23), Leuven, Belgium, 6–11 August 2006.

Sagamore XV: Electron Charge, Spin and Momentum Densities, Warwickshire, UK, 13–18 August 2006.

IUCr Teaching Commission Intensive School on Single-Crystal X-ray Structural Analysis, Siena, Italy, 27 August–2 September 2006.

Structural Analysis by X-ray Diffraction, Crystallography under Perturbation, Nancy, France, 28 August–2 September 2006.

Crystallography at High Pressure (Neutron, X-ray and Related Studies), Dubna, Russia, 28 September–1 October 2006.

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 two months before or after a meeting of a Regional Associate will not be considered for sponsorship unless the application has received the approval of the Chair of the Programme Committee of the Regional Associate meeting.

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

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

H. D. Flack attended the meeting The Future of the Research Information Chain – the Role of Publishers and Learned Societies, Budapest, Hungary, 17–18 March 2005, jointly organized by ALLEA (All European Academies – The European Federation of National Academies of Sciences and Humanities) and stm (The International Association of Scientific, Technical and Medical Publishers) at the headquarters of the Hungarian Academy of Science.

B. McMahon attended the Council of Science Editors Meeting in Atlanta, USA, 20–24 May 2005, and gave a presentation in the session on Emerging Tools.

B. McMahon attended the European University Information Systems (EUNIS) meeting in Manchester, UK, 21–24 June 2005, to which he submitted a paper on semantically rich metadata in crystallographic publishing.

The meeting attendances of the CODATA and ICSTI representatives, whose work is so closely related to that of the CEP, are recorded in their individual reports.

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

This year marks the fifteenth year since the Union adopted CIF (Crystallographic Information Framework, formerly Crystallographic Information File) as a standard for submission of crystal structure reports to the Union journals. Much has happened in that time and the Florence Congress provided an opportunity for COMCIFS to take stock of the project and plan its future directions.

The most notable achievement of the past fifteen years has been the preparation of an impressive array of CIF dictionaries that provide data names and definitions for the two thousand or so crystallographic terms that can appear in CIFs. No other discipline has a comparable set of dictionaries with such a wide community acceptance. These dictionaries are used in conjunction with the STAR file syntax as the format for the considerable archive of CIF-based structure reports. In the field of small-cell crystallography, CIF is now widely accepted as the standard for the submission of structure reports to many scientific journals, and for their archiving and downloading. In the macromolecular field CIF is used to archive the Protein Data Bank, but it does not yet have as wide community acceptance, most protein structure laboratories preferring to stay with the familiar, if inadequate, PDB format, and the macromolecular data centres favouring the use of XML.

XML is a markup language with many functional similarities to the STAR file structure used by CIF. Although a recent arrival, its development by the information technology community has earned it widespread acceptance in many scientific communities. It is more flexible than CIF, though this is not necessarily an advantage in an established field like crystallography. It allows users to develop their own semantics and define concepts in ways that may not be compatible with those defined by other users. Although XML users have access to an extensive suite of programs to manipulate their files, unless they agree on the semantics, *i.e.* the definitions and organization of the concepts of their discipline, they are unable to communicate with each other. CIF's suite of dictionaries provides a widely accepted semantic for crystallography that can be translated into an XML format for the benefit of XML users, though the reverse process is only possible if the XML file is written in a form designed to be compatible with CIF. COMCIFS is working to ensure that the information contained in CIFs and CIF dictionaries is available in XML format. Some conversion programs are already available and more work is planned.

Our goal is to enable CIFs to be read by generic programs that obtain all their crystallographic knowledge directly from the CIF dictionaries. This requires that all CIFs rigorously conform to the standard. In the early days this standard was not strictly enforced so as to avoid discouraging those who found CIF strange and unfamiliar, but over the years the degree of conformity has been steadily increased and the CIF standard itself has evolved in subtle ways as we became more aware of the possibilities inherent in the STAR syntax. Thus after preparing the coreCIF dictionary as a STAR file using the Dictionary Definition Language 1 (DDL1) it was decided that the macromolecular CIF dictionary should use advanced features that were only available in DDL2. The result was two incompatible CIF dialects, CIF1 and CIF2, using dictionaries based on DDL1 and DDL2, respectively. This required different programs for each dialect, or a duplication of effort to ensure that a single program could read both. While this decision made sense at the time, it has returned to haunt us as we strive to ensure that we retain compatibility between the CIF1 and CIF2 definitions even as the dictionaries evolve independently.

The problem of CIF dialects was discussed in Florence at the closed COMCIFS meeting. Here we developed a consensus that we should move towards a new dictionary language, DDL3, with corresponding CIF3 dictionaries. Programs designed to work with CIF3 dictionaries would be fully back-compatible and able to read any file written in either CIF1 or CIF2. A prototype has already been tested and an early approval of DDL3 will allow the conversion of the existing CIF1 and CIF2 dictionaries to CIF3. The opportunity is being taken to incorporate advanced features that were unimagined fifteen years ago. One of these is the development of an hierarchy of crystallographic concepts that would add flexibility and allow the dictionaries to evolve in parallel. Another innovation is the introduction of algorithms that instruct a program how the value of an item can be calculated on the fly from other items present in a CIF. These algorithms are computer-readable definitions that will enhance the ability of CIF dictionaries to serve as machine-readable repositories of crystallographic knowledge.

While these activities help to keep CIF at the forefront of information technology, COMCIFS is also concerned not to abandon those who find themselves still challenged by the demands of checkCIF. From the beginning, we knew that we would need a suite of tools to assist in preparing CIFs. The last couple of years has seen the appearance of a number of such programs, *e.g. enCIFer*, *publCIF* and *CIFedit*, that use the appropriate CIF dictionaries to assist users in writing fully conformant CIFs. *publCIF* has been developed by the IUCr editorial office and is well tuned to the publication requirements for small-cell structures. It will continue to be developed to handle macromolecular structure reports that are accompanied by structural data in mmCIF format, as the editorial production processes develop to handle such articles efficiently. Other tools are under development in an IUCr-sponsored project to upgrade some older CIF software to strict compliance with the latest CIF specifi-

cations. This project includes updates to *vcif*, a simple syntax checker, and to *CIFtbx*, a Fortran library; and the provision of a utility to manage the relaxation of the line and data name length restrictions in CIF version 1.1. As the existing dictionaries are converted to DDL3, we will encourage the preparation of CIF3-level programs that will be able to read any CIF whether written as CIF1, CIF2 or CIF3. We expect, however, that the existing dictionaries will continue in use until the advantages of CIF3 become sufficiently apparent that users voluntarily convert.

Among the routine business transacted during the course of the year were the preparation of new terms of reference expanding the mandate of COMCIFS to ensure that crystallographic information in digital form is compatible with standards in neighbouring fields. These terms were subsequently approved by the Executive Committee. COMCIFS also formally adopted responsibility for the maintenance of the DDL1 dictionary which had no organization designated to authorize and approve necessary changes. Finally, a complete documentation of CIF concepts and associated data dictionaries has been completed as Volume G of *International Tables for Crystallography*.

I. D. Brown, Chair

10. Committee on Crystallographic Databases

This Committee deals with matters that pertain to more than one database, and with issues that may come up from time to time that concern databases and data management in general. Following the decision of COMCIFS in Florence to integrate the DDL1 and DDL2 dictionaries, S. R. Hall and N. Spadaccini are finalizing the integrated dictionary with assistance from J. D. Westbrook (PDB). We thank the previous Chair, F. H. Allen, for coordinating the Committee activities in the previous triennium.

G. R. Desiraju, Chair

11. *IUCr Newsletter*

Four issues of the *IUCr Newsletter* were distributed in 2005 (Volume 12, No. 4, Volume 13, Nos. 1, 2 and 3). By the end of the year Volume 13, No. 4 was nearly complete and Volume 14, No. 1 was in preparation. This report will cover all four issues of Volume 13. All four issues were 32 pages in length. Coverage of the Florence Congress began in 13, No. 4 and will continue in 14, No. 1. As in previous years, the content covered activities of the IUCr and its Regional Associates, 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: the first two by W. L. Duax and the last two by Y. Ohashi. Issues 2 and 3 included an editorial written by J. L. Flippen-Anderson and in issue 4 the IUCr Congress reports were introduced by C. Mealli. Starting with issue 4 of 2005, editorial responsibility for the *Newsletter* will be shared by W. L. Duax and J. L. Flippen-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 Japan, edited by Y. Ohashi, in Volumes 13, Nos. 2 and 3. In addition to the initial articles describing crystallography in Japan Volume 13, No. 2 had reports describing the 2005 meeting of the Crystallographic Society of Japan and the annual meeting of the Japanese Society for Synchrotron Research.

Reports were published covering meetings in Germany, the Czech Republic, Singapore, Greece, Portugal, Italy, India, Mexico, France, Egypt, Indonesia, USA, Switzerland, Belgium, and Poland. Issue 13, No. 1 completed the coverage of ECM-22 in Budapest, Hungary, and had a special article celebrating the 40th anniversary of the Cambridge Crystallographic Data Centre. An article on NMR crystallography was also included in 13, No. 1. The online version of *International Tables* was announced in 13, No. 3 and the new IUCr Commission on Mathematical and Theoretical Crystallography was described in 13, No. 4.

The mailing list was 4% larger than in 2004 with an average distribution of 16,943. Twenty-one countries assist in the effective and economic distribution of the *Newsletter*. Individual distribution is sent to 83 additional countries. (Distributors: H. Fodil, Algeria; G. Jameson, Australia; J. Valderrama, Colombia; B. Kojic-Prodic, Croatia; J. Hasek, Czech Republic; C. Lecomte and Å. Kvick, France; A. Nangia and Executive Secretary, India; Ismunandar, Indonesia; P. Spadon, Italy; A. Satomi, Japan; A. Hamid Othman, Malaysia; R. Rendle, New Zealand; J. Lipkowski, Poland; M. Costa, Portugal; 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.)

W. L. Duax, Co-Editor
J. L. Flippen-Anderson, Co-Editor

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

The IUCr/OUP Book Series Committee reports with much pleasure that in 2005 the monumental monograph *Crystalline Molecular Complexes and Compounds Structures and Principles* by Frank H. Herbstein has been published in two volumes in the series IUCr Monographs on Crystallography.

New books are in the production phase. The Committee and the OUP editing staff reviewed a number of books and there were many contacts with authors about possible new volumes. The Committee and the science editor of OUP met at the Florence Congress to discuss progress and new plans and policies.

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). Also, 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

13. Regional Associates and Scientific Associates

13.1. American Crystallographic Association (ACA)

The 2005 ACA Spring Meeting was held in Orlando, Florida, 28 May–2 June. It was preceded by four one-day workshops on 27 May: (1) Structure Solution and Refinement of Difficult Structures, (2) Macromolecular Structure Validation, (3) Biology on the Colloid Nanoscale and (4) A Protein Crystallographic Toolbox: CCP4 Software Suite. The A. L. Patterson Award was granted to T. Alwyn Jones (University of Uppsala, Sweden) and the Margaret C. Etter Early Career Award was presented to Jennifer Swift (Georgetown University). The Transactions Symposium was dedicated to the subject New Horizons in Structure-Based Drug Design. Almost 750 crystallographers were present at the meeting, attending the 38

parallel sessions and having discussions with the authors of the more than 250 poster presentations. At the end of the meeting (2–3 June), a Summit on Crystallographic Education was organized by the Standing Committee on Continuing Education and the USNC/Cr. Once more, the organizers of the ACA Annual Meeting made special efforts to obtain funds to award travel grants to students and young scientists.

The 2005 ACA Summer School on Macromolecular Crystallography was held at the Illinois Institute of Technology (Chicago, IL) and the Advanced Photon Source (Argonne, IL), 18–30 July 2005. The school was designed for graduate students and postdoctoral researchers. Several scholarships were awarded to candidates from the USA and Latin-American countries to enable them to attend these courses, which are 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 Latin-American Country Membership, created by the ACA in 2004, was a very important step in the direction of establishing a more effective regional interaction with the countries in Central America, South America and Mexico. In early 2005, membership requests were submitted by Argentina and Brazil.

In 2005, on-line versions of Volumes 38 (Biological Neutron Diffraction) and 39 (Crystals in Supramolecular Chemistry) of the Transactions of the American Crystallographic Association were made available.

I. L. Torriani, IUCr Representative

13.2. Asian Crystallographic Association (AsCA)

The 13th AsCA Council meeting took place on 25 August 2005, during the Florence Congress. The meeting reviewed the arrangements for the joint meeting of AsCA and the Crystallographic Society of Japan (CrSJ) scheduled for 20–23 November 2006 in Tsukuba. A Programme Committee was set up with S. Wakatsuki as the Chair. The Council also held preliminary discussions on the AsCA meeting to be held in Taipei in late 2007 (AsCA'07). J. Simpson was appointed as the Chair of the Programme Committee. A long-felt need of AsCA has been that of a functional web site. A professionally designed web site of the Association has been constructed during 2005.

G. R. Desiraju, IUCr Representative

13.3. European Crystallographic Association (ECA)

The present membership of the ECA Executive Committee as appointed in 2003 is: President: H. Fuess (Germany); Past President: C. Lecomte (France); Vice-President: M. Jaskolski (Poland); Secretary: G. Filippini (Italy); Treasurer: M. T. Duarte (Portugal); Members: A. Liljas (Sweden), A. Roodt (South Africa), C. C. Wilson (UK)

The posts of President, Vice-President, Secretary, Treasurer and other members of the Executive become vacant at the Leuven ECA meeting in 2006, and elections will be held. The ECA Executive Committee proposes for the triennium 2006–2009: President: J. R. Helliwell (UK); Vice-President: S. Larsen (Denmark); Secretary: P. Bombicz (Hungary); Treasurer: R. Kuzel (Czech Republic); councillors who represent Individual and Corporate Affiliate Members on the ECA Council (to be elected 1 June 2006, to serve a three-year term): M. Nespolo (France), T. Borowiak (Poland).

The ECA has 13 Special Interest Groups (SIGS):

SIG1: Macromolecular Crystallography (Chair A. Liljas);

SIG2: Charge, Spin and Momentum Density (Chair H. Graafsma, Co-Chair U. Pietsch);

SIG3: Aperiodic Crystallography (Chair T. Janssen);

SIG4: Electron Crystallography (Chair T. E. Weirich);

SIG5: Mineralogical Crystallography (Chair W. Depmeier, Co-Chair A. R. Oganov);

SIG6: Instrumentation and Experimental Techniques (Chair J. R. Helliwell, Co-Chair J. L. Hodeau);

SIG7: Molecular Interaction and Recognition (Chair R. Boese, Co-Chair P. H. Van Rooyen);

SIG8: Powder Diffraction (Chair J. Rius, Co-Chair R. J. Cernik);

SIG9: Crystallographic Computing (Chair A. L. Spek);

SIG10: X-ray Diffraction and Optics (Chair M. Kovalchuk, Co-Chair B. Capelle);

SIG11: Crystallography under Extreme Conditions (Chair A. Polian, Co-Chair M. McMahon);

SIG12: Materials Science (Chair P. A. Thomas, Co-Chair P. Bordet);

SIG13: Molecular Structure and Chemical Properties (Coordinator C. C. Wilson).

Future meetings will be held as follows: Marrakech, Morocco, 22–27 August 2007; 2008 is an IUCr Congress year; Istanbul, Turkey, August 2009; Darmstadt, Germany; August 2010 (this will be held along with EPDIC XII).

The ECA has supported the following meetings in 2005.

(1) The regional Heart of Europe Biocrystallography Meeting (HEC-8), the eighth in the series, took place in Karlovy Vary, Czech Republic, 29 September–1 October 2005. The meeting was funded in part by the European Crystallographic Association, and also supported by the Czech and Slovak Crystallographic Association. The organizer was the Institute of Molecular Genetics, The Czech Academy of Sciences, Prague. The meeting was attended by about 100 participants and provided a forum for 32 presentations by young biocrystallographers from Germany, Poland, Austria and the hosting Czech Republic. A memorable HEC-8 Lecture on Phasing on Anomalous Scattering: Multi- *vs* Single-Wavelength was given by Z. Dauter from Argonne National Laboratory, USA.

(2) The 9th International Conference on Crystal Chemistry of Intermetallic Compounds was held in Lviv, Ukraine, 20–24 September 2005. This series of all-Union conferences was initiated in 1971 in context with the creation of the School on Crystal Chemistry at Lviv University and, since then, a meeting takes place approximately every third year.

(3) XVII International School on Physics and Chemistry of Condensed Matter and V International Symposium on Physics in Materials Science, Białowieża, Poland, 21–29 June 2005. The topic was Materials in Transition, and the organizer was The Institute of Experimental Physics, University of Bialystok, Poland. The School and Symposium gathered 65 participants from 10 countries. The programme was a natural continuation of the previous School (2004) on the Structural Aspects of Matter. The main emphasis was placed on the transient effects and time-resolved characteristics of structural phase transitions, especially those induced by light. Special attention was focused on catalytic phenomena and less-known halogen bonding. The school programme also covered the basics and up-to-date application of neutron scattering, muon spin rotation and various visualization techniques — all of which are essential in studies of phase transitions.

(4) International School on Mathematical and Theoretical Crystallography, Nancy, France, 20–24 June 2005. The school was attended by 61 registered participants from 20 countries with different backgrounds (chemistry, physics, mineralogy, mathematics, biology *etc.*).

The delegates were introduced to several aspects of modern theoretical crystallography by nine invited lecturers: Th. Hahn (Germany), H. Wondratschek (Germany), U. Müller (Germany), M. I. Aroyo (Spain), V. Kopsky (Czech Republic), M. Catti (Italy), A. R. Oganov (Switzerland), H. D. Flack (Switzerland) and T. Yamanaka (Japan). The school also included a poster session, with 23 posters presented. A Special Issue of *Acta Crystallographica* Section A will be published with articles from the lecturers and manuscripts submitted by the participants.

A new prize for young scientists, named after Erwin Lewy Bertaut, will start next year (subject to approval by the Council). The winner of the 2005 Perutz Prize was E. Dodson.

C. J. Gilmore, IUCr Representative

13.4. International Organization of Crystal Growth (IOCG)

In 2005 the major initiative supported by the IOCG was the Third International Workshop on Crystal Growth Technology, IWCGT-3, held at Beatenberg, above Interlaken, Switzerland, 10–19 September 2005. Co-Chairs were H. J. Scheel, Switzerland, S. Uda, Tohoku University, Japan, and D. Witter, Northrop Grumman, USA. The full report from this meeting was presented in the *IUCr Newsletter* [(2005), **13**(3), p. 26].

The UK Network for Crystal Growth and Nucleation and The British Association for Crystal Growth held a Summer School at Il Ciocco Conference Center, Lucca, Italy, 27 August–3 September 2005 (organized by N. de Leeuw and R. Catlow); this was dedicated to the latest applications in crystal growth and nucleation.

The American Association for Crystal Growth organized the 16th American Conference on Crystal Growth and Epitaxy (ACCGE 16), held jointly with the 12th US Biennial Workshop on Organometallic Vapor Phase Epitaxy (OMVPE) in Big Sky, Montana, USA, 10–14 July 2005 (http://www.crystalgrowth.org/old/conferences/2005/accge16/index.html). During this busy meeting, which is so important for the community, D. F. Bliss (who is an active member of the IUCr Commission on Crystal Growth and Characterization of Materials) was elected President of the American Association for Crystal Growth.

Another important event was the Gordon Conference on Thin Film and Crystal Growth Mechanism, Mount Holyoke College, South Hadley, Massachusetts, USA, 26 June–1 July 2005 (organized by M. Hines, Cornell University, and P. Vekilov, University of Houston).

Preparations 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; http://www.iocg.org/ICCG_15_flyer.pdf), 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) have also started.

H. A. Dabkowska, IUCr Representative

13.5. International Centre for Diffraction Data

R L. Snyder after many years of representing the ICDD (http://www.icdd.com/) at the CPD meetings has handed the responsibility over to J. A. Kaduk. We welcome Jim and thank Bob for his enthusiasm and commitment to the field of powder diffraction. 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: http://www.icdd.com/ and the IXAS web site: http://www.ixas.org/.

W. I. F. David, IUCr Representative

14. Representatives on Other Bodies

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

ICTNS met in Beijing, People's Republic of China, 16–17 August 2005. The IUCr Representative was unable to attend since the Florence Congress took place at approximately the same time. From the Minutes of the meeting, most of the points covered were of little interest for the IUCr. Of interest is the recommendation that the new definition of the kilogram be based on a definition of Planck's constant, rather than on a definition of Avogadro's constant that requires a measurement of the lattice parameter of silicon with an X-ray interferometer. The *IUPAC Handbook* has been updated and can be consulted at www.iupac.org/handbook.html. The *IUPAC Compendium of Chemical Terminology* (Gold Book) is being updated and can be consulted at http://gold.zvon.org.

A. Authier, IUCr Representative

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

The ICSTI General Assembly was held in Moscow, Russia, 25–29 May, at the invitation of VINITI, the all-Russian Institute for Scientific and Technical Information. The meeting included a one-day public conference entitled Information Services for Basic and Applied Sciences. Unfortunately, it was not possible for the undersigned to attend this meeting. However, the IUCr was represented/will be represented by H. D. Flack and J. R. Helliwell, respectively, at the following ICSTI meetings:

Winter committee meeting, 7–9 January 2005, Paris, France;

Winter committee meeting and public workshop on Information and Data in e-Science: Making Seamless Access a Reality, 3–5 February 2006, Paris, France. The new IUCr representative to ICSTI, J. R. Helliwell, has been invited to give a talk on The Role of Quality in Providing Seamless Access to Information and Data in e-Science at the public workshop.

In 2004/2005, the IUCr undertook a survey in conjunction with ICSTI to determine the extent to which policies and practices are in place to ensure the long-term availability of digital publications and data in the field of crystallography. Individual scientists and organizations were surveyed. The survey focused on formal refereed journal articles, informal publications, theses, published and unpublished data, and personal archives. The report of the findings and recommendations for action will be made available on the IUCr web site.

ICSTI maintains a public web site at http://www.icsti.org/, where the newsletter *ICSTI Forum* and other general information is made available. A private section is available only to members, the IUCr Representative sharing this opportunity with the IUCr's Sub-Committee on Electronic Publishing, Dissemination and Storage of Information (CEP).

In 2006, the ICSTI annual meeting will take place in Washington, DC, USA, 7–11 June, organized and sponsored by CENDI. The meeting includes a one-day public conference.

ICSTI is composed of a large spectrum of professionals from the STM and library sectors but with few scientists present. IUCr membership of ICSTI continues to fulfil its expectations by providing a source of current documentation and personal contacts in the field of scientific and technical information (electronic publishing).

P. R. Strickland, IUCr Representative 2002–August 2005
J. R. Helliwell, IUCr Representative August 2005–

14.3. International Council for Science (ICSU)

I represented the IUCr at the 28th General Assembly of ICSU (the International Council of Science) in Shanghai and Suzhou, People's Republic of China, 17–21 October 2005. Members of ICSU included 27 International Scientific Unions and 101 National Scientific Bodies. 219 representatives of 23 Scientific Unions and 55 nations attended the meeting. There were joint sessions for all attendees and sessions for which the Union representatives and the national representatives met separately. I found it more advantageous to attend the sessions for national representatives in order to have an opportunity to meet people from different countries (IUCr member countries and non-member countries). This gave me an unparalleled opportunity to meet leaders from the scientific community of many emerging nations.

One of the most important goals of ICSU is to build the infrastructure of science in emerging nations. ICSU is opening Regional Offices for African, Asian, Latin-American and Arab Nations. Because the Regional Associates of the IUCr (ACA, AsCA, ECA) have extensive programmes in these areas, I took the opportunity to describe their efforts to the Assembly of National Representatives.

I have begun correspondence with many of the people I met, including directors of the ICSU Regional Offices in South Africa and Malaysia. We need to explore how the IUCr and its Regional Associates can work together with the ICSU Regional Offices to bring the benefits and ultimately the technology of crystallography to countries in these regions.

Although the Board of ICSU has appropriate gender balance including a woman Past President and President Elect, less than 15% of the delegates from International Societies and National Academies of Sciences were women. I commented on the need for equitable representation by women at every level of the organization at the closing session. I also wrote to the General Secretary of ICSU to offer suggestions about ways to improve communication among delegates, the potential value of providing used instruments to suitably trained scientists in emerging countries, and the need to involve younger scientists in ICSU.

Communication. It was noted that there is need for more communication between the International Unions. We plan to add the names and addresses of all the International Union representatives who attended the ICSU Assembly to the mailing list of the *IUCr Newsletter*.

Posters and brief oral summary. Because so many representatives of International Unions attend the Triennial Assembly, it provides a good opportunity for the Unions to exchange information and share it with representatives of the National Academies of so many countries. It was impossible to contact all representatives independently during the very busy four days of the Assembly. A well organized poster session could help facilitate interaction between the Unions and national delegates. I recommended that at the next meeting the representatives of the International Unions be invited to prepare posters describing their goals, programmes and recent activities of greatest relevance to the long-range plans of ICSU. I also recommended an oral session at which a representative of each Union is allowed to present a 3 to 5 minute summary of the highlights of their poster.

Used Instrument Donations. ICSU does a wonderful job of ensuring and facilitating free travel and communication of scientists. Another way that ICSU could empower emerging nations to develop their scientific infrastructure and establish intellectual property rights to their unique natural resources would be to facilitate the transfer of used equipment to scientists with suitable training in emerging nations. ICSU could make this part of the guidelines for programmes that they support. ICSU might develop ways to support the installation, provision of replacement parts and long-term maintenance of such equipment.

Involvement of Youth. The ICSU General Assembly would benefit from more input from younger people. Many of the Unions have programmes for youth. The ACA has a young scientist special interest group that has revitalized the ACA. The ACA has also organized all-day symposia for high-school students and teachers in cities where the annual meeting has been held. I suggest that pre- and postdoctoral students from the site of the next ICSU General Assembly be invited to spend a day with the delegates, perhaps a day focused on ICSU programmes for students and young scientists.

W. L. Duax, IUCr Representative

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

Much of CODATA's work during 2005 was related to the second phase of the World Summit on the Information Society (WSIS, Tunis, November 2005). Following the discussions in the special session of the 19th International CODATA Conference (see http://www.iucr.org/iucr-top/data/docs/codata2004_berlin.html), a number of activities identified by the participants as important within the framework of WSIS commenced in January 2005.

In collaboration with the US National Academies, the US National Committee for CODATA, and wsis-online, CODATA compiled an inventory of more than 500 scientific activities that directly or indirectly related to the Agenda for Action and Declaration of Principles that came from the Geneva phase of the WSIS: http://www.wsis-online.net/science/home_EN/ and http://www.codata.org/wsis/CODATA-Inventory2Nov05.pdf.

An editorial on Science and the Digital Divide was published in the journal *Science* on 21 October 2005 (p. 405), written by S. Iwata (CODATA President) and R. Chen (CODATA Secretary General). A CODATA international workshop entitled Creating the Information Commons for e-Science: Toward Institutional Policies and Guidelines for Action was held at the UNESCO Headquarters in Paris, France, 1–2 September 2005. The meeting was sponsored by UNESCO, ICSU, TWAS, INASP and ICSTI, in collaboration with the OECD. The sponsoring organizations were supportive of further explorations of the feasibility of creating a Global Information Commons for Science Initiative. This initiative was officially launched at a round-table session organized by CODATA in Tunis on 14 November 2005. Panel participants included representatives of all the organizations sponsoring the UNESCO meeting, together with CERN and Science Commons (http://sciencecommons.org). CODATA also held a side event at WSIS on 17 November 2005 to highlight the Initiative for WSIS participants.

Other activities during the year included:

publication (February 2005) of the independent review conducted by CODATA of the Global Biodiversity Information Facility (GBIF);

Scientific Markup Languages Workshop in association with the NSF/National Science Digital Library (Denver, USA, 10–11 June 2005), at which I. D. Brown (Chair of COMCIFS) represented the IUCr in a presentation of the Crystallographic Information File format;

Annual Meeting of the CODATA Task Group on Fundamental Constants (Paris, France, 28 June 2005), confirming the schedule for publication of a revised set of recommended values for fundamental physical constants by the end of December 2006;

Workshop on Strategies for Permanent Access to Scientific Information in Southern Africa: Focus on Health and Environmental Information for Sustainable Development (Pretoria, South Africa, 5–7 September 2005), sponsored by the Task Group on Preservation of and Access to Scientific and Technical Data in Developing Countries (among the recommendations of this Workshop, focusing primarily on the African context, are mandates for scholars to expose their research *via* open access to preprints and e-prints, and for long-term curation of research outputs);

International Symposium on the Generalization of Information (Berlin, Germany, 14–16 September 2005);

International Symposium entitled Multimedia: Where Do We Go From Here? (Berlin, Germany, 19–20 September 2005), sponsored by the CODATA Task Group on Multimedia, Visualization, Data and Information;

formation of a Strategic Planning Committee arising from the recommendations for strategic development passed at the 24th CODATA General Assembly, in which the undersigned had some early involvement.

B. McMahon, IUCr Representative

14.5. ICSU Committee on Space Research (COSPAR)

COSPAR's objectives are to promote international level scientific research in space, with an emphasis on the exchange of results, information and opinions. COSPAR provides a forum, open to all scientists, for the discussion of problems that may affect scientific space research. These objectives are achieved through the organization of Scientific Assemblies, publications and other means.

COSPAR Colloquia and Workshops have been held regularly and Elsevier Science publishes the Proceedings in *Advances in Space Research*

The list of activities in 2005 is presented below:

UN/ESA/NASA Workshop on the International Heliophysical Year IHY 2007, Abu-Dhabi and Al-Ain, United Arab Emirates, 20–23 November 2005;

Solar Extreme Events: Fundamental Science and Applied Aspects (SEE 2005), Nor Amberd, Armenia, 26–30 September 2005;

Xth IUGG/IAGA Scientific Assembly, Toulouse, France, 18–29 July 2005;

URSI/COSPAR International Reference Ionosphere Workshop, Ebre Observatory, Roquetes, Spain, 27 June–1 July 2005;

15th Humans in Space Symposium, IAA, Graz, Austria, 22–26 May 2005;

4th European Conference on Space Debris, ESA, Darmstadt, Germany, 18–20 April 2005;

High Resolution and Hyperspectral Satellite Data Integration for Precision Farming, Environmental Monitoring and Possible New Applications, 21–22 February 2005.

The 68th COSPAR Bureau Meeting was held in Paris, France, 21–24 March 2005. The main issue was the formulation of a comprehensive list of recommendations from all the task groups involved in the reflection on the future of COSPAR, including interface with other organizations (particularly ICSU).

The next Bureau meeting is scheduled for the week of 20 March 2006. The next, 36th, COSPAR Scientific Assembly will be held in Beijing, People's Republic of China. Canada has issued an invitation to organize a COSPAR Assembly in 2008. Italy has also issued an informal invitation to COSPAR for either the same year or 2010.

As of 2005, the COSPAR President is R.-M. Bonnet (France) and the Vice-Presidents are W. Hermsen (The Netherlands) and E. C. Stone (USA).

The Scientific Commission on Materials Science in Space was chaired by R. Narayanan (USA), and co-Chaired by W.-R. Hu (People's Republic of China), V. Shevtsova (Belgium) and H. Kawamura (Japan).

H. A. Dabkowska, IUCr Representative

15. Finances

The Income and Expenditure account, Balance Sheet and Summary of Fund Accounts are given as Tables 2, 3 and 4, respectively (according to new auditing requirements, the full audited accounts must be made available exactly as prepared by the auditors and must not be reformatted for the journal). For comparison, the figures for 2004 are provided in italics. The accounts are presented in CHF. The full audited accounts are available from the IUCr electronic archives (Reference ES0355).[1]

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 2005 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, an apparent gain has arisen on the assets of the Union, in terms of CHF, amounting to CHF 314,091. The gain attributable to investment activities has been assigned to the General Fund and the gain attributable to trading activities has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 2005. It should be noted that this 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 2005.

The balance sheet shows that the assets of the Union, including the gain of CHF 314,091 resulting from fluctuations in rates of exchange, have increased during the year, from CHF 4,251,824 to CHF 4,710,914. The movement in market value of the investments was CHF 235,005 in 2005 (CHF 31,190 in 2004).

A transfer of CHF 150,000 was made to the Publications and Journals Development Fund from the *Acta Crystallographica* Fund. A transfer of CHF 150,000 was made to the Research and Education Fund from the *Acta Crystallographica* Fund. A transfer of CHF 40,000 was made to the Ewald Fund from the *Acta Crystallographica* Fund. A transfer of CHF 45,000 was made to the *Newsletter* Fund from the *Journal of Applied Crystallography* Fund. A transfer of CHF 15,000 was made to the President's Fund from the *Journal of Applied Crystallography* Fund. A transfer of CHF 75,000 was made to the Book 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 336,530, as compared with a deficit in 2004 of CHF 156,938. The administrative expenses were CHF 501,140 in 2005 as compared with CHF 476,276

[1] Services for accessing these data are described at the back of the journal.

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

	Swiss Francs			
	2005		*2004*	
Income				
Membership subscriptions		153,000		*142,246*
Sales				
Journals, back numbers and single issues	3,850,828		*3,731,939*	
Books	387,435		*345,896*	
Open Access Grant	72,475	4,310,738	*75,912*	*4,153,747*
Investment income				
Income from investments	153,116		*146,554*	
Bank interest	14,942		*14,897*	
(Loss)/profit on sale of investments	27,886	195,944	*21,019*	*182,470*
Other income				
Royalties and copyright fees	8,648		*8,340*	
Advertising income	240,022	248,670	*263,792*	*272,132*
Total Income		4,908,352		*4,750,595*
Expenditure				
Journals				
Publication costs	878,389		*892,027*	
Editorial expenses	363,937		*246,123*	
Technical editing	1,507,842		*1,481,533*	
Subscription administration	54,303	2,804,471	*50,841*	*2,670,524*
Books				
Publication costs	37,316		*62,527*	
Editorial expenses	100,350		*90,394*	
Technical editing	142,682	280,348	*57,776*	*210,697*
Newsletter				
Publication costs	93,268		*147,522*	
Editorial expenses	123,573	216,841	*82,199*	*229,721*
President's Fund Grants and Young Scientists' support		113,172		*130,618*
General Assembly costs		76,189		*19,589*
Ewald Prize		40,110		*743*
Committee meetings and expenses		123,345		*39,907*
Publications and journals development				
General	586,402		*561,216*	
Electronic Publishing Committee/Section Editors meeting expenses	1,997		*810*	
STAR/CIF	40,375		*57,243*	
Promotions Officer	173,082	801,856	*130,785*	*776,028*
Subscriptions paid		7,382		*8.968*
Visiting Professorship Programme		1,750		–
Administration expenses:				
General Secretary and Treasurer:				
Honorarium to Treasurer	11,377		*9,509*	
Audit and accountancy charges	72,169		*67,610*	
Legal and professional fees	14,549		*10,774*	
Travelling expenses	21,811		*18,981*	
Bank charges	2,423	122,329	*1,882*	*108,756*
Executive Secretary's office:				
Salaries and expenses	358,564		*350,500*	
Travel expenses of IUCr Representatives on other bodies	2,459		*6,437*	
Commission expenses	–		*8,928*	
Sponsorship of meetings	(17,282)		*13,923*	
President's secretary	6,780		*9,820*	
IUCr/FIZ agreement	(17,061)		(*14,492*)	
Bad debts	23,894	357,354	–	*375,116*
Depreciation		53,211		*63,307*
Total Expenditure		4,998,358		*4,633,974*

Table 2 (continued)

		2005		*2004*
		Swiss Francs		
(Deficit)/surplus) of income over expenditure		(90,006)		*116,621*
Movement in market value of investments in year		235,005		*31,190*
		144,999		*147,811*
Fluctuation in rates of exchange				
Trading activities	12,659		(*37,909*)	
Investment activities	301,432	314,091	(*260,745*)	(*298,654*)
Total recognized gains and losses relating to the year		459,090		(*150,843*)
Opening fund accounts at 1 January		4,251,824		*4,402,667*
Closing fund accounts at 31 December		4,710,914		*4,251,824*

All the income and expenditure related to continuing activities. Historic cost results would only differ from above by the loss 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.

in 2004. Of this amount, CHF 221,932 was charged to the publications of the Union.

The expenses of the Union Representatives on other bodies were CHF 2,459. The cost of the Finance Committee meetings held in 2005 was CHF 14,838, while the Executive Committee meeting cost CHF 108,507. The income from the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 17,061. The subscriptions from Adhering Bodies were CHF 153,000. Interest on bank accounts and investments credited to the General Fund was CHF 118,412.

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 1,866. Grants totalling CHF 15,500 were paid from the fund in 2005.

The *Acta Crystallographica* account for 2005 shows a surplus of CHF 402,141 before the transfer of CHF 340,000 to the other fund accounts, as compared with a surplus of CHF 535,564 in 2004 before the transfer of CHF 45,000 to the *Newsletter* Fund.

The subscription rates were increased for 2005. In 2005, the number of paid subscriptions to *Sections A+B+C(E)+D(F)* of *Acta*, including 22 (26) personal subscriptions, was 367 (429) (values for 2004 are given in parentheses). The number of paid subscriptions to *Sections A+B+C(E)*, including 7 (8) personal subscriptions, was 83 (105). The number of paid subscriptions to the separate sections of the journal were: *Section A* 230 (197 for 2004), *Section B* 201 (152), *Section C* 168 (118) and *Section D* 299 (263). 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 1,243,677 (for 12,986 published pages) as compared with CHF 1,156,794 in 2004 (10,175 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 144,262, as compared with a surplus of CHF 116,935 in 2004. In 2005, the number of paid subscriptions, including 86 (98 in 2004) personal subscriptions, was 608 (632 in 2004).

The *Journal of Synchrotron Radiation* account shows a deficit of CHF 81,791, as compared with a deficit of CHF 39,983 in 2004. In 2005, the number of paid subscriptions, including 59 (65 in 2004) personal subscriptions, was 213 (226 in 2004).

The *International Tables* account shows a surplus of CHF 28,025, as compared with a surplus of CHF 53,244 in 2004. The net sales income was CHF 287,893 in 2005 as compared with CHF 253,992 in 2004.

The Book Fund is credited with the sales of the remaining publications of the Union.

The *Newsletter* Fund account received a transfer of CHF 45,000 from the *Journal of Applied Crystallography* Fund in 2005 (CHF 45,000 from the *Acta Crystallographica* Fund in 2004). The cost to the Union of producing the *Newsletter* in 2005 was CHF 28,273 (CHF 50,592 in 2004).

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 2005, CHF 45,267 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 108,492 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.

Table 3
Balance sheet as at 31 December 2006.

	Swiss Francs			
	2005		*2004*	
FIXED ASSETS				
Tangible fixed assets		27,077		*34,536*
CURRENT ASSETS				
Stock		350,917		*330,864*
Cash at bank and in hand				
Current accounts	50,213		*3,620*	
Deposit and savings accounts	215,339		*78,571*	
Cash with Union officials	21,290	286,842	*17,812*	*100.003*
Investments at market value		3,867,338		*3,643,040*
Debtors, accrued income and payments in advance		611,534		*450,032*
Subscriptions due from Adhering Bodies		26,500		*27,485*
TOTAL CURRENT ASSETS		5,143,131		*4,550,424*
Creditors: amounts falling due within one year		(459,294)		(*333,136*)
NET CURRENT ASSETS		4,683,837		*4,217,288*
TOTAL FUNDS		4,710,914		*4,251,824*

Table 4
Summary of Fund Accounts as at 31 December 2006.

	Swiss Francs						
	As at 1 January 2005	Transfers between funds	(Deficit)/ excess of income over expenditure for the year	Increase in market value of investments	Fluctuations in exchange rates		Balance at 31 December 2005
					Trading	Investments	
FUND ACCOUNTS							
General Fund	350,512	–	(336,530)	235,005	716	301,432	551,135
President's Fund	90,155	15,000	(13,634)	–	264	–	91,785
Acta Crystallographica	972,497	(340,000)	402,141	–	2,979	–	1,037,617
Journal of Applied Crystallography	437,378	(135,000)	144,262	–	1,286	–	447,926
International Tables	107,795	–	28,025	–	391	–	136,211
Book Fund	(61,288)	75,000	(1,213)	–	36	–	12,535
Publications and Journals Development Fund	759,117	150,000	(79,157)	–	(2,390)	–	832,350
Research and Education Fund	903,618	150,000	(95,205)	–	2,759	–	961,172
Ewald Fund	499,285	40,000	(28,631)	–	1,470	–	512,124
Newsletter Fund	118,335	45,000	(28,273)	–	389	–	135,451
Journal of Synchrotron Radiation	74,420	–	(81,791)	–	(21)	–	(7,392)
	4,251,824	–	(90,006)	235,005	12,659	301,432	4,710,914