

Annex I

Appendices to the Agenda of the Twentieth General Assembly

1. Appendix A: Report of the Executive Committee

1.1. Executive Committee and Finance Committee meetings

The Executive Committee met in Geneva in August 2002 before and during the General Assembly, in Broome, Australia, in August 2003 at the time of the Joint meeting of AsCA '03 and Crystal-23 and in Budapest, Hungary, in August 2004 at the time of the Twenty-Second European Crystallographic Meeting. The Finance Committee met in March 2002, March 2003, March 2004 and August 2004, to prepare its advice and recommendations on finances, establishment and staff matters.

The most important items of business dealt with by the Executive Committee during the triennium were:

(1) editorial policy, pricing policy and subscription rates, consideration of appointment of new Editor-in-Chief and Editors for *Acta Cryst.* Sections D and F, approval of appointments of Co-editors and Book Review Editor, appeal procedure for aggrieved authors, electronic publishing, archival policy, Special Issues, open access, and other matters concerning the IUCr journals;

(2) launch of *Acta Cryst.* Section F *Structural Biology and Crystallization Communications*;

(3) Facility Information pages for *Journal of Synchrotron Radiation*;

(4) review of contract with Blackwell Munksgaard;

(5) review of structure and work of Promotion Committee;

(6) approval of the audited accounts;

(7) General Fund estimates and the level of the unit contribution, status of membership subscriptions;

(8) investment policy;

(9) funding and uses of the Publications and Journals Development Fund and the Research and Education Fund;

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

(11) Journal Grants Fund;

(12) cooperation with databases, open-access databases;

(13) progress with Volumes A, A1, B, C, D, E, F, F1 and G of *International Tables* and development of associated software, consideration of suggestions for new volumes, development work to put *International Tables* online;

(14) review of contract with Springer (formerly Kluwer);

(15) the *IUCr Newsletter*, the *World Directory of Crystallographers*;

(16) promotional activities;

(17) appointment of the Selection Committee for the seventh Ewald Prize;

(18) discussion of the arrangements for the Florence Congress;

(19) approval of the membership of the Programme Committee for the Florence Congress;

(20) level of financial support for the Florence Congress;

(21) nominations for Officers of the IUCr and for Chairs and members of Commissions, proposals from the National Committees for these positions.

(22) voting procedures for members of Executive Committee; size of Executive Committee.

Other items dealt with in this way were:

(23) implementation of the Crystallographic Information File (CIF) for *Acta Cryst.* and other uses of CIF, trademark application and adoption of the STAR file and CIF by other bodies, work of the Committee for the Maintenance of the CIF Standard (COMCIFS), provision of checking services to other publishers, support for mmCIF project and CIF handling software;

(24) approval of publications, jointly with Oxford University Press, in the IUCr/OUP Book Series;

(25) crystallography in Africa;

(26) relations with other Scientific Unions;

(27) Inter-Union Bioinformatics Group;

(28) review of the activities of Commissions;

(29) review of the activities of Regional Associates;

(30) review of the reports of IUCr Representatives on other bodies;

(31) review of the reports of the Committee on Crystallographic Databases;

Items concerning the Chester office were:

(32) staffing requirements in the IUCr office in Chester;

(33) preparation of revised job descriptions and revision of staffing structure;

(34) upgrading office technology in the IUCr office in Chester, provision of internet services.

1.2. Publications

The subscription prices of *Acta Crystallographica*, the *Journal of Applied Crystallography* and the *Journal of Synchrotron Radiation* were increased each year during the triennium.

The total annual number of pages published in 2002, 2003 and 2004 were:

	2002	2003	2004
<i>Acta Crystallographica Section A</i>	630	628	644
<i>Acta Crystallographica Section B</i>	1,088	821	763
<i>Acta Crystallographica Section C</i>	1,570	1,482	1,694
<i>Acta Crystallographica Section D</i>	2,243	2,385	2,406
<i>Acta Crystallographica Section E</i>	2,374	3,419	4,676
<i>Journal of Applied Crystallography</i>	760	1,505	1,041
<i>Journal of Synchrotron Radiation</i>	413	475	512
Total	9,078	10,715	11,736

In 2002, *Acta Cryst.* Section D contained the Proceedings of ICCBM-9, Jena, Germany, the Proceedings of the 2002 CCP4 Study Weekend on High-Throughput Structure Determination and a Special Issue on Databases jointly with Section B. In 2003, *JAC* contained papers presented at SAS 2002, Venice, Italy, and *Acta Cryst.* Section D contained the Proceedings of the 2003 CCP4 Study Weekend on Experimental Phasing. In 2004, *JSR* contained the

Proceedings of an International Symposium on Diffraction Structural Biology (ISDSB 03), Tsukuba, Japan, and *Acta Cryst.* Section D contained the Proceedings of the 2004 CCP4 Study Weekend on Model Building and Refinement. Various themed issues were also published during the triennium.

All the IUCr journals are available electronically through the **Crystallography Journals Online** service, including all back issues of the journals from 1948, and also through Blackwell Synergy.

The IUCr has two fully electronic journals available online only (*Acta Crystallographica* Section E: *Structure Reports Online* launched in 2001 and *Acta Crystallographica* Section F: *Structural Biology and Crystallization Communications* launched in 2005). Section E is available free of charge to subscribers to Section C, and Section F is available free of charge to subscribers to Section D.

The IUCr home page on the web (<http://www.iucr.org/>) continues to expand. It contains information in the following categories: The Union and its Components (including information on Adhering Bodies, Commissions, Regional Associates, Annual Reports, Congress Reports *etc.*); Journals and Other Publications (including information on the titles, synopses, structural schemes and contents of the IUCr journals); and Services (including the *World Database of Crystallographers* and *Crystallography News Online*). The number of requests per day is typically of the order of 155,000 from about 33,000 unique hosts.

Full details on the publication of volumes of *International Tables for Crystallography* are given in the Triennial Report of this Commission (Appendix D to the Agenda).

The *World Database of Crystallographers* continues to undergo major development to provide increased functionality and to allow online amendments and additions to be made by individual crystallographers.

The *IUCr Newsletter* is distributed free of charge to 587 libraries and 15,000 crystallographers and other interested individuals in 39 countries. J. L. Flippen-Anderson is the Editor with the editorial office at the Hauptman-Woodward Medical Research Institute at Buffalo, New York, USA, which also handles the distribution. A report on the *IUCr Newsletter* is given in Appendix H to the Agenda.

The IUCr/Oxford University Press Book Series continues to be successful. Details are given in Appendix I to the Agenda.

1.3. Sponsorship of meetings

The Sub-committee on the Union Calendar considers and advises the Executive Committee on requests for IUCr sponsorship and financial support of meetings. The Chair of the Sub-committee has been M. A. Carrondo in this triennium. A list of IUCr-sponsored meetings is given in Appendix J to the Agenda.

Applications for sponsorship are considered if they are submitted at least nine months in advance of the date of the meeting. Applications will be considered by the Committee four times a year at the end of March, June, September and December. Applications for sponsorship should be timed accordingly. For example, for a meeting to be held in June an application should be submitted by September of the previous year at the latest.

Requests from satellite meetings must be submitted, and possible financial support requested, through 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 requires the approval of the Chair of the

Congress Programme Committee. 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 (American Crystallographic Association, Asian Crystallographic Association, European Crystallographic Association) 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.

IUCr sponsorship can only be given to meetings that are international in character and open to participants from all countries. The membership of the Programme Committee is a good indication of this.

Active crystallographers should be involved in the organization of the conference and one or more sessions should deal with specific crystallographic topics. This does not automatically include any session on condensed matter physics, materials science or symmetry not related to crystallography. According to these criteria, all meetings organized by IUCr Commissions automatically qualify.

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

General financial support can be given to all meetings except those that form part of a continuing series. However, this restriction does not apply to schools or to meetings regularly organized by IUCr Commissions.

Explicit support from the relevant IUCr Commission(s) is strongly recommended for any meeting.

Travel support for young scientists is available for all meetings (including schools). This money should not be used for waiver of registration fees.

Consideration should be given as to whether the proposed meeting is appropriate in subject, form and timing with respect to other related meetings.

Except in special cases, IUCr funds should not be used to sponsor more than one event per year in the same location.

1.4. Commissions of the IUCr

Each Commission Chair is required to provide a written triennial report to the General Assembly. These reports are included as Appendices to the Agenda. Financial assistance has again been offered to the Commission Chairs, to enable them to attend the General Assembly for the presentation and discussion of their reports and to meet the Executive Committee prior to the General Assembly.

1.5. Regional Associates, Scientific Associates, and other bodies

The reports of the Representatives on these bodies are given as separate Appendices to the Agenda.

1.6. IUCr staff

There have been some staff changes during the triennium. The present members of staff in the IUCr offices in Chester are: M. H. Dacombe (Executive Secretary), M. J. Robinson (Administrative Assistant to the Executive Secretary), P. R. Strickland (Managing Editor), S. E. Barnes (Senior Technical Editor), B. McMahon (Research and Development Officer), C. A. Moore (Editorial Systems Developer), A. S. Berry, G. F. Holmes, L. E. Jones, J. K.

Bradshaw, S. Conway, A. Weight and N. J. Ashcroft (Technical Editors), S. Froggatt, S. Glynn and L. Stephenson (Assistant Technical Editors), M. A. Hoyland, D. Holden and D. Hoare (Systems Developers), L. Rathbone (Journals Production Assistant), C. Cook (Administrative Assistant) and A. J. Sharpe (Promotions Officer).

1.7. Acknowledgements

On behalf of the IUCr, the Executive Committee wishes to express its deep gratitude to the National Research Council and the Italian National Committee for Crystallography for the invitation to hold the Twentieth General Assembly and International Congress of Crystallography in Florence. It particularly wishes to thank the Chair of the Programme Committee, C. Mealli, and the Chair of the Organizing Committee, P. Paoli.

Finally, the Executive Committee wishes to thank all crystallographers who have assisted in the work of the IUCr in so many ways. This cooperation between crystallographers of different nationalities constitutes a most valuable aspect of the IUCr's activities.

2. Appendix B: Financial Report

The accounts of the IUCr for the calendar years 2002, 2003 and 2004 have already been published [*Acta Cryst.* (2003), **A59**, 374–433; (2005), **A61**, 265–299; (2005), **A61**, 586–620]. The accounts for the three years 2002, 2003 and 2004 are summarized in Tables 1–15. All amounts are expressed in Swiss Francs. The notations used in this report for the various currencies of the IUCr's activities are CHF = Swiss Franc, GBP = Pound Sterling, USD = US Dollar.

2.1. General financial development

Table 1 shows a comparison of the fund accounts at the beginning and the end of the triennium. The total assets have decreased by CHF 1,301,751 from CHF 5,553,575 to CHF 4,251,824, or 23%, over the triennium. These figures include the fluctuations in exchange rates. If the exchange-rate fluctuations are disregarded, the total assets decreased by CHF 1,383,526 from CHF 5,934,004 to CHF 4,550,478, or 23%, over the triennium. Part of this reduction is attributable to the volatility of the markets (see General Fund below).

Table 2 shows the distribution of the assets. The great majority of the amounts under debtors and creditors have been settled since year end.

The total holding of investments at 31 December 2004 is CHF 3,642,040 at market value, as shown in Table 2, of which 34% is held by Merrill Lynch and 66% by Close Brothers. The IUCr bank accounts and short-term deposits are held with the Union Bank of Switzerland, the National Westminster Bank and Merrill Lynch, involving the currencies CHF, GBP and USD.

As an association incorporated in Switzerland, the IUCr is exempt from Swiss Federal and Geneva Cantonal Tax. Under the terms of the United Kingdom/Switzerland Double Taxation Agreement dated 8 December 1977, investment income arising within the UK under present circumstances is not subject to United Kingdom tax. Investment income received from other countries with which Switzerland has a Double Taxation Agreement is also exempt from tax. In October 1985, a recognition of tax-exempt status in the USA was received from the Internal Revenue Service, Department of the US Treasury.

Table 1
Balance Sheet, Fund Accounts (Swiss Francs).

	31 December 2001	Fluctuations in rates of exchange	31 December 2004
General Fund	2,253,503	−791,637	350,512
President's Fund	56,803	−1,710	90,155
<i>Acta Crystallographica</i>	810,560	−15,740	972,497
<i>Journal of Applied Crystallography</i>	202,815	−7,700	437,378
<i>Journal of Synchrotron Radiation</i>	103,877	−2,060	74,420
<i>International Tables</i>	−2,025	−1,039	107,795
Book Fund	−31,489	258	−61,288
Publications and Journals			
Development Fund	567,419	−16,244	759,117
Research and Education Fund	959,904	−19,603	903,618
Ewald Fund	483,945	−9,803	499,285
Newsletter Fund	148,263	−2,376	118,335
Total accumulated balance	5,553,575	−867,654	4,251,824
Excluding exchange rates	5,934,004		4,550,478

Table 2
Balance sheet, Assets (Swiss Francs).

	31 December 2001	31 December 2004
Fixed assets		
Tangible fixed assets	97,216	34,536
Current assets		
Stock	77,359	330,864
Cash at banks and in hand		
Current accounts	62,708	3,620
Deposit and savings accounts	244,167	78,571
Cash with Union officials	29,466	17,812
Investments at market value	4,772,261	3,642,040
Debtors, accrued income and payments in advance	450,736	450,032
Subscriptions due	23,874	27,485
Total current assets	5,660,571	4,550,424
Deduct Creditors and accrued charges	−204,212	−333,136
Net current assets	5,456,359	4,217,288
Total assets	5,553,575	4,251,824

Income and expenditure account

In order to present an overall picture of the state of the Union's affairs an income and expenditure account for the triennium is included (based on ICSU format) as Table 3. This shows that following a period when the Union was operating at a loss owing to the investment in developing **Crystallography Journals Online** and new and revised versions of *International Tables for Crystallography*, it is now operating with a small surplus of income over expenditure. The Union is predicted to continue to operate with a small surplus in the coming triennium.

2.2. General Fund

Table 4 shows the accounts for the General Fund and Table 5 compares these accounts for the triennium with the budget approved by the Geneva General Assembly. This fund carries the income and expenditure related to the IUCr's administration and its regular scientific activities, other than publications. The income has two main sources, the subscriptions from Adhering Bodies and the interest

international union of crystallography

Table 3
Income and expenditure (ICSU format).

	2002		2003		2004	
Income						
Contributions from national members		148,000		148,215		142,246
Sales of publications, royalties		4,263,605		3,671,094		4,425,879
Bank interest/investment income						
plus profit on disposals		94,464		207,830		182,470
Other income		14,874		16,960		14,492
Total income			4,520,943		4,044,099	4,765,087
Expenditure						
<i>(a) Scientific activities</i>						
General Assembly	57,155			-924		19,589
Scientific meetings: symposia/research and education	167,317		175,441		138,345	
Representation at scientific meetings	3,379		4,322		6,437	
Grants to individuals/organizations	19,891		0		6,196	
Other	49,005	297,368	8,957	190,484	9,671	237,481
<i>Routine meetings</i>						
Executive Committee/Finance Committee		104,458		65,886		39,907
Publications		3,611,188	4,013,014	3,325,234	3,581,604	3,829,727
						4,107,115
<i>(b) Other activities</i>						
Contribution to ICSU	9,003			8,837		7,987
Contribution to other ICSU bodies (ICSTI)	968	9,971	963	9,800	981	8,968
<i>Administrative expenses</i>						
Salaries and related charges	281,247		275,808		280,400	
General office expenses	92,929		98,285		108,410	
Office equipment	75,127		70,526		63,307	
Audit fees, legal fees	86,414		69,510		78,384	
Bank charges	2,772	538,489	548,460	1,437	515,566	525,366
Total expenditure			4,561,474		4,106,970	532,383
						541,351
						4,648,466
Excess/deficit of income over expenditure			-40,531			-62,871
Increase/decrease in market value of investments			-751,472			272,966
Profit/loss on exchange rate fluctuations			-278,387			-290,613
Accumulated balance at 1 January			5,553,575			4,483,185
Accumulated balance at 31 December			4,483,185			4,402,667
						4,251,824

income from investments and bank accounts. The subscriptions from Adhering Bodies are based on the unit contribution, which was CHF 1,000 for 2002, 2003 and 2004. The total number of membership units was 154 for 2002 and 149 for 2003 and 2004. The yield from investments is less than the budgeted amount by CHF 478,827. This is mainly because the holdings that had been with Foreign & Colonial had to be moved in 2003 when the Funds were closed. Favourable arrangements were made with Close Brothers for the transfer of the holdings at no cost but the income that would otherwise have been derived from the Foreign & Colonial holdings in 2003 was not realized. Instead, this income was included in the market value. The decline in the world markets adversely affected the assets of the IUCr during the triennium (especially during 2002). However, it should be noted that the investments are held primarily for long-term gain and now that the Union is operating with a surplus there should be no need to realize any of the investments to any significant extent. There has been a move to increase the proportion of the investments held as bonds and cash to about 40% (from about 30% at the time of the Geneva Congress).

The administration expenses for the journals are calculated as 45% of the general administration costs of the IUCr, including the work of the Executive Secretary and his office and of the General Secretary and Treasurer. The Executive Committee met annually, while the Finance Committee held one meeting in each of 2002 and 2003 and

two meetings in 2004. The cost of these meetings varies, as seen from Table 4, depending on the location and the circumstances. In Table 5 they are included in the expenses of administrative meetings, together with the costs of the IUCr representatives on other bodies. The expenses of scientific meetings in Table 5 include the travel grants and other expenses for the Geneva Congress in 2002, the cost of the 2004 meeting of the Programme Committee for the Florence Congress, the expenses of the non-publishing Commissions, financial support to meetings and schools, and the IUCr/FIZ Agreement (which generated income in each year of the triennium). Proportions of the Research and Development and promotion costs are charged to the General Fund. The financial support for young scientists attending meetings and schools is charged to the Research and Education Fund, see Table 13.

In Table 5, the unfavourable deviation from budget of CHF 508,038 is almost entirely accounted for by the low income from investments mentioned above. Overall expenditure over the triennium was 1.3% higher than predicted.

2.3. President's Fund

Table 6 gives the account for the President's Fund. It is intended mainly for use in emergencies and under special or difficult circumstances, to help crystallographers from countries with currency

Table 4
General Fund (Swiss Francs).

	2002	2003	2004
Income			
Subscriptions from Adhering Bodies	148,000	148,215	142,246
Yield from investments and bank accounts (including profit/loss on disposal of investments)	-13,077	157,173	127,077
Amount charged to other Funds:			
<i>Acta Crystallographica</i>	181,534	160,712	181,948
<i>Journal of Applied Crystallography</i>	17,107	27,793	18,599
<i>Journal of Synchrotron Radiation</i>	9,469	9,028	9,142
	<u>343,033</u>	<u>502,921</u>	<u>479,012</u>
Expenditure			
Administration	472,764	449,259	476,276
Subscriptions to ICSU/ICSU bodies	9,971	9,800	10,568
Executive Committee	92,439	54,125	28,990
Finance Committee	12,019	11,761	10,917
19th General Assembly and Congress expenses	57,155	-924	-
20th General Assembly and Congress Programme Committee	-	-	19,589
IUCr Representatives on other bodies	3,379	4,323	6,437
Expenses of Commissions	-	8,957	8,928
Sponsorship of meetings	46,764	16,426	13,923
President's secretarial	4,135	9,542	9,820
IUCr/FIZ Agreement	-14,874	-13,609	-14,492
Promotion	16,892	14,517	17,400
Programming and development costs	43,828	44,405	49,194
	<u>744,472</u>	<u>608,582</u>	<u>635,950</u>
<i>Excess/deficit of income over expenditure</i>	<u>-401,439</u>	<u>-105,661</u>	<u>-156,938</u>
Fluctuations in rates of exchange	<u>-254,507</u>	<u>-271,249</u>	<u>-265,881</u>
Movement in market value	<u>-751,472</u>	<u>272,966</u>	<u>31,190</u>
Accumulated balance at end of year	<u>846,085</u>	<u>742,141</u>	<u>350,512</u>

Table 5
General Fund. Comparison of budget and accounts for the years 2002–2004 inclusive (Swiss Francs).

	Budget		Accounts		Difference	
Income						
Subscriptions from Adhering Bodies	450,000		438,461		-11,539	
Yield from investments and bank accounts (including profit/loss on disposal of investments)	750,000		271,173		-478,827	
Grants from UNESCO/ICSU	0	1,200,000	0	709,634	0	-490,366
Expenditure						
Administration (net)	940,000		992,700		52,700	
Subscriptions to ICSU/ICSU bodies	33,000		28,739		-4,261	
Administrative meetings	272,500		224,390		-48,110	
Scientific meetings	110,500		127,843		17,343	
Transfers to other Funds	0	1,356,000	0	1,373,672	0	17,672
Unfavourable variant from budget						-508,038
Estimated profit or deficit		<u>-156,000</u>				<u>-156,000</u>
<i>Deficit of income over expenditure</i>				<u>-664,038</u>		<u>-664,038</u>

problems to take part in the activities of the IUCr (especially in connection with the triennial Congresses).

2.4. Journals Funds

Tables 7, 8 and 9 give the accounts for *Acta Crystallographica* (*Acta*), the *Journal of Applied Crystallography* (*JAC*) and the *Journal of Synchrotron Radiation* (*JSR*). The total numbers of pages printed

for *Acta*, *JAC* and *JSR* were 9,078, 10,715 and 11,736 in 2002, 2003 and 2004, respectively. The Finance Committee and the Executive Committee have monitored the financial development for all journals very closely. The total number of subscriptions (including full and reduced-rate) decreased by about 5% p.a. over the triennium. The **Crystallography Journals Online** service has been available throughout the triennium and has been a great success. It is accessed by more than 33,000 unique hosts and receives on average about

Table 6
President's Fund (Swiss Francs).

	2002	2003	2004
Income			
Donations, transfers and interest	2,215	1,717	2,217
Expenditure			
Grants	19,891	0	6,196
<i>Excess of income over expenditure</i>	<i>-17,676</i>	<i>1,717</i>	<i>-3,979</i>
Transfers from other Funds:			
<i>Acta Crystallographica</i>	30,000	25,000	-
Fluctuations in rates of exchange	-451	-502	-757
Accumulated balance at end of year	68,676	94,891	90,155

155,000 requests per day. The online-only *Acta* Section E *Structure Reports Online* was launched at the beginning of 2001 and is accessible free of charge to subscribers to *Acta* Section C. The online-only *Acta* Section F *Structural Biology and Crystallization Communications* was launched at the beginning of 2005 and is accessible free of charge to subscribers to *Acta* Section D. For further details see the Triennial Report by the Chair of the Commission on Journals (Appendix D to the Agenda).

2.5. International Tables

The *International Tables* accounts are shown in Table 10. Volume A (*Space-Group Symmetry*) had been out of print in 2000 and 2001 and a large number of orders had built up for the revised edition that was published in 2002. New Volumes published in the triennium were Volume A1 (*Symmetry Relations between Space Groups*) and Volume D (*Physical Properties of Crystals*). Volume E (*Subperiodic Groups*) was published in December 2002. For further details see the Triennial Report by the Chair of the Commission on International Tables (Appendix D to the Agenda).

2.6. Book Fund

Table 11 gives the accounts of the Book Fund. The accumulated balance of this fund became negative during 2004 as a result of the large amount of work involved with updating and re-structuring the *World Database of Crystallographers*.

2.7. Publications and Journals Development Fund

Table 12 shows the accounts of the Publications and Journals Development Fund. This fund was established in 1984 and has been built up through transfers from other funds. In order to build up the fund further and in a systematic way, with the goal to make it self-supporting, in 1989 the Executive Committee decided to increase its balance by crediting it with interest currently calculated as 2.5% of the balance of the fund, as shown in Table 12. During the triennium the major expenses are related to the purchase of computer hardware and software, programming and development, promotion, a digitization project to make all back issues of the journals available online, Special Issue costs and a project for the preparation of a list of mmCIF data items and templates to enable data deposited with the Protein Data Bank to be suitable for submission to IUCr journals. It

remains the policy of the Executive Committee to support and encourage the IUCr's highly qualified staff by supplying them with the best equipment. Also charged to this fund are costs of maintaining **Crystallography News Online**, the crystallographic neXus project (for making CD-ROMs containing a wealth of crystallographic software, extracts of web sites *etc.* available free of charge to those in developing countries who do not have ready access to the web) and support for the Journal Grants Fund. As the programming and development activities underpin much of the Union's activity, in 1997 the Executive Committee decided that the associated costs should be assigned to the Journals Funds, the *International Tables* Fund and the General Fund. In 2001, this principle was extended to the promotion expenses.

2.8. Research and Education Fund

Table 13 shows the accounts of the Research and Education Fund. The fund was also established in 1984 and, like the Publication and Journals Development Fund, has been built up through transfers from other funds. This fund is currently increased by 2.5% p.a., taken from the interest income. CHF 378,238 was given as young scientist's support during the triennium. Other expenditure involved the Visiting Professorship Programme and a project to support a PhD student as part of the Crystallography in Africa initiative.

2.9. Ewald Fund

The accounts of the Ewald Fund are given in Table 14. The interest on the capital is intended to cover the costs of the Prize. It is calculated as 2.5% of the balance in the fund, and is taken from the total annual interest income received from the IUCr's investments, in the same way as for the interest credited to the Publications and Journals Development Fund and to the Research and Education Fund. The balance of the interest from the investments is credited to the General Fund. An additional CHF 25,000 has been transferred to the fund during the triennium.

2.10. Newsletter Fund

Table 15 shows the accounts of the *Newsletter* Fund. The fund was established in 1994 following the successful launch of the *IUCr Newsletter* in 1993 (when the expenses were charged to the General Fund). The *IUCr Newsletter* is currently distributed free of charge to 587 libraries and 15,000 crystallographers and other interested individuals in 39 countries. The costs to the IUCr were CHF 87,795 in 2002, CHF 29,165 in 2003 and CHF 50,592 in 2004.

3. Appendix C: Ewald Prize

The establishment of the Ewald Prize, for outstanding contributions to the science of crystallography, was announced in February 1986 and was given wide publicity. The name of the Prize was chosen with the kind consent of the late Paul Peter Ewald, to recognize Professor Ewald's significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography, especially his services as the President of the Provisional International Crystallographic Committee from 1946 to 1948, as the first Editor of the IUCr's publication *Acta Crystallographica* from 1948 to 1959, and as the President of the IUCr from 1960 to 1963.

Shortly after the death of Professor Ewald in 1985, his family informed the President that Professor Ewald had wished to make a

Table 7
Acta Crystallographica (Swiss Francs).

	2002	2003	2004		
Income					
Subscriptions and sales of back numbers and single issues	2,831,674	2,393,390	3,052,467		
Distribution costs charged to subscribers	100,147	94,201	–		
Special Issue income	45,771	22,637	13,305		
Royalties, copyright fees	22,510	17,827	23,353		
Pay per view and secondary services (net)	10,364	9,634	19,924	3,010,466	2,537,689
<i>Less</i> Publisher's commission	–205,091	–172,494	–350,478		
Yield from advertisements	8,134	16,565	33,126		
Recharge/Recredit to Publications and Journals Development Fund for Special Issues	–1,615	–11,692	–	2,811,894	2,370,068
Expenditure					
Publication expenses					
Production	431,187	344,023	336,646		
Distribution and postage	86,030	88,220	–		
Net profit on offprints	–24,862	–31,637	–14,308		
Special Issue costs	44,156	10,945	13,305		
Editorial expenses, including Promotion	1,336,280	1,338,365	1,487,161		
Programming and development	180,133	259,763	251,381		
Administration expenses	181,534	160,712	181,948	2,234,458	2,170,391
<i>Excess of income over expenditure</i>				577,436	199,677
Transfers to other Funds:					
President's Fund	–30,000	–25,000	–		
Publications and Journals Development Fund	–270,000	–250,000	–		
<i>Journal of Synchrotron Radiation</i>	–50,000	–30,000	–		
Research and Education Fund	–50,000	–30,000	–		
Book Fund	120,000	20,000	–		
<i>Newsletter</i> Fund	–25,000	–	–45,000	–625,000	–465,000
Fluctuations in rates of exchange	–4,977	–2,593	–8,170		
Accumulated balance at end of year				758,019	490,103

bequest to the IUCr. After consulting Mrs Ewald, this generous bequest, together with a donation from the Ewald family and a donation from the IUCr, was used as starting capital for the Ewald Prize. The interest from this capital and further donations from the IUCr are used to finance the Prize.

The Prize consists of a medal, a certificate and an award of USD 30,000. It is presented once every three years during the triennial International Congresses of Crystallography. The first Prize was presented during the Perth Congress, being awarded jointly to J. M. Cowley and A. F. Moodie. The second Prize was presented during the Bordeaux Congress to B. K. Vainshtein. The third Prize was presented during the Beijing Congress to N. Kato. The fourth Prize was presented during the Seattle Congress to M. G. Ross-mann. The fifth Prize was presented during the Glasgow Congress to G. N. Ramachandran. The sixth Prize was presented during the Geneva Congress to M. M. Woolfson. In January 2005, it was announced that the seventh Ewald Prize had been awarded to Professor P. Coppens for his contributions to developing the fields of electron density determination and the crystallography of molecular excited states, and for his contributions to the education and inspiration of young crystallographers as an enthusiastic teacher by participating in and organizing many courses and workshops.

The presentation of the Ewald Prize was made during the Congress Opening Ceremony.

4. Appendix D: Reports of Commissions of the Union

4.1. Commission on Journals

4.1.1. Overview. Comparing the year-ends of the last three triennia, 11,736 journal pages were published in 2004, compared with 9,215 in 2001 and 7,937 in 1998. This increase in the number of pages has been accompanied by a major reduction in publication times for all sections of *Acta Cryst.*, *J. Appl. Cryst.* and *J. Synchrotron Rad.* Thus, for *Acta Cryst.* Sections A, B, C and D in 2004 publication times were 6.2, 4.8, 2.3 and 4.3 months *versus* 12 months for each in 1995; the 2004 times for *Acta Cryst.* Section E, *J. Appl. Cryst.* and *J. Synchrotron Rad.* were 0.8, 6.7 and 6.5 months, respectively. This improvement has happened owing to measures introduced to metricate individual Co-editor review times and to improved efficiency in the technical editing, all aided by e-mail and use of the web. The latest initiative aimed at efficiency, an electronic submission system for articles, introduced in 2003, has been very popular with Co-editors and authors.

Financially, the overall subscriptions situation has remained positive in a challenging climate. There is an annual attrition of subscriptions but at approximately 5% this is less than the average of 7% generally experienced by science journals. Prudent attention to setting of year-on-year subscription rates by the IUCr Finance Committee through the triennium has kept IUCr journals generating a surplus overall. Strong challenges have surfaced in 2004 as the US

international union of crystallography

Table 8

Journal of Applied Crystallography (Swiss Francs).

	2002	2003	2004
Income			
Subscriptions and sales of back numbers and single issues	436,036	372,954	459,611
Distribution costs charged to subscribers	14,623	14,741	–
Special Issue income	–	12,321	127
Royalties, copyright fees	3,575	2,368	2,120
Pay per view and secondary services (net)	2,960	1,666	2,037
	<u>457,194</u>	<u>406,001</u>	<u>465,662</u>
<i>Less</i> Publisher's commission	–31,375	–27,067	–68,332
Yield from advertisements	11,245	8,850	9,106
Recharge/Recredit to Publications and Journals			
Development Fund for Special Issues	–	41,380	–127
	<u>437,064</u>	<u>429,164</u>	<u>406,309</u>
Expenditure			
Publication expenses			
Production	43,874	67,494	68,595
Distribution and postage	12,080	27,457	–
Net profit on offprints	–3,376	–3,611	–6,406
Special Issue costs	–	53,701	–
Editorial expenses, including Promotion	187,139	135,546	187,704
Programming and development	28,050	22,646	31,976
Administration expenses	17,107	27,793	18,599
	<u>284,874</u>	<u>331,026</u>	<u>289,374</u>
<i>Excess of income over expenditure</i>	<u>152,190</u>	<u>98,138</u>	<u>116,935</u>
Transfers to other Funds:			
<i>Newsletter</i> Fund	–25,000	–45,000	–
Book Fund	–	–	–30,000
Ewald Fund	–	–25,000	–
	<u>–25,000</u>	<u>–70,000</u>	<u>–30,000</u>
Fluctuations in rates of exchange	–2,153	–1,873	–3,674
Accumulated balance at end of year	<u>327,852</u>	<u>354,117</u>	<u>437,378</u>

Table 9

Journal of Synchrotron Radiation (Swiss Francs).

	2002	2003	2004
Income			
Subscriptions and sales of back numbers and single issues	159,325	146,093	205,596
Distribution costs charged to subscribers	2,441	4,521	–
Special Issue income	659	1,177	30,024
Royalties, copyright fees	1,209	1,928	3,372
Pay per view and secondary services (net)	1,480	542	1,002
	<u>165,114</u>	<u>154,261</u>	<u>239,994</u>
<i>Less</i> Publisher's commission	–11,230	–10,534	–49,896
Yield from advertisements and Facility Information pages	5,504	11,367	42,431
Recharge/Recredit to Publications and Journals			
Development Fund for Special Issues	–659	15,086	28,813
	<u>158,729</u>	<u>170,180</u>	<u>261,342</u>
Expenditure			
Publication expenses			
Production	27,682	27,553	31,571
Distribution and postage	4,444	4,654	–
Net profit on offprints	–3,562	–190	–1,394
Special Issue costs	–	16,263	58,837
Editorial expenses, including Promotion	138,727	129,517	171,193
Programming and development	9,204	23,534	31,976
Administration expenses	9,469	9,028	9,142
	<u>185,964</u>	<u>210,359</u>	<u>301,325</u>
<i>Excess/Deficit of income over expenditure</i>	<u>–27,235</u>	<u>–40,179</u>	<u>–39,983</u>
Transfers from other Funds:			
<i>Acta Crystallographica</i>	50,000	30,000	–
<i>Journal of Applied Crystallography</i>	–	–	–
	<u>50,000</u>	<u>30,000</u>	<u>–</u>
Fluctuations in rates of exchange	–826	–609	–625
Accumulated balance at end of year	<u>125,816</u>	<u>115,028</u>	<u>74,420</u>

Table 10
International Tables (Swiss Francs).

	2002		2003		2004	
Income						
Sales:						
Volume A	259,939		70,678		97,519	
Volume A Teaching Edition	16,079		8,417		116	
Volume A1	–		–		20,687	
Volume B	43,539		27,481		25,463	
Volume C	39,735		25,029		70,854	
Volume D	–		50,644		57,085	
Volume E	6,561		55,493		17,968	
Volume F	114,311		60,893		47,236	
Less Publisher's commission	–124,449	355,715	–77,304	221,331	–88,837	253,992
Expenditure						
Production Volume A	26,386		9,056		10,354	
Production Volume A Teaching Edition	266		3,000		2,123	
Production Volume A1	–		–		4,901	
Production Volume B	5,096		3,291		2,639	
Production Volume C	4,948		4,235		12,521	
Production Volume D	–		7,974		18,231	
Production Volume E	5,645		4,253		3,848	
Production Volume F	13,209		6,589		6,542	
Editorial expenses	187,384		39,067		67,583	
Promotion	16,891		14,517		17,400	
Programming and development	118,335	378,160	49,289	141,271	54,606	200,748
Excess/Deficit of income over expenditure		–22,445		80,060		53,244
Fluctuations in rates of exchange		160		–293		–906
Accumulated balance at end of year		–24,310		55,457		107,795

Table 11
Book Fund (Swiss Francs).

	2002		2003		2004	
Income						
Sales:						
<i>Historical Atlas of Crystallography</i>	86		2		138	
<i>World Directory of Crystallographers</i>	1		4,030		2,821	
<i>Escher Kaleidozyklen</i>	45		176		–	
<i>Structure Reports</i>	70		964		406	
Sundry publications	–		–		108	
Royalties						
IUCr/OUP Book Series	3,653	3,855	2,479	7,651	1,081	4,554
Expenditure						
<i>World Directory of Crystallographers</i>	1,824		1,584		1,368	
Programming and development	48,211		19,538		94,784	
Promotion	16,891	66,926	14,517	35,639	17,400	113,552
Deficit of income over expenditure		–63,071		–27,988		–108,998
Transfers from other Funds:						
<i>Journal of Applied Crystallography</i>	–		–		30,000	
<i>Acta Crystallographica</i>	120,000	120,000	20,000	20,000	–	30,000
Fluctuations in rates of exchange		–166		–91		515
Accumulated balance at end of year		25,274		17,195		–61,288

National Institutes of Health (NIH) and the UK Science and Technology Parliamentary Committee have both investigated science publishing and recommended that for government-funded research the results and data should be made freely available within 12 months of publication. These developments will require very careful discussion within the IUCr Finance Committee.

The citation impact of IUCr journals continued to be high, effectively occupying two or three of the top five ranking positions in crystallography.

The overall withdrawal plus rejection rate for the journals was 26% in 2004, up compared with 2003 (20%) and 2002 (18%). Looking into this there is a noticeable effect from *Acta Cryst.* Section C in 2004 of

Table 12
Publication and Journals Development Fund (Swiss Francs).

	2002	2003	2004
Income			
Investment income		28,869	16,055
			18,671
Expenditure			
Computer expenses:			
Programming and development	438,279	444,039	586,059
Programming and development recharged to other Funds	-438,279	-444,039	-586,059
Electronic Publishing Committee/Section Editors' meeting	1,458	2,576	810
STAR/CIF	621	2,688	57,243
Promotions Representative	152,174	130,785	156,759
Promotions Representative recharged to other Funds	-152,174	-130,785	-156,759
Web input	2,981	2,931	998
Special Issue costs (surplus) recharged to (from) other Funds	-2,274	44,773	28,686
Journal Grants Fund subsidies	19,088	30,094	46,301
Digitization project	15,987	-	-
Crystallographic neXus	2,141	3,422	-
Depreciation of computer equipment	46,262	46,262	132,746
		86,264	22,605
			156,643
<i>Deficit of income over expenditure</i>		-57,395	-116,691
			-137,972
Transfers from other Funds:			
<i>Acta Crystallographica</i>	270,000	270,000	250,000
		250,000	250,000
			-
			-
Fluctuations in rates of exchange		-5,088	-4,779
			-6,377
Accumulated balance at end of year		774,936	903,466
			759,117

Table 13
Research and Education Fund (Swiss Francs).

	2002	2003	2004
Income			
Investment income	50,361	21,433	22,225
Donation	-	50,361	3,288
			24,721
			22,225
Expenditure			
Young scientist support	111,983	146,873	119,382
Visiting Professorship Programme	8,570	6,179	-
Grants/Africa PhD support	-	102,553	5,963
			159,015
			5,040
			124,422
<i>Deficit of income over expenditure</i>		-70,192	-134,294
			-102,197
Transfers from other Funds:			
<i>Acta Crystallographica</i>	130,000	130,000	140,000
		140,000	140,000
			-
			-
Fluctuations in rates of exchange		-6,651	-5,361
			-7,591
Accumulated balance at end of year		1,013,061	1,013,406
			903,618

49% versus 38% in both 2002 and 2003, which in turn analyses as being heavily biased by high rejection rate by country of origin.

An open-access option for authors was introduced on a fee payment basis in 2004. In the case of authors from the UK, however, a grant from the UK Joint Information Systems Committee allowed all UK papers to be published as open access in 2004 and another award made this possible for 2005.

Acta E is attracting ever-increasing numbers of electronic structure reports; the number of electronic pages produced in 2004 is approximately 85% of all the printed pages published for *Acta Cryst.* in 2002! This success has required an expansion of the *Acta E* Editorial Board. This is a major achievement to publish so many papers, all of which are of course citable and citation ranked by ISI.

Acta C has not suffered from the *Acta E* launch. *Acta C* subscribers in any case receive *Acta E* within the *Acta C* subscription. Rather,

Acta C is now showing that it is increasingly the premier home of important and high-quality crystal structure communications; evidence that this is happening is in the citation impact rising from 0.571 in 2001, to 0.659 in 2002 and 0.828 in 2003.

Discussions concerning a new Section of *Acta Cryst.* catering for high-throughput crystallization communications started in about 1997. As structural genomics programmes became funded in the early 2000s, the issue broadened as to how to handle high-throughput short structural biology communications. In terms of quantity, approximately half of any single issue of *Acta D* had become regularly devoted to crystallization communications. The structural genomics funding, in addition, was very healthy and a journal outlet might be optimized for them as well. Thus, through 2003 and 2004, the situations of crystallization and high-throughput structural biology/genomics reports were monitored carefully by IUCr journals staff and

Table 14
Ewald Fund (Swiss Francs).

	2002		2003		2004	
Income						
Investment income	26,096		11,452		12,280	
Grants	–	26,096	63	11,515	–	12,280
Expenditure						
Ewald Prize/Selection Committee		49,005		–		743
<i>Excess/Deficit of income over expenditure</i>		–22,909		11,515		11,537
Transfers from other Funds:						
<i>Journal of Applied Crystallography</i>	–	–	25,000	25,000	–	–
Fluctuations in rates of exchange		–3,007		–2,602		–4,194
Accumulated balance at end of year		458,029		491,942		499,285

Table 15
Newsletter Fund (Swiss Francs).

	2002		2003		2004	
Income						
Advertisements	122,668		230,075		179,129	
Reimbursement of 19GAC circular	–739	121,929	–	230,075	–	179,129
Expenditure						
Editorial honoraria	7,284		6,000		5,760	
Editorial expenses	78,567		70,473		76,439	
Printing and distribution	93,207		125,523		102,739	
Advertising costs	30,666	209,724	57,514	259,240	44,783	229,721
<i>Deficit of income over expenditure</i>		–87,795		–29,165	50,592	–36,429
Transfers from other Funds:						
<i>Acta Crystallographica</i>	25,000		–		45,000	
<i>Journal of Applied Crystallography</i>	25,000	50,000	45,000	45,000	–	45,000
Fluctuations in rates of exchange		–721		–661		–994
Accumulated balance at end of year		109,747		124,921		118,335

the Editor-in-Chief. In 2004, the final decision was taken to bud part of *Acta D* into a new *Acta F*. The launch of *Acta F* was agreed in mid-2004 with a launch date of January 2005. The name of *Acta F* was also finalized as *Structural Biology and Crystallization Communications*. New Section Editors (H. M. Einspahr and J. M. Guss) and a new Editorial Board were appointed. Extensive work has been made jointly with the Protein Data Bank by H. M. Einspahr concerning streamlined deposition-to-publication methodologies. We acknowledge the cooperation of the Protein Data Bank in this work. The first issue was published in January 2005. *Acta D* subscribers receive *Acta F* free.

This is my final triennial report. I have greatly appreciated the high professional interactions and knowledge of the IUCr Chester staff, notably Peter Strickland (Managing Editor), Brian McMahon (Research and Development Officer), Andrea Sharpe (Promotions Officer) and Mike Dacombe (Executive Secretary), and indeed all the IUCr staff at Chester. I have enjoyed many science interactions with fellow IUCr journals' Editors and Co-editors (*Acta Cryst.*, *J. Appl. Cryst.* and *J. Synchrotron Rad.*) and with our submitting authors, as well as with many fellow diffraction physicists, crystal-

lographers and structural scientists who care deeply about the IUCr, through my nine years as Editor-in-Chief of *Acta Cryst.* I acknowledge also very good collaborations with the Executive and Finance Committees and with the *IUCr Newsletter* Editors. I thank here also, most heartily, the many scientists who helped me as referees. Overall I wish to record here that to have had the chance to contribute to the International Union of Crystallography by serving the IUCr journals learned society style of publishing enterprise, as well as authors, subscribers and readers, has been a deeply fulfilling experience for me.

J. R. Helliwell, Editor-in-Chief, *Acta Crystallographica* and Chair of Commission

4.1.2. *Acta Crystallographica* Section A. Basic statistics for Section A are shown in the following table.

Pages for science comprise only Research Papers, Short Communications and Letters to the Editor; publication time applies to research papers; the origin of articles binned for Europe, Asia+Australia and the Americas comprises Research Papers

Statistics for Section A

Year	Total pages	Pages for science	No. of Research Papers	No. of Short Communications	Average length of Research Papers	Publication time (months)	Europe (%)	Asia (%)	Americas (%)
2002	630	551	65	14	8.0	5.6	50	25	25
2002	375	372	Supplement, Abstracts of the Geneva Congress						
2003	628	474	58	6	7.9	4.5	54	10	36
2004	644	626	78	7	7.8	6.2	61	14	25
2004	308	308	Abstracts of ECM-22						

and Short Communications counted as integral or half-integral numbers.

Section A published 18 issues, 6 per year. The numbers for 2002 are comparable to those for 2000, but lower than those for 2001 by 10 Research Papers. A further notable dip occurs in 2003, but the results for 2004 again reach levels comparable to those of 2001. This appears to indicate that Section A on average retains its volumetric importance. The good results for 2004 are in part due to the September Special Issue containing 21 articles in 160 pages (see below). Still, the five regular issues of 2004 comprise as many pages and articles as the six issues of 2003. The rejection plus withdrawal rates oscillate around 33%, being 29, 40 and 32%, respectively. The geographical origins of the papers show a European preponderance. The electronic submission procedure works very well and is used by a large majority of authors.

In 2002 and 2003, no Lead Articles, Topical Reviews or Special Issues were published. In 2004, two contributions to the Microsymposium on Quantum Crystallography of the Geneva Congress in 2002 were published with an introduction by the Chair S. Manninen. In September 2004, a Special Issue was published on New Information from Modern Charge Density Methods, containing work presented at the Third European Charge Density Meeting ECDM-III at Sandbjerg Estate, Denmark. The Guest Editor was the conference organizer, F. K. Larsen.

Section A covers a broad interdisciplinary spectrum of the exact sciences. It has retained its comparative international rating during the past five years with impact factors oscillating between 1.42 and 1.75. It is indubitably the leading journal for work in Foundations of Crystallography. We hope to publish in the near future two Special Issues and three Lead Articles/Topical Reviews. I thank the Co-editors and the referees for their work.

D. Schwarzenbach, Editor

4.1.3. Acta Crystallographica Section B. During the triennium 2002–2004, Section B published six issues per year. In the years 2002–2004, the numbers of articles were 132, 88 and 87, with the high value for 2002 a partial consequence of a very successful Special Issue (jointly with Section D) on crystallographic databases. The numbers of pages per year were 1,088, 821, and 763. Papers came from 27 different countries. All papers were written in English.

A comparison of the statistics for the years 2002–2004 shows that the distribution of articles between the inorganic, metal-organic and organic sections of the journal varies from year to year. Overall, the ratio of papers that discuss inorganic and molecular compounds is about 35:65.

A comparison of numbers of articles and pages for this and the previous triennium indicates that the number of pages per year has been decreasing. It may be that work is now being reported in a more concise way. Because access to archived CIFs and to other Supplementary Material is now easy, the number of tables in the printed

papers can be reduced. On the other hand, the number of papers per year is also down. It is possible that some papers that would in the past have appeared in Section B are now appearing in Section C because structures that were once considered difficult or unusual (e.g. because of twinning or a large number of molecules in the asymmetric unit) have become more routine. This factor might

help explain the rise of the combined rejection/withdrawal rate for Section B from 17% in 1999–2001 to ca 35% in 2003–2004. Finally, it seems almost certain that competition from *CrystEngComm* (started in 1999 by the Royal Society of Chemistry) and *Cryst. Growth Design* (started in 2001 by the American Chemical Society) is a factor in the decreased number of papers. Ways of enhancing the competitive position of Section B are being considered. One Topical Review was published in 2004. Another is being written and several others are in the discussion stage.

A very positive development is the continuing increase of the impact factor from 1.73 for 2000 (announced in 2001) to 3.64 for 2003 (announced in 2004). This increase has brought Section B greater visibility and very favourable publicity. The heavily cited 2002 Special Issue on databases is an important factor in the rise.

The electronic submission system first implemented in 2003 is now fully operational. The system is popular with both authors and editors. Time to publication dropped from 7.2 months in 2001 to 4.8 months in 2004. Communication between authors, Co-editors, referees and the Chester Office is now essentially instantaneous and all file processing is highly automated.

Colour figures have become so common that the journal pages look quite different compared to three years ago. The colour enhances the visual appeal, but more colour is being used than seems necessary.

It is, as always, a pleasure to thank the Chester staff for their skill in producing attractive journal pages that are easily read. Placing the many tables, figures and footnotes in logical positions relative to the text is no easy task. The considerable work necessary to make sure the text conforms to reasonable standards is also very much appreciated.

C. P. Brock, Editor

4.1.4. Acta Crystallographica Section C. Section C continues to specialize in the rapid publication of high-quality studies of novel and challenging crystal and molecular structures. Publication times continue their downward trend with the majority of technically correct and well written papers appearing online (<http://journals.iucr.org/c>) within one to two months of submission. In 2003, Section C published 478 papers (49 inorganic, 186 metal-organic and 243 organic) in a total of 1,482 pages. In 2004, Section C published 554 papers (42 inorganic, 227 metal-organic, 285 organic) in a total of 1,686 pages – a 15% increase in papers and pages over 2003. Section C is now showing that it is increasingly the premier home of important and high-quality crystal structure communications; evidence that this is happening is in the citation impact rising from 0.571 in 2001, to 0.659 in 2002 and 0.828 in 2003.

There has been a significant increase in the number of submissions to Section C in the last triennium and this has resulted in a major increase in editorial workload. Some 39% of original technically correct submissions to Section C in 2003 were subsequently with-

drawn or rejected; this withdrawal/rejection rate climbed to 48% in 2004. The principal reasons for this significant increase in the withdrawal/rejection rate were either that 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 (increasingly) that the text in the *Comment* section was very poorly crafted and difficult to understand.

Some changes have been made to the 2005 *Notes for Authors* in an attempt to improve the quality of initial submissions. It is a requirement that the text sections of the paper be written in clear and correct English (or one of the other accepted languages). Papers with text sections containing consistently poor grammar or incomprehensible statements are now being rejected promptly by the assigned Co-editor. While the editors and Chester editorial office staff are very willing to provide help with any technical CIF problems, they cannot be expected to assist with major corrections or re-drafting of inadequately prepared text. To assist Co-editors with the initial review of new submissions, we are now asking that the submitting author consider providing in the `_publ_contact_letter` section of the CIF a brief statement of what is new, novel or interesting about the structure(s) in the submitted CIF that merits publication in the printed form in Section C. Given the ever increasing number of structures determined, the pressure on space in Section C is such that we must serve our chemical and materials-structure communities by keeping Section C as a premier outlet for the best crystal structures, both technically and scientifically.

It was with deep regret that we learned of the death in 2004 of Professor Mario Nardelli, a highly respected and long-time member of the Section C Editorial Board.

It is always a pleasure to thank the many Co-editors, referees, and the Chester staff for their superb work in the preparation of Section C; their fine efforts make my job as Editor much easier and I look forward to our continuing partnership.

G. Ferguson, Editor

4.1.5. *Acta Crystallographica* Section D. The past three years have seen major changes, both in Section D and in biological crystallography itself. First and foremost has been the retirement of our founding Editor, Jenny Glusker. Jenny approached her task of developing the new journal, from its inception in 1993, with enormous wisdom and personal commitment, and for this we owe her a huge debt of gratitude. Perhaps significantly, it has taken the two of us, E. N. Baker and Z. Dauter, to replace her! Coinciding with Jenny's retirement as Editor, and celebrating 10 years of publication of Section D, a number of invited articles were published from leading crystallographers.

The first 10 years of Section D coincided with a boom in biological crystallography that shows no sign of stopping. In 1993, there were less than 2,000 experimentally determined protein structures in the Protein Data Bank; in 2003 there were 22,000 and today there are more than 30,000. This growth in biological crystallography is driven by the importance of protein structures for biotechnology, medicine and functional genomics. In parallel, there have been many changes in crystallographic methods, technologies and practice, including the development of crystallization robotics, the much wider use of anomalous scattering (MAD and SAD), automated map interpretation and model building, many improved protocols for structure solution and refinement, and major synchrotron developments.

The task of Section D is to capture the dynamism of this field, and provide a high-quality publication venue for the biological crystallography community. The journal looks superb, and the quality of

production is excellent. The electronic submission system, which was introduced in 2003, works very well for authors, reviewers and Co-editors, and has also helped reduce average publication times; these have steadily decreased from 5.2 months for full articles in 2002, to 4.9 months in 2003, to 4.3 months in 2004. The journal has also grown, from 2,243 pages in 2002 to 2,406 in 2004.

In terms of content, Section D remains pre-eminent in the publication of new methods in biological crystallography. This makes it a very important resource for the crystallographic community, and many of these methodological papers are highly cited. The publication of the very popular CCP4 study weekend series (see below) is also important. In some other respects the journal is not yet meeting its full potential, however. The number of structural papers published averages about 10 per issue, but we wish to increase this and attract more high-profile structures. Of some concern here is the impact factor, which was 1.76 in 2002 and 2.21 in 2003, lower than some competitor structural biology journals.

The place of crystallization papers has stimulated much discussion. Whereas the number of full research articles has remained steady at about 12 per monthly issue, the number of crystallization papers has increased from an average of 16.8 in 2002, to 20.6 in 2003, to 24.6 in 2004; in 2004, crystallization papers accounted for 60% of articles and 37% of pages. Crystal growth is a key part of crystallography, often requiring great skill, and full documentation of protein production and crystallization is essential for the reproducibility of a crystallographic structure determination. Paradoxically, despite the importance of these papers, they are seldom cited and thus depress the impact factor of the journal. From 2005, they will instead be published in the new all-electronic journal, *Acta F*, leaving *Acta D* to focus on crystallographic methods and structures.

Notable features of the past three years have been the Special Issues devoted to methods. These are also available as stand-alone publications. The CCP4 study weekend issue is published towards the end of each year, with Guest Editors who are responsible for the issue. In 2002, the topic was high-throughput structure determination, with guest editors R. Esnouf, D. Stuart and K. Wilson; in 2003, A. McCoy and N. McDonald were Guest Editors for an issue focusing on experimental phasing; and in 2004 the topic was model building and refinement, with Guest Editors A. Perrakis and M. Noble. These are always eagerly awaited issues, and the papers give a snapshot of the leading edge of the field. We are enormously grateful both to CCP4 and to the Guest Editors for the continued publication of this series. The other Special Issue from the past three years, in October 2002, presented the Proceedings of the 9th International Conference on the Crystallization of Biological Macromolecules. Again, this contains seminal methodological papers, and we are very grateful to the Guest Editors M. Riès-Kautt and R. Hilgenfeld.

Finally, we thank the many people who contribute to the success of the journal: our authors and readers; the reviewers whose efforts are critical for maintaining quality; our Co-editors who give their time and wisdom in shepherding papers through to acceptance; Louise Jones and Simon Glynn for their efforts at Chester in maintaining superb production quality; and Peter Strickland, Managing Editor, and John Helliwell, Editor-in-Chief, for their guidance and management.

E. N. Baker and **Z. Dauter**, Editors

4.1.6. *Acta Crystallographica* Section E. This is the first full triennial report for the journal; three years ago, we were able to give a report for only one year, 2001, the first year of publication. A great deal has happened since then! From its inception in 2001, Section E of

Acta Crystallographica has experienced a steady and remarkable growth, as evidenced by the statistics reported in the following table for the three years covered by this report.

Statistics for Section E			
	2002	2003	2004
Manuscripts received	1,036	1,595	2,383
Manuscripts accepted	937	1,370	1,899
Manuscripts rejected	37	81	253
Manuscripts withdrawn	67	117	203
Inorganic papers	49	59	57
Metal-organic papers	295	444	743
Organic papers	577	794	1,003
Total papers published	922	1,305	1,811
Pages published	2,374	3,419	4,676

In terms of both published papers and pages, the journal in 2004 was well over twice the size of 2001. This rate of growth shows no sign of abating.

Over the same period, there has been a slight decrease in the average time taken from receipt to publication, from 1 month to 0.8 months. Authors are asked to make revisions within one month, otherwise papers are considered to be withdrawn; in some cases, more than one round of revision is necessary, so a small proportion of papers have quite long publication times. Publication times as short as 3 days from receipt to online availability have occasionally been achieved.

Over these years, the greatest proportion of published papers has originated in the People's Republic of China, reaching 38.9% in 2004; the next highest proportions in 2004 were USA (7.7%), Turkey (6.8%), UK (6.4%) and India (5.7%).

Most published papers have a length of 2–3 pages. Each reports the structure of a single material; reports of multiple structures are not accepted, in order to achieve maximum automation in procedures and publishing efficiency.

The journal has two joint Section Editors, whose activities include providing advice to Co-editors, selecting monthly electronic cover illustrations for the journal's web site, and proof-reading all papers before publication to ensure consistency and conformity with journal policies. They also serve as Co-editors.

The number of Co-editors has risen each year in response to the growth of the journal itself: 19 in 2002, 25 in 2003, and 31 in 2004; more Co-editors have already been appointed early in 2005. Unfortunately, we have lost the services of one Co-editor, Professor Mario Nardelli, who had served from the very beginning of the journal; his death in 2004 was a significant loss to the IUCr as a whole. The distribution of Co-editors by country (at the end of 2004) is Australia (2), Austria (1), Canada (3), China (1), Croatia (1), France (1), Germany (2), India (1), Italy (1), Japan (2), Malaysia (1), New Zealand (1), Russia (2), Sweden (1), Switzerland (1), UK (3 plus 2 Section Editors), USA (5).

The journal is served mainly by two members of editorial staff in the Chester IUCr offices, Gillian Holmes and Sean Conway, under the guidance and supervision of Peter Strickland. This level of central editorial staffing has not changed during the lifetime of the journal, and the efficiency and dedication of the staff with their much increased workload are much appreciated.

The basic manuscript submission, handling and editorial procedures set up at the launch of the journal have remained broadly the same during this period, though there have been a number of changes and improvements in response to the increasing number of papers. These include some streamlining of e-mail and other correspondence with authors; significant development of web resources for Co-editors including online status lists and access to the documents associated

with each paper (a very positive development for the Section Editors at the proof-reading stage); a two-stage proof checking procedure (Section Editors make some corrections and raise queries before the proofs are made available to authors); the automatic return of submissions to authors for correction before formal receipt and allocation to a Co-editor if serious problems are detected in the automatic checking process; and automated Section Editor feedback to Co-editors from the proof-reading.

More significant developments in the manuscript submission procedure are currently underway, for implementation during 2005, and will be presented in the next annual and triennial reports.

Improvements in services for authors over the three-year period include the release (and later update) of the CIF editing tool enCIFer, provided by the Cambridge Crystallographic Data Centre, and a preliminary version of a utility for editing CIF-based submissions through Microsoft Word, using a template with embedded macros developed in the IUCr editorial office. A wide range of web-based author interfaces for submission, proofs and electronic reprints is provided in a single location on the journal's home-page, together with access for readers and subscribers, only one step away from the main **Crystallography Journals Online** web site.

The journal has proved very popular with authors, especially those in countries of the Middle and Far East. Attractive features are the rapid publication, the ease of submission, availability of useful author services, full-colour publication with no charge, and the opportunity to publish crystal structures without an extended discussion of the results. It is also widely appreciated that Section E, along with other IUCr journals, maintains very high technical standards of production and encourages rigour and care in the determination of crystal structures.

Section E provides a complementary service to that of Section C, where a more substantial discussion of results is required, and where papers can be published describing two or more related structures. Its rapid growth has eased pressure on Section C, while at the same time leading to a substantial increase overall in the publication of crystal structures in the IUCr journals, and it has attracted many new authors.

The journal received ISI accreditation within one year of its launch; papers published in it are thus certified as undergoing peer review, and they are fully indexed and used in citation analyses, which is an important consideration for many authors.

Although the journal's impact factor, calculated for the first time in 2004, is rather low at 0.453, this is to be expected from the nature of the journal and its relationship to Section C (which has a higher value of 0.828, climbing from its previous value of 0.659, possibly due in some measure to the launch of Section E), and it is higher than those of other journals with a similar remit (*J. Chem. Crystallogr.* at 0.400 and *Z. Kristallogr. New Cryst. Struct.* at 0.349).

D. G. Watson and W. Clegg, Editors

4.1.7. Journal of Applied Crystallography. *JAC* published 760 pages in 2002, 1,009 pages in 2003 (plus 496 pages of Conference Proceedings of the 12th International Conference on Small-Angle Scattering held in Venice, Italy, in 2002), and 1,041 pages in 2004. The increase in the number of pages (small-angle scattering not included) is due to an increase in the number of articles, but also, to a lesser extent (~7%), to the increased length of individual articles. The increase in the number of papers reflects the appointment of very successful new Co-editors in the USA but, among the main subscriber countries, more papers may still be desirable from the USA and Japan. There was a further decrease of the average publication time

(from 7.1 to 6.7 months) owing to the reduction of editing time, while the average review time remained constant at about 4.5 months. Manuscripts are now almost exclusively submitted and reviewed electronically. The combined rejection and withdrawal rate remained at 25 to 27% (without small-angle scattering). The impact factor continues at a high level, among the IUCr journals only second to *Acta B*, and *JAC* was ranked fifth in crystallography journals (2003).

A relatively large number of Co-editors will retire this year; the great service to the journal by S. S. Hasnain, J. R. Helliwell, A. M. Moore, Å. Oskarsson, D. Pandey and H. Zimmermann is highly appreciated. Some new appointments will be considered during the current and the forthcoming years.

G. Kostorz, Editor

4.1.8. Journal of Synchrotron Radiation. October 2004 marked the 10th anniversary of *JSR*. A total of 230 research articles comprising 1,265 pages were published during the period 2002–2004. This is less than past three-year periods reflecting a change in emphasis of the journal from publishing large proceedings from major synchrotron-radiation conferences to more focused special editions with focused themes. Although this approach reduces the total number of pages published per year, we believe the quality of the papers has increased. During this time, the impact factor rose from 0.885 in 2002 to 1.144 in 2003. We hope that this trend continues during the upcoming years. The average publication time has been sporadic during this three-year period, starting with 6.6 months in 2002, shooting upwards to 8.2 months in 2003, and recovering to 6.5 months in 2004. This seems to be driven in large part by an increase in review time during this triennium. We, as Main Editors, will have to be increasingly vigilant to ensure that all editors encourage rapid reviewing by referees and timely editing by authors.

In the next triennium, we expect the interest in this field will continue to grow as new approaches to the generation of radiation in the range from VUV to hard X-rays, such as energy recover linacs (ERLs) and free electron lasers (FELs), are developed. We fully expect that *JSR* will remain the pre-eminent journal dedicated to reporting scientific and instrument advancements, regardless of the source technology, in the years to come.

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

4.2. Commission on *International Tables*

The present set of *International Tables* was extended by the publication of three new volumes, Volumes E, D and A1, during 2002, 2003 and 2004, respectively. A further new volume, Volume G, will be published during 2005. Work on the online version of the Tables is in progress. The extension of the present set of volumes is also being discussed.

Th. Hahn resigned as Chair of the Commission during the Geneva Congress. All members of the Commission wish to express their deep

gratitude to him. He will, however, continue to act as Editor of Volume A. At the end of 2003, Professor H. Fuess was appointed as his successor as Chair of the Commission.

Details of the scope and the contents of the different volumes of *International Tables* can be found at the home page of the Commission, which is maintained at Tel Aviv University by U. Shmueli at the URL <http://crystal.tau.ac.il/xtal/comit/index.html>.

The table below summarizes sales and stock figures for the volumes for the last three years.

4.2.1. Volume A. Space-Group Symmetry; Editor Th. Hahn. The Fifth Editions of Volume A and the Teaching Edition of Volume A were published in 2002. A reprint with corrections of errors and small improvements is scheduled for 2005. The volume still remains the flagship of the series and sells well.

4.2.2. Volume A1. Symmetry Relations between Space Groups; Editors H. Wondratschek and U. Müller. Volume A1 was published in 2004. It contains a list of maximal subgroups of the space groups. Part 1 deals with group-theoretical aspects of space groups, group-subgroup relations and the underlying mathematical background. Part 2 contains complete listings of all maximal subgroups for each space group, including their general positions or their generators, their conjugacy relations and transformations to conventional settings. Part 3 lists the relations between the Wyckoff positions for every maximal subgroup of every space group, including the cell transformations and coordinate transformations. In both Parts 2 and 3, the infinitely many isomorphic subgroups have been included in a parametrized form.

4.2.3. Volume B. Reciprocal Space; Editor U. Shmueli. Editorial activities during the last two years have been mainly dedicated to the preparation of the Third Edition of Volume B. The subdivision of the Volume into five parts will remain unchanged, but several changes are envisaged within most parts. Major revisions will be to: the discussion of applications of direct methods to macromolecular crystallography; electron diffraction and microscopy and their relation to structure determination; molecular modelling; and diffuse scattering.

4.2.4. Volume C. Mathematical, Physical and Chemical Tables; Editor E. Prince/H. Fuess. The Third Edition of Volume C was published in 2003, with corrections and revisions of a total of 11 chapters. E. Prince then retired as the Editor of Volume C. The members of the Commission wish to express their very great thanks to him for all his work. H. Fuess has taken over the role of Editor of Volume C and will work on the production of the next edition of this volume.

4.2.5. Volume D. Physical Properties of Crystals; Editor A. Authier. The Commission is grateful to A. Authier for the completion of Volume D, sales of which are off to a good start. The volume is a tremendous achievement and is a valuable reference work not only for crystallographers and mineralogists but also for all scientists interested in the solid state and in materials science. The volume has 536 pages and 18 chapters distributed within three parts: (1) tensorial aspects of physical properties; (2) symmetry aspects of excitations; and (3) symmetry aspects of structural phase transitions, twinning and domain structures. It is accompanied by a CD-ROM.

4.2.6. Volume E. Subperiodic Groups; Editors V. Kopsky and D. B. Litvin. The Volume has been on sale since 2002. A list of corrections has been collected and will be discussed with users.

4.2.7. Volume F. Macromolecular Crystallography; Editors M. G. Rossmann and E. A. Arnold. Volume F turned out to be a solid base for

Volume	A	A1	Brief A	B	C	D	E	F
Dates of printing and reprinting	1983 1984 1987 1989 1992 1995 1996 1998	2004	1985 1988 1989 1993 1996	1993 1996 2001	1992 1995 1999	2003	2002	2001
Sales 2002–2004	1,911	177	1,258	437	572	534	426	831
Total sales	10,056	177	6,690	3,068	3,773	534	426	1,315
Stock at 31 December 2004	53	546	214	485	675	917	311	659

scientists studying biological macromolecules. In addition to Volume F, a version of Volume A on noncentrosymmetric space groups for use in protein crystallography (Volume F1) is under discussion.

4.2.8. Volume G. Crystallographic Information; Editors B. McMahon and S. R. Hall. In cooperation with COMCIFS, the IUCr Committee for the Maintenance of the CIF Standard, a revision cycle of a number of CIF dictionaries during 2003 was linked to the production schedule of the volume. The outstanding chapters for the application section were reviewed in 2004 and the volume will be published in 2005.

H. Fuess, Chair

4.3. Commission on Aperiodic Crystals

The Commission, including several new members, was reappointed by the Geneva General Assembly. Official meetings of the Commission took place during the Geneva Congress and during Aperiodic 2003 in Belo Horizonte, Brazil. Many Commission members had the opportunity to hold discussions at various international conferences.

The activities of the Commission were focused on the organization of international conferences and the coordination of activities between the different communities working on quasicrystals and incommensurate structures.

At the Geneva Congress, an Open Commission Meeting was organized around the question 'What is a crystal?' Although seemingly a simple question, it requires careful consideration of the properties we want to assign to crystalline materials. One property that does not characterize the crystalline state is a periodic atomic structure. Aperiodic crystals are crystals that lack three-dimensional (3D) translational symmetry. A property that can be assigned to an ideal crystal structure is that it will have infinitely sharp Bragg peaks in the diffraction. For aperiodic crystals, these Bragg reflections cannot be indexed on the basis of a 3D reciprocal lattice. In 1993, 'an essentially discrete diffraction diagram' was used by the IUCr as a definition of the crystalline state. [See the 1991 Annual Report of the Executive Committee [*Acta Cryst.* (1992), **A48**, 922–946].] Thus a motivation for the discussion was to try to develop a definition that generalizes the notion of a periodic array of atoms towards aperiodic crystals, and thus does not require the understanding of diffraction. In this way a definition could be designed that could be made easily understandable for non-specialists. At the Open Meeting of the Commission, these questions were introduced by S. van Smaalen, W. Steurer and D. Pandey. Subsequently, they were discussed with many contributions from the audience. An agreement on one particular definition was not obtained, but the discussion led to three statements that each by itself might characterize the crystalline state:

- (1) a solid with an essentially discrete diffraction diagram;
- (2) a solid with an atomic structure with long-range order;
- (3) a solid with an atomic structure that can be obtained as a section of an n -dimensional periodic structure ($n = 3, 4, \dots$).

Advantages of and problems with each of these definitions were discussed.

The most important event was the International Congress on Aperiodic Crystals, Aperiodic 2003, that took place 8–13 September 2003 at the Federal University of Minas Gerais in Belo Horizonte (Brazil). This meeting was organized by N. Speziali. Aperiodic 2003 was the eighth in a series of triennial meetings that have the goal to bring together scientists studying the atomic structures and physical properties of quasicrystals, incommensurately modulated crystals, incommensurate composite crystals and polytypes. It was attended by 90 participants from 22 countries in 5 continents. Participation was

negatively affected by the difficulties of travel that have existed since approximately 2002. At least two intended participants, both invited speakers, could not go to Belo Horizonte, because they did not obtain a transit visa for the USA in time. The Proceedings of Aperiodic 2003 have been published as Volume 305 (2004) of *Ferroelectrics*. A detailed report of this meeting can be viewed on the web site of the Commission. This report and many photographs can be viewed at the web site of Aperiodic 2003 at <http://agora.grude.ufmg.br/aperiodic2003>.

The series of workshops on aperiodic crystallography in Bayreuth, Germany, was continued by the 4th Workshop on Structural Analysis of Aperiodic Crystals, which took place 6–8 March 2003 at the University of Bayreuth; this Workshop was organized by S. van Smaalen. Approximately 40 participants could attend lectures on structure determination, symmetry aspects, and the interpretation of structures by M. Dusek and V. Petricek (Prague, Czech Republic), J. M. Perez-Mato (Bilbao, Spain), A. Schonleber (Lausanne, Switzerland), and L. Palatinus and S. van Smaalen (Bayreuth, Germany). In the afternoons, the participants had the opportunity to practise structural analysis of incommensurate crystals with the computer program *JANA2000* and a script with several worked-out examples that treated different aspects of structure solution and structure analysis.

As part of the AsCA '03/Crystal-23 meeting in Broome, Australia (10–13 August 2003), a half-day workshop 'Introduction to Modulated Structure' was organized by S. Schmid.

The Commission continued to promote activities on the crystallography of aperiodic crystals at national and international meetings. Microsymposia on aperiodic crystals were organized at the Geneva Congress in 2002, at the annual meetings of the American Crystallographic Association (ACA), at the Asian Crystallographic Meetings, at the European Crystallographic Meetings, at the annual meetings of the German Crystallographic Association (DGK), and at the annual meetings of the Society of Crystallographers in Australia and New Zealand (SCANZ).

Following previous work, the CIF dictionary for modulated structures was completed in February 2002. Based on this new CIF dictionary, a database of incommensurately modulated structures and composite crystals was developed. Both projects evolved under the direction of G. Madariaga (Bilbao, Spain) in cooperation with the Committee for the Maintenance of the CIF Standard. The CIF standard is available at the IUCr web site. The database is available at the Bilbao Crystallography Server at <http://www.cryst.ehu.es/icsdb/index.html>.

Aperiodic 2006, the next in the series of triennial Aperiodic meetings, will take place 17–22 September 2006, in Zao (near Sendai), Japan. This meeting is organized by A. Yamamoto (Chair), An Pang Tsai (Vice-Chair), Y. Gotoh, Y. Michiue, Y. Miyazaki and K. Saitoh.

A workshop on aperiodic crystallography will take place on the first day of the Florence Congress. The goal of this workshop is to give an overview of the state of the art of crystallographic analysis of incommensurate crystals and quasicrystals. Introductory lectures will present the fundamentals of the superspace theory for the description of incommensurate crystal structures. The afternoon session will be devoted to recent developments and applications of superspace crystallography. The Fifth Workshop on Structural Analysis of Aperiodic Crystals at the University of Bayreuth, Germany, will be organized 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>.

S. van Smaalen, Chair

4.4. Commission on Biological Macromolecules

In keeping with the triennial cycle, at the start and end of its term the Commission dealt with matters relating to the Congress and General Assembly. For each meeting, the Commission provided advice regarding topics for Microsymposia and suggested Chairs and speakers for plenary sessions. In keeping with the trends of recent years, the macromolecular community was strongly represented at the Geneva meeting with 13 of the Keynote Lectures and 29 of the Microsymposia in the area of macromolecular crystallography, in addition to the hundreds of posters. Spurred to some degree by the requirements for high throughput generated by structural genomics initiatives, the Congress highlighted new and improved methods ranging from protein crystallization to applications of direct methods and automated structure refinement. We expect that the final programme in Florence will have an equally strong representation from the macromolecular community.

The major activity of the Commission at the Geneva Congress was a Joint Open Meeting of the Commissions on Journals and Biological Macromolecules. The purpose of the meeting was to bring to the attention of the community initiatives by the IUCr journals to provide for high-throughput electronic publication of macromolecular structures. These structures might result from structural genomics or, for example, from studies of complexes arising from drug screening. The meeting discussed the need for close liaison with the Protein Data Bank (PDB) to coordinate data deposition and publication. H. M. Berman, from the PDB, outlined procedures being developed jointly with the editorial staff of *Acta Crystallographica* to provide details required by the journal directly to the author for incorporation in the electronic publication. It is also envisaged that referees will be provided with copies of the structure verification data compiled by the PDB for every Data Bank submission. These activities were significantly boosted when the IUCr established the all-electronic Section F of *Acta Crystallographica* to provide a convenient and rapid means of publication of short structural communications and crystallization notes for macromolecular crystallography. The first issue of *Acta F* went online in January 2005. One of the joint Editors of *Acta F*, H. M. Einspahr, has been working closely with the PDB and the staff in Chester to define new data items and inaugurate procedures for the return of data from the PDB to the journal.

The question of the revised requirements for the deposition of coordinates and diffraction data was resolved early in the three-year term of the Commission. Letters were written to the editors of all journals that publish macromolecular crystal structures with generally positive responses. Most journals now enforce the minimum recommendations of the IUCr although some, for commercial reasons, have not enforced the deposition of structure-factor data despite the arguments that these data need to be properly curated to prevent loss. All members of the community should deposit such data and encourage their colleagues to do so. There is now increased pressure from some parts of the community to remove any post-publication delay in the release of coordinate and structure-factor data. The incoming Commission may need to revisit this issue.

Members of the Commission have been actively engaged in the planning of national crystallographic meetings and of meetings of the

Regional Associates of the IUCr. There was also a strong representation from the Commission at the meetings of the International Structural Genomics Organization held in Berlin, Germany, in November 2002, and in Washington, DC, USA, in November 2004. This new body seeks to provide a forum for the discussion and planning of structural genomics initiatives and has by its nature a large crystallographic membership. Many new resources including synchrotron beamlines, automation for macromolecular crystallography and software systems are making their way from structural genomics groups into the general community.

The Commission has provided active support for meetings and workshops held in Asia, South America, Europe and Australia. These focused workshops provide a very cost effective means of keeping students and other young scientists in touch with the latest developments in the field. Support from the IUCr is used to provide access to these meetings for students. Most requests to the Commission have been enthusiastically received subject to some questions of timing and access.

The Commission plans to hold an Open Meeting during the Florence Congress on software standards in macromolecular crystallography. This meeting aims to address practical aspects of common file formats as well as fundamental issues regarding the need for access to source codes for verification of calculations.

J. M. Guss, Chair

4.5. Commission on Charge, Spin and Momentum Densities

During the triennium, the Commission was actively engaged in the organization of meeting sessions to promote the field among young scientists (not only crystallographers, but physicists, chemists, materials scientists and biologists) and these are described in the annual reports. Charge, spin and momentum densities special sessions were organized by the Commission or with the help of the Commission for the following crystallographic meetings: Geneva Congress in 2002, ECM-20 in 2003 (Durban, South Africa), ECM-21 in 2004 (Budapest, Hungary), AsCA '03 in 2003 (Broome, Australia) and AsCA '04 in 2004 (Hong Kong, People's Republic of China). It is regrettable that ACA meetings no longer provide any special sessions on electron distribution.

International special charge density meetings were also very successfully attended (see the annual reports for more details). Sagamore XIV (Broome, 2003) was organized by M. A. Spackman; the next will be organized by M. J. Cooper (UK in 2006). The last Gordon Conference (Mount Holyoke, 2004) was organized by J. C. H. Spence; the next will be chaired by C. Gatti.

Europe is very active in the field of electron density with the organization every two years of the European Charge Density Meeting. ECDM3 was organized by B. Iversen and F. K. Larsen at Sandbjerg Estate (Denmark) in June 2003, immediately after a PESC Workshop (ESF) on new information from modern charge density. The next will be organized in 2006 by U. Pietsch (Potsdam, Germany).

The oral presentations and some posters of Sagamore XIV were published in 2004 in *J. Phys. Chem. Solids* and the ESF and ECDM3 conferences will be reported in a Special Issue of *Acta A* in 2005.

The Multipolar Refinement Project results were published in *Acta A* in 2003 and all other running projects have been ended (MEM, Fermiology) owing to non-activity. A new project begins in 2005 proposed by D. Jayatilaka concerning the possibility (or not) of extracting from the X-ray and polarized neutron data an experimental wavefunction. This project was launched during the 2004 Gordon Research Conference (GRC). Seven groups participate and

we expect the first results to be discussed during the Florence Congress.

The 5th International Conference on Inelastic X-ray Scattering was held at Argonne National Laboratory in September 2004 and was organized by E. Ercan Alp and A. Bansil (130 participants). The attendance was twice as large as the other meetings, an indication of the impact of the inelastic X-ray scattering dedicated beam lines at third-generation synchrotrons. The programme may be found at <http://www.aps.anl.gov/ixs04/agenda.html>.

In general, I believe that the field covering electron, spin and momentum density found a new youth due to the combination of human, experimental, theoretical and technical factors. The community is becoming younger as proved, for example, by the fact that 55% of the GRC attendees were less than 40 years old. It not only attracts crystallographers but also chemists, physicists, biologists and materials scientists. The community is open to new complementary techniques such as convergent-beam diffraction, surface diffraction, synchrotron and inelastic scattering, new DFT techniques – it opens its traditional subjects (chemical bonds, Fermiology, spin density) to new materials, molecular materials, cuprates, manganites, ferroelectrics, thermoelectronics, macromolecules, surface science – and to new cutting-edge projects, electron density of atoms, molecules and crystals under thermodynamic constraints: pressure, electric field, photoexcitation, time-resolved experiments.

All these projects mentioned above will be the future of our field experimentally and theoretically: new unexpected experimental results will need new theoretical approaches (not simply by pushing a button to run a program).

The need for education becomes more and more important at a time where most 'old timers' are retiring or will retire. Therefore, in order to develop the field with all our new young colleagues, a school is certainly important; this school must be opened to scientists from Africa and South America because these two continents did not participate in the GRC or Sagamore meetings: people from developing countries are expected to contribute to the field because – it is a paradox – their research has few financial means but also is not driven by politics, which imposes more and more on day-to-day research (I give you money today, I have to have the results tomorrow). I think this observation holds for most fields of crystallography: fundamental and methodological research will be performed in countries where money is scarce. By comparison, in the USA, the best confirmation is the almost disappearance of our field because almost all the 'crystallographic money' is provided to biocrystallographers and to crystallographic staff.

C. Lecomte, Chair

4.6. Commission on Crystal Growth and Characterization of Materials

As usual, the Commission directed most of its activity to the organization of international schools for young scientists. Moreover, during the triennium, the Commission also helped to organize several topical workshops. The complete list of organized/supported events is given below:

(1) Latin-American Summer School on Crystal Growth, chaired by E. Dieguez, took place 3–7 July 2002 at the Universidad Autonoma de Madrid, Spain. Two Commission members were enrolled as lecturers at the school.

(2) International School on the Crystal Growth of Technologically Important Electronic Materials (ISCGTIEM) organized by K. Byrappa and R. Fornari at the University of Mysore, India, 20–28 January 2003. The school was supported financially by the IUCr,

through a grant which allowed the participation of 15 needy students. The school had about 90 students and 30 tutors, from 20 different countries representing all five continents. All participants received a copy of the book entitled *Crystal Growth of Technologically Important Electronic Materials* edited by K. Byrappa, T. Ohachi, H. Klapper and R. Fornari and published by Allied Science Publishers, New Delhi, India. Ten members and consultants of our Commission participated in the school as lecturers.

(3) International School on Crystal Growth, Characterization and Applications (ISCGChA), held in La Pedera, Uruguay, 9–13 December 2003, chaired by L. Fornaro. The objective of ISCGChA was to foster activities connected with the growth and characterization of crystals, especially in Latin-American countries. ISCGChA was aimed at promoting the training of young students and researchers in the principles and the methods of crystal growth, and in the different characterizations and applications of crystals. The ISCGChA included a series of lectures from European, Japanese, North American and Latin-American lecturers as well as poster sessions, where the participants presented their activities. The presentations of Latin-American participants will appear in a special issue of *Cryst. Res. Technol.* The school was attended by about 60 participants. Two members of the Commission gave lectures at the school, while two additional Commission members were involved in the International Advisory Committee.

(4) 12th International Summer School on Crystal Growth (ISSCG-12), held in Berlin, Germany, 1–7 August 2004. This was a very successful school, which attracted over 120 young participants from 28 countries. The technical programme included 30 excellent lectures and tutorial seminars held by internationally recognized specialists. It is worth mentioning that 66 students from needy countries were supported by the organizers thanks to the generous sponsorship of various agencies and organizations, among which was the IUCr. The school Proceedings were published by Elsevier Science in a book entitled *Crystal Growth – from Fundamentals to Technology* edited by G. Mueller, J. J. Metois and P. Rudolph.

(5) International Conference on Crystal Growth (ICCG-14), held in Grenoble, France, 9–13 August 2004, in conjunction with the 12th International Conference on Vapour Growth and Epitaxy. This is a most important forum for crystal growers and many members of our Commission were involved in the organization of the different sessions. Altogether the programme included 943 papers, ranging from growth of traditional semiconductors to oxides to nanomaterials and nanoclusters. The Proceedings, edited by T. Duffar, M. Heuken and J. Villain, are partly published in *J. Cryst. Growth* and partly distributed on CD-ROM. The conference was sponsored by the IUCr.

(6) International Workshop on Nanomagnetism, La Habana, Cuba, 15–19 November 2004. The Commission supported this meeting and recommended its sponsorship by the IUCr. The meeting was considered successful as it attracted about 85 participants from 17 countries. Important to note is that one quarter of the participants were students, six of which could participate thanks to the IUCr sponsorship. The Proceedings of the meeting should appear soon in *Journal of Magnetism and Magnetic Materials*.

The Commission positively concluded the activity of the triennium with an international school 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. The participants numbered about 45, mostly from Mexico, but with a consistent participation from other Latin-American countries. Sixteen lecturers from Canada, France, Germany, Uruguay, Mexico, Spain, Switzerland and 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, ferroelectric materials, solution growth of biocrystals, structural studies and defects in real crystals. Four members of the Commission were enrolled as lecturers at the school.

R. Fornari, Chair

4.7. Commission on Crystallographic Computing

The major focus of the Commission during the triennium was threefold:

(1) The creation and maintenance of a web site of the Commission (<http://www.iucr.org/iucr-top/comm/ccom/>), including five bi-annual Newsletters. Every issue was organized around a central theme for which a number of authors were invited for a contribution. In addition, there were stories about early crystallographic computing. All issues are still online.

(2) The proposal and implementation of Microsymposia for the Florence Congress. In that context, nine computing-related sessions were arranged covering the various areas of interest (small molecule, macromolecule, charge density, powder diffraction *etc.*)

(3) The organization of an IUCr crystallographic computing school to be held in Siena, Italy, prior to the Florence Congress. This school will address the generally felt need for the education of the next generation of scientific crystallographic software developers. The current generation of crystallographic software was produced and is maintained by a generation that will soon retire or is retired already.

This is in particular an issue in the non-macrocrystallography community. Currently used software is written in a language that is no longer mainstream and extremely difficult to maintain by the next generation of maintainers. The current software user community expects menu-driven software with a button for everything he/she wishes to be executed to address their particular problem. Everything that is not behind a button will soon be lost or considered impossible. Somebody has to know how to arrange for that. This is a task for a scientist with an interest in software development. The current software 'speak' is no longer Fortran but C++ and scripting languages like Python. The school will be held in a former cloister just outside Siena with an attendance of about 80 to 85 participants. The all-in school fee could be kept at the reasonable amount of EUR 500, reduced to EUR 50 by a number of bursaries for young scientists thanks to several generous sponsors.

A. L. Spek, Chair

4.8. Commission on Crystallographic Nomenclature

The Commission met in closed session at the Geneva Congress. Two working groups had been previously established (one on Phase Identifiers and one on Co-Crystal Nomenclature). A third, on Synchrotron Radiation Nomenclature, was established in Geneva

Working Group on Synchrotron Radiation Nomenclature [D. Mills (Chair), A. Kvik, T. Ohta, I. A. Robinson, A. Authier; J. R. Helliwell was invited to join in the course of the triennium]. The group has produced a report regarding the uses of the terms 'brilliance' and 'brightness'. Its recommendation is that the quantity characterizing the radiation properties of third-generation sources, namely the number of photons emitted per second per bandwidth per unit solid angle and unit area of the source [$\text{photons s}^{-1} \text{mm}^{-2} \text{mrad}^{-2}$ ($0.1\% \text{ bandwidth}^{-1}$)] is best described by the term 'spectral brightness'. The report has been adopted by the Commission.

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. D. Westbrook, B. McMahon (consultant); J.-C. Toledano resigned in the course of the triennium and we have to deplore the passing away of M. Berndt]. The group is charged with developing an identifier for crystalline phases. It has examined a number of ways to formulate an identifier that will uniquely label crystal structure phases stored in a computer database and has listed the properties that should under normal circumstances uniquely characterize each crystalline phase. Its efforts have been coordinated with the Committee developing an IUPAC–NIST Chemical Identifier (InChI) since it was they who initially requested the phase identifier. Both groups independently had adopted very similar approaches. The final report of the Working Group is practically complete and is expected to be submitted in the near future.

Working Group on Co-Crystal Nomenclature [F. H. Allen (Chair), J. Atwood, J. D. Dunitz, U. Griesser, F. H. Herbstein, L. R. Nassimbeni, A. Authier]. The group had been established to examine the nomenclature of co-crystals, for which a wide variety of terminologies currently exist, *e.g.* inclusion compound, clathrate, molecular complex, adduct *etc.* An initial meeting was held in Geneva in August 2002. However, the Chair reported in 2003 that there was in fact little input from the members of the working group, which seemed to show a certain lack of interest in the topic. Furthermore, owing to the additional responsibilities he had had to take up, the Chair asked to be relieved of the chairmanship. There was therefore no further activity on this topic during the triennium. If there is any interest in reviving it, this can be discussed during the next closed meeting in Florence.

The IUPAC Interdivisional Committee on Nomenclature and Symbols has been restructured and renamed Interdivisional Committee on Terminology, Nomenclature and Symbols, thus recognizing the importance of terminology. A new Chair, J. Lorimer, has been appointed and the IUCr representative, S. C. Abrahams, reported an increased level of activity in 2004. For instance, there is a proposal for the use of the name 'uno', symbol U, for the unit one so that dimensionless numbers may be treated in the same way as all other SI units. Thus, a second phase in a material detected at a $15 \mu\text{g/kg}$ level, for example, would be expressed as 15 nU (15 nanouno) of that phase.

COMCIFS. In preparing CIF dictionaries, COMCIFS has to define concepts very tightly and to invent CIF names for these. The Chair of COMCIFS, I. D. Brown, reports that no nomenclature issue has arisen during the triennium. During 2004, COMCIFS has put considerable energy into the publication of *International Tables for Crystallography*, Volume G, the volume that will contain a comprehensive account of the CIF project. It is expected to be published in 2005.

A. Authier, Chair

4.9. Commission on Crystallographic Teaching

The members of the Commission as agreed in Geneva during the General Assembly in August 2002 were: R. B. Neder (Chair, Germany), J. D. Barnes (USA), G. Chapuis (Switzerland), L. M. D. Cranswick (Canada), K. Crenell (UK), M. E. Kastner (USA), K. Ogawa (Japan), S. Parthasarathy (India), P. Spadon (Italy), V. S. Urusov (Russia). The Commission was not active for the first two years and in September 2004 the Executive Committee decided to appoint P. Spadon as Chair.

Contacts were established *via* e-mail and the first action was to make suggestions for the preparation of the scientific programme for

the Florence Congress. During the same Congress, a meeting is planned in order to agree on the future activity of the Commission and for this it will be particularly important to suggest new qualified and active members to be appointed for the triennium 2005–2008.

Recently, contacts have been established with the Informal Working Group on Mathematical and Theoretical Crystallography (MaThCryst) in order to contribute to the organization of a 'Winter School' in Havana, Cuba, with young scientists of the Caribbean region as potential public. A programme and list of speakers is under discussion. P. Spadon is a member of the Scientific Programme Committee for the Florence Congress.

P. Spadon, Chair

4.10. Commission on Electron Diffraction

The last three years have been a time of great excitement in electron diffraction and microscopy, resulting partly from the boom in nanoscience and partly from breakthroughs in new instrumentation. These have included the commercial development of aberration-correctors and monochromators, and of field-emission scanning transmission instruments (STEMs) and TEMs capable of imaging and spectroscopy with sub-ångstrom spatial resolution, a long-sought goal finally attained. The field-emission source (brighter than current-generation synchrotron/undulator systems) has allowed inner-shell energy-loss spectra and images of individual dopant atoms in crystals to be obtained, while Professor Zewail's Nobel Prize has spurred the development of subpicosecond electron diffraction systems. The discovery of the carbon nanotube by high-resolution TEM has stimulated much new high-resolution *in situ* imaging at high pressures for catalysts, while the new electron precession camera has been fully developed and applied. Oxygen ordering in high- T_c materials and defects at interfaces continue to be imaged at atomic resolution, while a major development has been the achievement of tomographic imaging in materials science by TEM at subnanometre resolution for mesoporous materials. The subnanometre probe of the STEM, and the much greater sensitivity of electron structure factors to ionicity than X-ray structure factors, at low angles, has allowed highly accurate extinction-free quantification of convergent-beam electron diffraction patterns to produce charge-density maps of unprecedented precision for the study of bonding. In biology, cryo-EM has produced whole-cell tomographic images at 5 nm resolution, while single-particle work continues to explore the ribosome and other macromolecules and membrane proteins, which cannot be crystallized at subnanometre resolution.

These years have been crowded with teaching activity and conferences, some of which included the well attended (90 attendees) Erice/NATO school in Sicily, Italy, in summer 2004 on electron crystallography, and workshops on time-resolved electron diffraction and imaging at Livermore, USA, in summer 2004, international and national conferences on electron microscopy in many countries, the 2004 Gordon Conference on charge densities, a school on electron crystallography at Berkeley, USA, in April 2004, similar schools in Beijing, People's Republic of China (100 attendees in December 2002) and Moscow, Russia, amongst many others. D. L. Dorset won the Patterson award of the ACA in 2002 for his work in electron crystallography of organic materials. There have been several special issues of journals devoted to electron crystallography and atomic resolution electron microscopy.

The Commission now has a web page, accessed through the IUCr web page and Commission links, which contains a list of teaching materials including books and free software. Also given is a list of conferences and links to web pages of many active research groups,

arranged by applications in materials science and biology. The Commission, chaired by J. C. H. Spence, will meet at the Florence Congress.

J. C. H. Spence, Chair

4.11. Commission on High Pressure

The third triennium for the Commission started with some important changes in its membership. Most prominently, R. J. Nelmes, the *spiritus rector* and driving force of the Commission, stepped down as Chair and was replaced by M. Kunz (then Switzerland, now USA). Furthermore, S. Tolbert (USA), R. Winter (Germany), J. S. Loveday (UK), J. Tse (Canada), M. Mezouar (France) and N. Hamaya (Japan) were newly elected to the Commission. A. Katrusiak (Poland) and S. K. Sikka (India) as well as the outgoing Chair R. J. Nelmes were appointed as new consultants to the Commission. The past three years have brought further development in high-pressure crystallography. On the one hand, established high-pressure techniques are applied in new fields such as protein crystallography or nanomaterials science; on the other hand, high-pressure crystallography is newly combined with experimental methods (*e.g.* inelastic scattering, small-angle scattering, X-ray spectroscopy and X-ray radiography), which opens new possibilities to solve problems in a variety of disciplines. At the same time, the continuing development of established techniques allows the application of high-pressure crystallography to more and more sophisticated problems. This development is strongly supported by the expansion and perfection of dedicated high-pressure experimental stations at synchrotron and neutron sources all over the world. Tremendous progress in computational techniques continues to support strongly or even lead the way in the structural exploration of matter at extreme conditions.

In order to support interaction between the individuals in the broad field of high-pressure crystallography, the main activity of the Commission in the past three years was the organization of symposia, workshops and a summer school. These events are also used as a forum, which should allow outsiders to learn about the potential that high-pressure crystallography could offer for their research. We also put a specific effort into supporting young scientists in order to encourage them for a continuation of their career in science.

4.11.1. Symposia, workshops and summer school. During the Geneva Congress, the Commission organized six Microsymposia, which were all well attended. These six Microsymposia were complemented by two Open Commission meetings focusing on technical development and application of high pressure in protein crystallography.

Following this large event in 2002, a more focused workshop entitled Non-Ambient Crystallography: The Science of Change was organized in 2003 at the Lawrence Berkeley National Laboratory in Berkeley, California, USA, by S. Clark (LBL), A. Kavner (UCLA) and Commission member S. Tolbert (UCLA). In addition to a range of interesting Microsymposia (anisotropy in P/T deformations, kinetics of structural change; theory of structure under pressure; transport under pressure; phase transitions; synthesis at high pressure), this workshop also offered four hands-on introductory courses on: high-pressure infrared spectroscopy; high-pressure powder diffraction; laser-heated diamond anvil cells; and general alignment and maintenance of diamond anvil cells. These hands-on courses were especially appreciated by the 20 students, who benefited from IUCr travel support.

The year 2003 also saw the very successful realization of the first high-pressure crystallography summer school, held 4–15 June in

Erice, Sicily, Italy. Commission consultant A. Katrusiak (Poland) acted as course director together with P. McMillan (UK). 30 international experts held lectures and workshops on practical aspects of both experimental and computational work in high-pressure crystallography. 88 selected participants from 21 countries were on site for the summer school and were joined by numerous 'virtual' participants, who made use of the first live broadcast of the Erice summer school *via* the internet and were able to pose questions to the speakers through a web chat-room.

In 2004, the Commission held a workshop covering the full scope of its activities at the Canadian Light Source in Saskatoon, 18–21 August 2004. Commission member J. Tse coordinated the organization and chaired the Programme Committee. The scientific programme covered many scientific and technological areas of interest to the high-pressure community. The workshop was arranged in 11 sessions over three and a half days. Each session focused on a particular subject and was led by a Keynote Lecture introducing the state-of-the-art of the field. There were a total of 47 oral presentations covering diverse topical subjects such as structural studies on biological materials, liquid–liquid transition, amorphous solids, structural chemistry of novel materials and structures, superconductivity and magnetism, computational crystallography and the latest developments in instrumentation and methodologies for structural determination. A large portion of the presentations was given by young scientists (10 lectures by recent post-doctorals and students). In addition to formal presentations, a poster session with 22 contributions provided an alternative forum for further scientific discussions.

As in previous Congresses, the Commission put a lot of effort into shaping the programme at the Florence Congress. Commission member J. B. Parise is a member of the Programme Committee. He was instrumental in planning six Microsymposia organized by the Commission. On top of these six Microsymposia, Commission members J. S. Loveday and I. N. Goncharenko are organizing two Open Commission meetings, focusing on high-pressure single-crystal crystallography and technical developments. This together with two Keynote Lectures (J. Tse and M. McMahon) will form a well rounded high-pressure 'workshop' within the Congress.

4.11.2. Commission meetings. The main meeting of this triennium was held during the 2004 workshop in Saskatoon, Canada. Six members and consultants were present. Topics discussed were the creation of a high-pressure-specific CIF code, the shaping of the Florence Congress and possible sites of future Commission workshops, as well as maintaining the Commission web page.

4.11.3. Future plans and activities. The upcoming triennium is very promising for the high-pressure crystallography community. Recent progress in the artificial growth of diamonds and the upcoming dedicated high-pressure beamline at the newly constructed Spallation Neutron Source in Oak Ridge, USA, together with new or improved dedicated high-pressure synchrotron beamlines, will open an array of new experiments. Especially interesting for crystallographers is also the newly revived interest in high-pressure single-crystal diffraction, which may enable the extraction of detailed structural information experimentally at megabar pressures.

The Commission plans more of its workshops in the years 2006 and 2007. In order to help in the expansion of the high-pressure community into Eastern Europe, it was decided to hold the 2006 workshop in Dubna, Russia, where we obtained support from the Joint Institute of Nuclear Research. The 2007 workshop is planned to be held at the DIAMOND Synchrotron Source in the UK. Commission member J. S. Loveday will act as the local organizer. Also, first steps have been undertaken to organize a Commission

workshop in 2009 in China, again with the aim to reach out to less represented countries.

M. Kunz, Chair

4.12. Commission on Inorganic and Mineral Structures

4.12.1. Preface. Following a proposal submitted by G. Ferraris, the formation of the Commission (CIMS) was approved at the Geneva General Assembly in August 2002. With this act, it was recognized that, even if research on inorganic structures is to some extent related to areas covered by other IUCr Commissions (*e.g.* those dealing with instrumentation and methods), the establishment of a Commission could better attract within the IUCr orbit more inorganic crystallography, particularly that related to materials and minerals science.

The main aims of CIMS are as follows:

To strengthen links and interactions of structural inorganic scientists with the crystallographic community.

To promote the presence at the IUCr meetings of Microsymposia specifically dedicated to the Commission purposes.

To promote the publication of inorganic crystallography in the journals of the Union.

To promote and organize symposia, workshops and schools of interest to the crystallographic inorganic community.

4.12.2. Contacts between members and consultants. 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/> set up and administered by M. Nespolo.

Occasions for personal contacts of some of the CIMS members have been: Geneva Congress (August 2002); 18th General Meeting of the International Mineralogical Association (Edinburgh, UK, September 2002); ECM-21 (Durban, South Africa, August 2003); ECM-22 (Budapest, Hungary, August 2004); Symposium on Micro- and Mesoporous Mineral Phases (Rome, Italy, December 2004).

4.12.3. Co-organization and support of scientific meetings. The following conferences have been supported by CIMS; most have been (co-)organized by members of the Commission, as indicated:

9th European Conference on Solid State Chemistry (3–6 September 2003, Stuttgart, Germany); co-organizer, M. Jansen.

XV International Conference on X-ray Analysis and Crystal Chemistry of Minerals (St Petersburg, Russia, 15–19 September 2003); members of the Programme Committee: G. Ferraris and D. Yu. Pushcharovsky.

Anniversary Fedorov Session 2003 (St Petersburg, Russia, 9–10 December 2003); members of the Programme Committee: G. Ferraris and D. Yu. Pushcharovsky.

Satellite Meeting of ECM-22: Crystallography at the Start of the 21st Century: Mathematical and Symmetry Aspects (Budapest, Hungary, 24–26 August 2004); organizer: M. Nespolo; lecturers from CIMS: M. Nespolo and W. Depmeier.

Micro- and Mesoporous Mineral Phases (Rome, Italy, 6–7 December 2004); co-organizer: G. Ferraris. This has been the main conference organized by CIMS and has been financially supported by the IUCr. A full report is available at <http://www.lcm3b.uhp-nancy.fr/cims/pdf/Confreport-Rome.pdf>. The conference was devoted to inorganic porous materials other than zeolites. Over 100 delegates from 20 countries with 32 oral and 53 poster presentations attended the meeting. The extended abstracts filled 324 pages of a book of pre-prints. The contributions of twelve oral presentations are printed as volume 57 (same title as the meeting) of the series *Reviews in Mineralogy and Geochemistry* (Editors G. Ferraris and S. Merlino). A number of other contributions are in press in a dedicated issue of the

European Journal of Mineralogy. Lecturers from CIMS: W. Depmeier, G. Ferraris and L. B. McCusker.

International School on Mathematical and Theoretical Crystallography (Nancy, France, 20–24 June 2005); organizer: M. Nespolo.

The following sessions of conferences have been proposed by CIMS; most have been convened by members of the Commission, as indicated.

ECM-21 (Durban, South Africa, August 2003): Mineralogical Crystallography (convener: E. Tillmanns); Perovskites Ancient and Modern (convener: A. M. Glazer); invited speakers from CIMS: G. Ferraris and A. M. Glazer.

32nd International Geological Congress (Florence, Italy, 20–28 August 2004): Microstructures, Modularity, Modulations in Minerals (convener: G. Ferraris); Crystal Structures of Minerals: Topology and Classification (conveners: D. Yu. Pushcharovsky and E. Tillmanns).

ECM-22 (Budapest, Hungary, August 2004): Investigation Techniques in Mineral Science (convener: M. Nespolo); Advances in Powder Diffraction Methods (convener: J. Rius); invited speakers from CIMS: W. Depmeier and G. Ferraris.

Florence Congress: Open Commission Meeting (convener: G. Ferraris); MS7: Crystal Chemistry of Inorganic and Mineral compounds (convener: W. Depmeier); MS35: Polytypism and Twinning (convener: G. Ferraris); MS79: Inorganic and Mineral Structures Solved and Refined by Powder Diffraction Data (convener: J. Rius); MS14: Modularity and Modulation in Inorganic and Mineral Structures; MS28: Structure/Properties Relationships of Technologically Relevant Inorganic and Mineral Compounds; Keynote Lecturer from CIMS: L. B. McCusker; Keynote Lecturer proposed by CIMS: T. J. White (Singapore).

4.12.4. Other activities of CIMS members. The following activities of members related to CIMS purposes and not yet mentioned above have been reported to the Chair for the period 2002–2005.

I. D. Brown is author of the IUCr Monograph *The Chemical Bond in Inorganic Chemistry*.

W. Depmeier is co-organizer of the meeting Mineralogical Museums (St Petersburg, Russia, June 2005) and President of the German Crystallographic Association.

G. Ferraris is co-author with E. Makovicky and S. Merlino of the IUCr Monograph *Crystallography of Modular Materials*. He is a member of the Programme Committee and convener of the 19th Meeting of the International Mineralogical Association (IMA) (Kobe, Japan, 23–28 July 2006); he is Vice-Chair of the Commission on New Minerals and Mineral Names (CNMMN) of IMA.

M. Matsui is Chair of the Meeting Secretariat for IMA 2006 (Kobe, Japan) and Editor of *Physics and Chemistry of Minerals*.

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) (Vienna, 2010).

L. B. McCusker was a member of the Advisory Board for the 14th International Zeolite Conference (Cape Town, South Africa, 2004); she lectured at NHSC-33 (Pune, India), the 14th International Zeolite Conference (Cape Town, South Africa) and CPDIC-9 (Prague, Czech Republic); she was a Guest Co-editor of a special issue of *Zeitschrift für Kristallographie* devoted to Structure Determination from Powder Diffraction Data; she is a member of the Organizing/Programme Committees of EPDIC-10 (Geneva, Switzerland, 2006) and ZMPC 2006 (Yanago, Japan, 2006); she co-maintains the IZA websites on zeolites, <http://www.iza-online.org/> and <http://www.iza-structure.org/>.

M. Nespolo is Associate Editor of the *European Journal of Mineralogy*, Secretary of the Special Interest Group SIG5 Miner-

alogical Crystallography of the European Crystallographic Association (ECA), and webmaster of the ECA.

D. Yu. Pushcharovsky represents CIMS on the Programme Committee of the Florence Congress.

J. Rius is a member of the ESRF Review Committee in the Chemistry area, of the Spanish Committee of Crystallography and of the Scientific Committee of EPDIC-9 (Prague, Czech Republic 2004); he is Chair of the Special Interest Group (SIG8) of the ECA; he is an Associate Editor of the *European Journal of Mineralogy*.

G. Ferraris, Chair

4.13. Commission on Neutron Scattering

With regard to the past triennium (2002–2004), the present perspectives of the neutron community are worldwide positive and promising. On the one hand, the most powerful sources such as ILL or ISIS have been refurbished or are being expanded. On the other hand, a few medium-flux sources have been closed or the decision has been taken to shut them down in the near future as, for example, with the Jülich reactor in Germany or the reactor in Studsvik (Sweden). But the decommissioning of these sources, very important for the scientific community in the past, will be fully compensated by the new high-flux sources like the new German research reactor FRM-II in Garching near Munich, which came into operation in 2004, and the new ANSTO facility OPAL in Australia starting at the end of 2005. In addition, the new next-generation neutron sources, the spallation sources SNS in the USA and J-PARC in Japan, are currently under construction; in particular, the SNS in the USA is due to start working in 2006. These very intense sources will open up new horizons in neutron scattering research for the coming decades.

Referring to the topics of the corresponding research, there is an increasing demand from industry to use neutrons as a probe in materials research in order to optimize production processes or to improve the long life cycle of technical components. At the sources, efforts are being made to provide dedicated instruments for these applications satisfying the special requests of the industrial users. In addition, an increasing number of users with biological or soft-matter questions are applying for beamtime at neutron sources. But this growing demand should be best met by the new very intense spallation sources. More and more special sample environments play an important role in neutron experiments; for instance, in research on high- T_c superconductors or in strongly correlated magnetic systems. Therefore, several facilities offer not only very high magnetic fields, but also unique possibilities such as laboratories for crystal growth, isotopic exchange or thermodynamic experiments to extend the on-site potential and to improve conditions for the users.

4.13.1. International meetings. In order to present new scientific areas and innovative methods to the users as well as to broaden the neutron community, a large number of international meetings and workshops on neutron scattering took place all over the world during the last three years. An overview of the most important meetings is given below.

The XVI ICANS (International Collaboration on Advanced Neutron Sources) meeting took place in Neuss, Germany, in May 2003. The meeting was hosted by the Forschungszentrum Jülich, Germany, and was co-sponsored amongst others by Hahn–Meitner-Institut, Berlin, Germany. Some of the major topics of the meeting concerned neutron scattering instrumentation, as well as target and moderator systems.

The 3rd European Conference on Neutron Scattering (ECNS) hosted by the European Neutron Scattering Association (ENSA) was held at Montpellier, France, in September 2003 with 615 participants

from 30 countries. The conference focused amongst other topics on advances in instrumentation.

In September 2002, the 4th International Workshop on Polarized Neutrons in Condensed Matter Investigations (PNCMI) was held in Jülich, Germany, and the 5th PNCMI Workshop was held in Washington, DC, USA, in June 2004.

The 21st and 22nd European Crystallographic Meetings (ECM) were held in August 2003 in Durban, South Africa, and in August 2004 in Budapest, Hungary, respectively. During these meetings, several satellite meetings were also held.

In April 2005, the XVII ICANS Meeting was held in Santa Fe, USA. The next important meeting in 2005, besides the Florence Congress, will be the International Conference on Neutron Scattering (ICNS) that will take place in Sydney, Australia, at the end of November/beginning of December. On this occasion, the ANSTO research reactor OPAL (Open Pool Australian Light-water) will come into operation.

In addition, the Institut Laue–Langevin (ILL), Grenoble, France, regularly organizes topical workshops that have become a real tradition. These workshops also address young researchers; indeed, at ILL much importance is attached to training of researchers.

4.13.2. Neutron sources – international cooperation. In the last three years, many changes occurred in Europe concerning neutron sources with some old sources being closed and new ones being built or refurbished. For instance, the new research reactor FRM-II in Munich, Germany, was inaugurated in the middle of 2004 and routine operation started in the spring of 2005 after some teething troubles. The first experiments have already been carried out successfully. The research reactor BER-II, operated by Hahn–Meitner-Institut, Berlin, Germany, remains the second long-term neutron source in Germany. In January 2005, a new second Neutron Guide Hall was completed at this source. In the coming years, new advanced instruments such as the Extreme Environment Diffractometer (EXED) and a High-Resolution Small-Angle Scattering instrument (VSANS) will be installed in the hall in order to comply with the users' needs. In 2004, the decision was taken to shut down the reactor FRJ-2 at Forschungszentrum Jülich, Germany, by May 2006. A contract to install an outstation of the Forschungszentrum Jülich at the site of FRM-II was agreed between the Technical University Munich and the Forschungszentrum Jülich in June 2004. The mid-term closure of the reactor FRG-1 (Forschungszentrum Geesthacht, Germany) was decided.

The research reactor in Studsvik, Sweden, will be closed down by summer of 2005.

The financial situation of the French reactor Orphée, operated by Laboratoire Léon Brillouin (LLB), could be secured for the years to come.

The only continuous spallation neutron source worldwide SINQ, located at Paul-Scherrer-Institut, Villigen, Switzerland, is running successfully and provides the best opportunities for fruitful experiments.

In December 2004, ISIS, the world's leading spallation neutron source at Rutherford Appleton Laboratory, UK, celebrated the 20th anniversary of its first neutron production. A second target station is being built in order to meet the users' requirements. It will open new opportunities in biomolecular science, nanoscale science, advanced materials and soft condensed matter. The completion of the target installation is expected to occur in 2007.

The ILL in Grenoble, France, as the central European facility and most powerful neutron source in the world, attracts European researchers as well as scientists from all over the world. In 2000, the ILL launched the so-called Millennium Programme, a five-year

development programme, with the aim to renew the instrumentation. Other points like the optimization of the range of neutron beams or the upgrade of the neutron guide system are also part of this programme. A refit programme to secure the long-term operation of the reactor, presently causing a reduction of the operation cycles, is successfully on the way and will be finished in 2006. By then normal routine operation with the usual $4\frac{1}{2}$ cycles per year will restart.

The ESS (European Spallation Source) project has been almost fully designed, but was not financed after evaluation in 2002. However, it remains an important project for the future of neutron scattering in Europe. The discussion about such a source is going on in different European countries.

The China Advanced Research Reactor (CARR), a 60 MW facility, is expected to become critical at the end of 2006.

The construction of the new Australian research reactor OPAL (Open Pool Australian Light-water) began in April 2002 and the commissioning phase will start at the end of 2005. Eight instruments are planned for the facility so far, but a future expansion is possible.

The Japanese research reactor JRR-3M, the high-performance neutron source of JAERI, is still successfully in operation and allows multipurpose research with various neutron experiments.

Concerning the JAERI–KEK Joint Facility for High Intensity Proton Accelerators, called the J-PARC Project, the commissioning of equipment was started in the linac and 3 GeV synchrotron building. The construction of the final part of the 50 GeV accelerator tunnel will be ordered soon.

The Spallation Neutron Source SNS is being built at Oak Ridge National Laboratory, USA. The facility will have one target station with 24 instruments and will provide the most intense neutron beams in the world. Since SNS is nearly completed, the first neutrons are expected in 2006. The SNS will attract 1,000 to 2,000 scientists and engineers each year from universities, industry and laboratories from the USA as well as from other countries. The diverse applications of neutron scattering research will provide hitherto not yet reached scientific and technical opportunities for experts.

M. Steiner, Chair

4.14. Commission on Powder Diffraction

The Commission (CPD) has again been quite active during the last three years. CPD round robins and the *Newsletter* are still the main pillars of CPD activity. In addition, the CPD also feels a strong commitment toward teaching and is now engaged in a major textbook project *Powder Diffraction in Theory and Practice* at a graduate level. In addition, several courses on powder diffraction were supported or organized by the CPD and its members.

4.14.1. Newsletter. Every CPD *Newsletter* is devoted to a particular topic, providing up-to-date information in that particular branch of powder diffraction, well before the information finds its way into textbooks, thus making it a valuable source of information. The *Newsletter* has considerably increased in size, quality and the number of subscribers. Started by our previous Chair P. Scardi, we have now finished the task of transferring all of the older CPD *Newsletters* from paper to electronic format. All issues of the scanned *Newsletters* have finally been corrected for scanning and typographical errors and can be downloaded from <http://www.mpi-stuttgart.mpg.de/cpd/html/newsletter.html>. All *Newsletters* easily fit on a 'collectors' CD-ROM. The wide availability of fast internet connections and the provision of a powerful server by the MPI for Solid State Research means that most people nowadays download the *Newsletter* from the web, which is fast, cheap and convenient. We recognize that people in some developing countries do not have

appropriate internet access, which still requires a costly printed version of the *Newsletter*. In future, it might well be that the CPD *Newsletter* will convert to an entirely electronic version, while still keeping an ISSN number.

During 2002, two issues of the CPD *Newsletter* were published. The summer issue (No. 27) was edited by L. M. D. Cranswick and G. J. Kruger and was entitled Powder Diffraction in Mining and Minerals. The winter issue (No. 28) was edited by P. Scardi and was entitled XRD Line Profile Analysis. These two issues can both be considered as state-of-the-art contributions and important references. In 2003, the summer issue (No. 29) of the CPD *Newsletter* was edited by A. N. Fitch and was entitled Powder Diffraction in Action. As can be seen from the title, this *Newsletter* is devoted to the various aspects on *in situ* powder diffraction. It nicely reflects current achievements in this rapidly growing area and underlines the importance of the CPD *Newsletter* in reporting recent achievements and trends in powder diffraction. *Newsletter* No. 30 edited by C. Hubbard was delayed and will be combined with the winter issue of 2004 (No. 32) edited by R. Delhez. In 2004, the summer issue (No. 31) edited by N. Masciocchi on powder diffraction of molecular functional materials had reached a record size of 75 pages presenting a variety of methods for solving complicated materials of general interest.

The popularity of the computer software pages by L. M. D. Cranswick is still very high. These pages are much appreciated by readers for their informative content and their effective presentation. News from ICDD and IXAS is also present in all issues, together with news on forthcoming events. In an attempt to keep production costs as low as possible, the *Newsletters* are printed and distributed from Venezuela. Special thanks go to M. Delgado who voluntarily offered his help in this matter. The CPD is also grateful to the sponsors of the *Newsletter* who help cover the high printing and distribution costs.

4.14.2. Web site. The CPD web site is still the reference point for powder diffractionists around the world and has undergone a major reorganization. Besides links and information on events related to PD (including the CPD round robins), the web site gives free access to the CPD *Newsletter* archive, from which recent and past issues can be downloaded in pdf (Acrobat) format. The CPD tries to increase its activity in teaching. A new section for 'educational exercises' and 'teaching pamphlets' has been added. These provisions have greatly increased the number of readers. In particular, the exercise on how to distinguish between the different isomers of Alq₃ (a 'hot candidate' for blue LEDs) using high-resolution powder diffraction data is challenging. The teaching section is still in its infancy and we strongly hope that more people will send in their contributions, which would be for the benefit of everyone in the community.

4.14.3. CPD projects. Round robins. Round robins are long-term projects and there is usually some overlap between consecutive triennia, as in the case of the Quantitative Phase Analysis Round Robin (QPA-RR) and the Size-Strain Round Robin (SS-RR). The first part of the comprehensive QPA-RR was reported in a publication by I. C. Madsen *et al.* [*J. Appl. Cryst.* (2001), **34**, 409–426], distributed as a free offprint together with CPD *Newsletter* No. 25. The second part was published later by N. V. Y. Scarlett *et al.* [*J. Appl. Cryst.* (2002), **35**, 383–400] and was distributed as a reprint with *Newsletter* No. 27. Readers can refer to these papers for an exhaustive discussion on the results of the QPA-RR. Both parts can be freely downloaded from the CPD web site, where additional information and original data files can be found.

The results of the round robin on size-strain line broadening that was conducted some time ago and a comparative analysis using three different line-broadening methods were published as Size-Strain Line-Broadening Analysis of the Ceria Round-Robin Sample {D.

Balzar, N. Audebrand, M. Daymond, A. N. Fitch, A. Hewat, J. I. Langford, A. Le Bail, D. Louër, O. Masson, C. N. McCowan, N. C. Popa, P. W. Stephens & B. Toby [*J. Appl. Cryst.* (2004), **37**, 911–924]]. The reprint will be distributed with the current *Newsletter* (No. 32).

Further round robins, *e.g.* on organic standards for Rietveld refinement or performance of 2D detectors, are planned and will be realized in the next triennium.

Textbook. The most ambitious current project of the CPD is a textbook entitled *Powder Diffraction in Theory and Practice* at a graduate level; this will be published by the Royal Society of Chemistry (UK). Editors are the current Chair and S. Billinge from Michigan State University. Several members of the CPD have agreed to write chapters for this book.

4.14.4. Meetings/workshops/schools. The year 2002 was dominated by the Geneva Congress, a real success in terms of attendance and scientific quality. Powder diffraction (PD) was very well represented with more than 11 Microsymposia directly related to powder diffraction. Support was given to a variety of conferences, schools and workshops. Meetings of interest for the CPD in 2002 included the 8th European Powder Diffraction Conference in Uppsala (May 2002, Chair R. Tellgren). After the establishment of the EPDIC Committee ECA-SIG, the CPD regularly takes part in the planning activity for the EPDIC conference. The CPD supported the II International School on Powder Diffraction, organized by the Indian Association for the Cultivation of Science (Jadavpur, Calcutta, India, January 2002). Meetings of interest for the CPD in 2003 included the 21st European Crystallographic Meeting in Durban, South Africa, 24–29 August 2003, where a CPD meeting also took place. The CPD supported a Workshop on Radiation Based Techniques, 24–27 October 2003, in Cape Town, South Africa, and the conference Structure Solution from Powder Diffraction Data, 14–19 September 2003, in Stara Lesna, Slovak Republic. In 2004, the CPD endorsed various meetings: Recent Advances in X-ray Powder Diffraction, 27 November–2 December 2004, Assiut, Egypt, organized by the Egyptian Society of Crystallography and its Applications (ESCA), EPDIC IX, European Powder Diffraction Conference, in Prague, Czech Republic, 2–5 September 2004, which was also the host for the yearly CPD meeting, and the Fifth Canadian Powder Diffraction Workshop (including neutron diffraction), 28–29 May 2004, at the University of Waterloo, Waterloo, Ontario, Canada. With W. I. F. David a member of the Programme Committee, the CPD was engaged in the planning of the powder sessions for the upcoming Florence Congress, verifying that powder diffraction is well represented with nine Microsymposia and one Keynote Lecture. Under the auspices of the CPD, an International Workshop on Powder Diffraction at Non-Ambient Conditions has been organized and attracted a great deal of interest. The workshop will take place 5–7 October 2005 at the Max-Planck Institute for Solid State Research in Stuttgart, Germany. The CPD also agreed to sponsor the regular Reynolds Cup.

R. Dinnebier, Chair

4.15. Commission on Small-Angle Scattering

The details of the Commission's activities are presented in the annual reports of the Commission. The present report aims at providing an overview of these activities and to outline the directions of the future work and activities.

4.15.1. Meetings. *The triennial Small-Angle Scattering (SAS) meeting.* The International Conference on Small-Angle Scattering has been held on a triennial basis for nearly forty years. It is the main

occasion for scientists practising small-angle scattering to meet and exchange ideas related to the technique itself across the boundaries of the various scientific disciplines and its broad range of applications. The conference has been organized independently of the IUCr and the venue of the next conference is decided by the participants of the current one. In the past, the conference has coincided with the years of the IUCr Congress and this has caused problems concerning the possibility to seek support from the IUCr when the SAS conference could not be considered as a satellite meeting to the IUCr Congress. At SAS 2002 in Venice, this issue was raised by those of the Commission members who were also members of the International Advisory Board and the problems were discussed. The Board decided to recommend that the next conference be moved by one year, so that such a conflict will be avoided. This was accepted by the participants and the next conference is to be held in 2006 in Japan. T. Hashimoto (University of Kyoto) will Chair the conference and Y. Amemiya of the Commission is a member of the Organizing Committee. Members of the Commission are also serving on the International Advisory Committee of SAS 2006. The Commission will also take an active role in supporting the future SAS conferences and in providing guidance as well as 'institutional memory' for future organizers.

The IUCr Congress. The Commission has provided input on Microsymposium topics for the Florence Congress. Suggestions for speakers and Chairs were given. The recommendations made by the Commission have largely been followed and have resulted in several SAS-related Microsymposia and a Keynote Lecture. Y. Amemiya and I. Torriani are involved in organizing a Microsymposium on Analysis of Anisotropic Materials.

4.15.2. Education. Commission members are in general very active in organizing and participating in summer schools and tutorial workshops to promote small-angle-scattering techniques (see annual reports for details). In connection with the IUCr Congresses, the Commission takes responsibility for organizing tutorial workshops. In 2002, the Commission (J. D. Barnes, Chair) organized a well attended tutorial workshop at the Geneva Congress. In connection with the Florence Congress, the Commission (J. S. Pedersen, Chair) is organizing a one-day tutorial workshop on small-angle scattering. Several Commission members will give tutorial lectures so that a broad expertise is present at the workshop.

Since several Commission members are instrument-responsible for SAXS and SANS facilities, they interact regularly with user groups, and they educate and train students and post docs in the practical aspects of small-angle scattering.

4.15.3. Publication. The Proceedings of SAS 2002 (Venice) were published in *Journal of Applied Crystallography (JAC)*. This impressive volume is an important reference for the community and the high quality of the published papers is thanks to G. Kostorz (consultant of the Commission and Editor of *JAC*).

G. Kostorz will continue his efforts for the publication of the Proceedings for SAS 2006 in *JAC*, as for previous Proceedings. It is important that the papers of the conference are collected in a highly ranked journal such as *JAC*, since each of these Proceedings constitutes an important milestone as a collection of SAS literature. Therefore, the effort of publication in *JAC* is strongly supported by the Commission, which is most grateful to G. Kostorz for once again offering his help with editing the Proceedings.

4.15.4. Software development. The Commission will continue to provide 'moral support' for future canSAS and NOBUGS conferences related to software, data handling and analysis. In addition, software is developed by Commission members on an individual basis. P. Thiyagarajan provides a SAS analysis software package to the students and faculty who visit IPNS and APS for experiments. D.

Svergun offers his programs for analysis of SAS data to the community by making them publicly available on the EMBL web site.

4.15.5. Community building. The Commission (D. I. Svergun and J. S. Pedersen) made a call in 2002 through the SAS list-server for SAS-related links to web pages on hardware and software. The response to the call was limited and hence the web pages are unfortunately rather incomplete. The material that was received was edited by D. I. Svergun and J. S. Pedersen and placed on the Commission's web pages.

The Commission has an SAS list-server at the IUCr web site for communication among the subscribing SAS users. However, the use of the list-server has decreased significantly, which might be a result of the fact that the Commission itself has used it to a limited extent. It is desirable to appoint a Commission member to be responsible for the list-server, so that its use can be boosted and the subscription list can be updated. Commission members serve on the scientific committees of several large-scale facilities, national as well as international. In this connection, they not only evaluate beamtime applications but also participate in important discussions on the future instrumentation and development strategies at these facilities.

4.15.6. Prizes. At SAS 2002, the Commission, together with the organizers, took the initiative to award SAS prizes. There were three Young Scientist Prizes, named after O. Kratky, P. W. Schmidt and H. Brumberger, which were given for the best contributions related to experimental aspects, theory and applications, respectively. The prizes were sponsored by some of the SAS instrumentation companies (Bruker AXS, Anton Paar and Osmics). In addition, a prize, named after A. Guinier, was given to a scientist for a significant (breakthrough or life-long) contribution to the advancement of the SAS technique. This prize was sponsored from the IUCr President's Fund.

The Commission has the impression that the prize initiative was well received by the SAS community. The Commission will take responsibility for the SAS prizes (administration, funding and support) at future SAS conferences.

4.15.7. Technical issues. The Commission has been discussing an extension to the web page to include important references on technical issues such as absolute calibration, q calibration, smearing effects and data analysis. It has also been suggested that more introductory material should be included. Currently, there is a reference/link to an introduction from S. King. The Commission believes that it would be very useful to include lecture notes from some of the many SAS schools that have taken place in the past. Although there are several new textbooks on the market, lecture notes often have a special pedagogical touch that make them very accessible to newcomers. This effort should be enhanced during the next three-year period.

The Commission has discussed initiating a round robin with inter-laboratory checks of calibration procedures for SAXS. There are still different opinions about the usefulness of such a task, which would be very time-consuming. However, even if the results of comparing calibration procedures at individual laboratories are not published, it is still an important exercise for each of the laboratories to scrutinize their procedures and the possible sources of error through such comparisons. Commission member A. Allen (from NIST) is exploring the potential for developing a NIST Standard Reference Material (SRM) for SAS intensity calibration, particularly for SAXS. A calibration standard sample and a NIST-certified calibration curve for the measured SAXS intensity could also be used for comparison of individual calibration procedures.

4.15.8. Summary. There is a broad range of highly relevant tasks on which the Commission has made progress, and it will continue to

work on these over the next three-year period. However, advancing these tasks and projects will depend critically on how much time and effort the individual members can devote to them.

J. S. Pedersen, Chair

4.16. Commission on Structural Chemistry

The main activity of 2002 was the Geneva Congress. The meeting contained numerous Microsymposia of interest to the structural chemistry community. Commission members G. Punte and L. Brammer served as Microsymposia organizers and four others (V. Belsky, J. L. Flippen-Anderson, T. W. Hambley and D. C. Levendis) served as co-organizers for Microsymposia.

The Commission met during the Congress and discussed the scope of what we define as 'structural chemistry' as well as where the interests of the Commission overlap or intersect with other Commissions, such as (i) Inorganic and Mineral Structures, (ii) Charge, Spin and Momentum Densities, (iii) Crystal Growth and Characterization of Materials, and (iv) Powder Diffraction. The potential for supporting joint Microsymposia with these neighbouring Commissions was recognized for future IUCr Congresses. With regards to other meetings, the Commission discussed the possibility of providing input in the area of structural chemistry to the organization of the AsCA regional meeting, and possibly also the ECM meeting. *Acta Crystallographica*, Section B, the IUCr journal that is perhaps most closely associated with the Commission, is considering a series of Special Issues in areas such as drug design and polymorphism. The Commission noted that it should aim to provide useful input into these and similar initiatives.

The Commission endorsed the 3rd National Russian Crystal Chemistry Conference and the Indaba IV meeting, entitled Patterns in Nature, to be held in 2003 (see comments later in this report).

Commission members felt that the current requirement for meeting organizers to apply for IUCr support nine months in advance of a meeting was too long a lead-time. Commission Chair L. Brammer requested that the Sub-committee on the Union Calendar should consider reducing this period to six months. The Sub-committee subsequently decided that it would not take up the Commission's recommendation. (Adequate time has to be allowed for subsequent visa applications *etc.*)

Some issues discussed in the previous year required updating. There had been previous discussion in the Commission about the inclusion of new data items (*e.g.* for twinning) in the CIFs generated for small-molecule structures. L. Brammer contacted B. McMahon to ascertain the current status of any developments. An informal working party has been established to look into this. L. Brammer will check on future progress. There was also discussion of the possible need to include more data entries on area detectors in the small-molecule CIF.

There had also been previous discussion in the Commission of the value of providing a mechanism for archiving structure factors. L. Brammer checked with B. McMahon regarding the status of this idea. The IUCr appear to be open to considering some form of repository for structure factors from other journals or database depositions, but would need to be convinced that there was genuine scientific need. It is likely also that any costs for such a project would need to be recovered.

In 2003, the Commission was asked to nominate members with interests in structural chemistry for inclusion in the IUCr Scientific Programme Committee (SPC) for the Florence Congress. L. Brammer (UK) was recommended as a SPC member by the

Commission and was subsequently appointed together with F. Lahoz (Spain), SPC Chair C. Mealli (Italy) and past SPC Chair M. Kaftory (Israel) who also have interests in structural chemistry.

No requests were received during 2003 from organizers of conferences and symposia for Commission support in seeking IUCr funds.

Commission member D. Braga organized and served as Chair of a Euroconference on Molecular Crystal Engineering, held in Maratea, Italy, in June 2003.

Two meetings organized by Commission members and for which IUCr support had been sought were held in 2003. The 3rd National Russian Crystal Chemistry Conference was held 19–23 May in Moscow and funds were committed by the IUCr in support of the meeting. The Programme Chair was Commission member V. Belsky. The Indaba IV meeting, entitled Patterns in Nature, chaired by P. van Rooyen, was held in Skukuza in the Kruger National Park, South Africa, 17–21 August 2003, as a satellite of the ECM-21 in Durban, South Africa. Commission member D. C. Levendis served on the Organizing Committee, while L. Brammer and G. R. Desiraju served on the Programme Committee. In attendance there were 83 people from 15 countries, with 26 young scientists supported by IUCr grants.

Commission members made a significant contribution to convening many of the Microsymposia at ECM-21 in Durban, South Africa, 17–23 August 2003, and the satellite meeting The African Neutron Diffraction Meeting, 21–23 August 2003 (C. C. Wilson, Programme Chair).

In 2004, activities were mostly concentrated on developing a strong programme in the area of structural chemistry for the upcoming Florence Congress. The Commission sought input on topics for Microsymposia, potential symposia organizers/Chairs and on Keynote speakers by e-mail from its own membership and from a wide range of scientists around the world with interests in all aspects of structural chemistry. The response was excellent and the Commission through its representation on the Programme Committee was able to assemble a very strong programme that will run continuously through the Congress covering topics including design and synthesis of crystalline materials, intermolecular interactions and crystal packing, functional crystalline materials, chemical reactions in crystals, and topology of crystalline networks; study of crystals under non-ambient conditions, and with spectroscopic as well as various crystallographic methods; symposia on drug design, catalysis and supramolecular chemistry were also included.

The Commission endorsed the next in the series of highly successful Indaba meetings, Indaba-V, to be held in Kruger National Park, South Africa, in 2006. The principal organizer is Commission member D. C. Levendis. The Commission also endorsed, together with the Commission on Crystal Growth and Characterization of Materials, a proposed full day Workshop on Small-Molecule Crystallization to be organized in conjunction with the Florence Congress.

Commission members D. Braga and L. Brammer were among the Organizing/Programme Committee of the *CrystEngComm* Discussion 2 meeting held in Nottingham, UK, in September 2004. The meeting brought together a multidisciplinary group of scientists and many students working in the area of crystal engineering. Presented papers were also published in the RSC journal *CrystEngComm*.

L. Brammer, Chair

4.17. Commission on Synchrotron Radiation

The mission of the Commission is to promote access of crystallographers worldwide to the world's synchrotron radiation (SR) facilities. A subcharge is to promote the development of crystal-

lographic instrumentation technology and standards, particularly in the direction of X-ray detectors. To foster communication, we endorse (and sometimes sponsor) international meetings as the best means to achieve these goals.

The Commission endorsed conference activities in several scientific areas where SR meets crystallography, sending letters specifically to:

(i) V. Holy and Z. Sourek of the University of Prague, Czech Republic, who organized the XTOP conference in Prague in September 2004. The programme was very interesting and was trying to add some new crystallographic directions to the traditional subject of X-ray topography.

(ii) D. C. Creagh, Professor of Physics at the University of Canberra, Australia, for the International Radiation Physics Society's Triennial Symposium in Cape Town, South Africa, 27–31 October 2003, preceded by a Workshop on Radiation Based Analytical Techniques. The latter dealt with the interaction of radiation with matter, in particular synchrotron radiation and neutrons, and the Rietveld technique.

(iii) Å. Kvik of ESRF, Grenoble, France, and N. Greaves of the University of Wales, UK, who organized the Fourth Conference on Synchrotron Radiation in Materials Science (SRMS-4) in Grenoble 23–25 August 2004. The conference covered the following subject areas: nanostructures; semiconductors and opto-electronics materials; clusters, micro/mesoporous materials; biomaterials and polymers; magnetic materials, charge, spin and orbital ordering; engineering materials; surfaces and interfaces; ceramics and glasses; extreme conditions and techniques.

(iv) E. E. Vogel, Departamento de Ciencias Físicas, Universidad de La Frontera, Temuco, Chile, to endorse the application for IUCr support of the Latin-American Workshop on Magnetism, Magnetic Materials and their Applications that he was organizing. This meeting included many speakers using SR methods on its Agenda in both the programme and the list of invited speakers. The organizers were encouraged to contact the LNLS facility in Campinas, Brazil, which is active in hosting users of SR and is building a base of South American users. J. Brum, Director of LNLS, also indicated support.

In anticipation of the Florence Congress, we nominated R. Felici of ESRF to attend the planning meeting and to promote the appearance of SR speakers and symposia in the programme. He was very successful in this mission and we can all look forward to an exciting Congress.

An election was held to select from the candidates for new members of the Commission proposed by the various National Committees for Crystallography

4.17.1. Detector workshops. (1) The Commission was represented at the detector workshop, which was part of the Advanced Photon Source (APS) user's meeting, held 6 May 2004. J. Quintana introduced the workshop by reminding attendees that there is often a wide gap between the knowledge and experience of beamline users and the technologies that are available. He considers this to be a major obstacle to progress in the development of SR methods. This is precisely why the Commission is trying to communicate with IUCr members about technological advances.

At the workshop, Jin Wang presented an overview of detector technologies and described how the APS 'detector pool' operates. S. Ross described the advances made to develop Avalanche Photodiode Detectors (APD). Apart from the difficulty of obtaining the devices, they appear to be attractive for their moderately high energy resolution and good time resolution: when used with a suitable gated integrator, they should be able to pick out individual pulses from the 1296 bunch mode of APS, corresponding to a 2.8 ns spacing.

E. Westbrooke described his recent developments of detectors for Protein Crystallography (PX) at the Berkeley-based Molecular Biology Consortium. Collaborating with Optics1 Inc., he presented promising development work on lens coupling of a CCD to a phosphor. One advantage is that it allows overlap of the borders between the 'tiles' of the multi-CCD arrays. It will be interesting to see if his technology will be superior to earlier attempts that suffered from degradation of the optical surfaces with time. He also described two emerging technologies: the JPL Hybrid Imaging Technology (HIT), which uses 'bump bonding' of CMOS electronics to a conventional CCD sensor array; and the 3DX concept of S. Parker (Hawaii) involving micro-machining of Si sensor blocks with poly-Si electrodes drilled into them to form a new type of pixel array.

G. Darbyshire gave a full account of the detectors being developed for the DIAMOND Light Source (UK), which demonstrated that the new facility takes detectors very seriously. He advocated different short-, medium- and long-term solutions for each technique to be served. Crystallography users would have available new 'diffex' strip detectors for powder diffraction with customized energy resolution on each channel and a very large number of channels available simultaneously. In the long run, PX would be served by Monolithic Active Pixel Sensor (MAPS) arrays, which are currently being developed in a $3K \times 4K$ format with $5 \mu\text{m}$ pixels. These are based entirely on CMOS, including the sensor itself, so will be easy to mass-produce. He expects MAPS to replace current CCD technology eventually.

(2) The Commission helped sponsor a detector workshop at the ESRF user's meeting, which was very successful. A verbal summary was provided by the organizer, H. Graafsma (ESRF). A USA–European collaboration on new thin phosphors was established. Alternative materials for sensor layers, such as CdSe, were discussed. Detector development of the popular FRELON CCD readout system is advancing well at ESRF, but there is no easy way to commercialize it so that it can be adopted by other sources. Four components are generally required for a CCD: phosphor, coupling, sensor and readout. The future looks very bright for a new detector technology, called a pixel detector, which should ultimately replace CCDs. The technology offers photon counting and energy resolution at high count rate in every pixel. The ESRF pixel detector project is benefiting strongly by tying in development efforts of CERN and the medical imaging industry. A 256×256 prototype, called 'Medipix' was being tested at BM05 (ESRF) in April 2003. A low-doped $300 \mu\text{m}$ Si drift detector array of $55 \mu\text{m}^2$ pixels is biased to about 300 V. The bottom electrode is bump-bonded to a readout circuit occupying the same area as each pixel. Each circuit contains the amplifiers, discriminators and 13-bit scaler needed to obtain four decades of dynamic range. The design is a prototype that would partially satisfy the potential needs of two communities: for medical imaging applications, the sensitivity at high energies is insufficient, while the dynamic range is rather poor for crystallographic uses. Both applications will eventually need considerably larger arrays, which might be available in about five years' time, according to ESRF detector group leader H. Graafsma.

A summary of the workshop programme was abstracted from the <http://www.esrf.fr> web site. X-ray Detectors: The Way to Get More Out of Your Beamline! was held 13–14 February 2003 with a Scientific Organizing Committee comprising H. Graafsma (Chair), M. Kocsis, T. Martin and C. Ponchut. The objectives of the meeting were to review the current status of detectors, how they are used, what is needed and what is coming. The workshop intended to bring the synchrotron user community and the detector developers together, with an explicit goal to inform the detector developers of the forth-

coming needs and requirements and to inform the user community of the worldwide state of the art as well as future perspectives.

A Special Issue on X-ray detectors for synchrotron radiation was published by the *Journal of Synchrotron Radiation*. All workshop attendees were sponsored by the IUCr to receive a free copy. Meanwhile presentation materials from most of the talks are available from the web site at <http://www.esrf.fr/Conferences/UsersMeeting2003/Detectors/Speakers/>.

Another Special Issue of *Journal of Synchrotron Radiation* on X-ray detectors is in preparation in May 2005. So far ten contributions have been received and are in the refereeing process. The edition is expected to be completed by the end of 2005.

(3) An American detector workshop was held in Washington, DC, 30–31 October 2000. The workshop resulted in a white paper 'A Program in Detector Development for the US Synchrotron Radiation Community' by A. Thompson (ALS, LBNL), D. M. Mills (APS, ANL), S. Naday (ANL), J. Hormes (Center for Advanced Microstructures and Devices, CAMD), S. Gruner (Cornell High-Energy Synchrotron Source, CHESS), P. Siddons (NSLS, BNL), J. Arthur (SSRL), R. Wehlitz (University of Wisconsin Synchrotron Research Center, SRC) and H. Padmore (ALS, LBNL). S. Gruner attended the meeting and forwarded the document. The summary page is included here:

"There is a clear gulf between the capabilities of modern synchrotrons to deliver high photon fluxes, and the capabilities of detectors to measure the resulting photon, electron or ion signals. While a huge investment has been made in storage ring technology, there has not to date been a commensurate investment in detector systems. With appropriate detector technology, gains in data rates could be 3 to 4 orders of magnitude in some cases. The US community working in detector technology is under-funded and fragmented and works without the long-term funding commitment required for development of the most advanced detector systems. It is becoming apparent that the US is falling behind its international competitors in provision of state of the art detector technology for cutting edge synchrotron radiation based experiments.

There is thus an urgent need for a coordinated national program in detector research and development for synchrotron radiation research. Several new technologies are becoming available that could revolutionize the capabilities of detectors. One of the most important advances is the massive integration of parallel electronics into detectors on a pixel by pixel basis. Such detectors have the capability not only to work at very high rates, in some cases approaching 1 THz, but to include 'smart processing' of information on chip. Other important areas include the revolution in low temperature X-ray detectors capable of high energy resolution, and, if used in the form of arrays, potentially high counting rates. The science enabled by such detectors will be spread across the whole spectrum of synchrotron radiation research. For example, the study of the 3D structure of systems with short-range order using X-ray fluorescence holography (XFH), microsecond dynamics in polymers and magnetic systems studied using photon correlation spectroscopy, environmental chemistry studied using fluorescence yield micro-XAS, the study of chemical and electronic structure *via* photoemission and X-ray emission, and many more areas will be revolutionized by the use of advanced detectors."

The principal conclusions of the Washington workshop were that:

(i) Funding of advanced detectors is the most cost effective way of increasing the effectiveness of both existing and planned future synchrotron facilities.

(ii) Funding agencies should make provision for use of the most advanced present-day detectors on existing facilities; there are

examples of multi-million-dollar 3rd generation beamline facilities with 1st generation detectors.

(iii) There should be a nationally coordinated programme to provide funding of long-range strategic research in a number of highlight areas.

(iv) An organization modelled after the successful BioSync dealing with biological applications of synchrotron radiation, 'DetectorSync', should be formed to coordinate the area of detector research, and to represent the communities needs to funding agencies.

4.17.2. Outreach activities. (1) The Commission sent a letter of support for the proposal of H. Padmore from the Advanced Light Source in Berkeley, USA. The proposal is for construction of a full-scale pixel detector, with every pixel having energy encoding and time stamping. The plan is to make a detector that is fairly 'universal', although the basic framework is quite flexible and will allow many upgrades and customization for specific experiments. It is based on a deeply deplete (300 μm) Si PIN diode sensor, and therefore this will only give good performance for energies up to around 15 keV. For higher energies, it is proposed in parallel to develop a GaAs sensor and to test this at the single chip level, which would give good performance up to 30 keV. The options of photon-correlation on the chip would be particularly appealing: this is achieved by time stamping each photon it sees with a precision of 10 ns. The time-stamped data are then pipelined to a bank of FPGA processors to calculate the time autocorrelation, or cross correlation functions.

Pixel detectors appear to be the best 'new' technology on the horizon for future SR needs. There are several parallel efforts worldwide that would benefit greatly from the communication efforts of the Commission and other bodies. There are technology transfer activities at CERN through the so-called Medipix consortium. This aims to develop their existing pixel technology for medical imaging, which is all GaAs based. There are also development efforts at Rutherford Appleton Laboratory (RAL) on some aspects of pixel design; RAL has responsibility to build pixel detector systems for the DIAMOND SR source.

(2) There has been a SR nomenclature discussion between D. M. Mills of APS and the Chair of the Commission on Crystallographic Nomenclature (A. Authier) on behalf of a working group of that Commission. They have prepared a draft report that will be published in *Acta A* and *JSR*.

The discussion concluded that there was a slight preference for use of the terms 'brightness' or 'spectral brightness' rather than 'brilliance'. They came to the conclusion that 'spectral brightness' is the best term as it specifically calls out the importance not only of the number of photons per second per unit source size and unit divergence, but also of the number of photons in a particular bandwidth.

(3) An Indo-US Workshop on Radiation Physics with Synchrotrons and Other New Sources was held at Argonne National Laboratory, Argonne, IL, USA, 13–16 May 2003. It was sponsored by the Indo-US Forum (a joint venture of the National Academy of Sciences and the Department of Science and Technology of India), with 12 participants from India, 12 from around the USA and about 20 from local institutions. The aim of the workshop was to foster closer scientific ties between Indian and US scientists and to identify new opportunities resulting from the synchrotron and high-power laser sources in both countries. These include the behaviour of correlated many-particle systems in intense fields and other environments. The meeting was organized by L. Young and S. Roy.

I. Robinson, Chair

4.18. Commission on XAFS

The Commission continued with D. Arvanitis as Chair after the Geneva Congress in August 2002. Owing to long-term lack of activity of the Commission, the Executive Committee decided to appoint A. M. Molenbroek as Chair from 1 October 2004. It turned out that both R. F. Pettifer and K. Baberschke had resigned from the Commission, so from October 2004 the Commission members have been D. Arvanitis, K. Asakura, B. Hedman, A. Michalowicz, S. Mobilio, A. M. Molenbroek (Chair) and S. S. Hasnain (Consultant).

Contacts have been initiated and maintained among the members mainly *via* e-mail. At a meeting at the Florence Congress the future goals and plans of this Commission will be agreed. B. Hedman is a member of the Scientific Programme Committee of the Florence Congress.

The main goals until now have been:

To suggest active and qualified members for the future Commission, to be appointed at the Florence Congress. It turned out that the responses to whether or not this Commission should continue were so positive that a higher level of activity can be expected from now on.

To help organize a Microsymposium on XAFS at the Florence Congress. S. Mobilio and J. Garcia-Ruiz will chair a session on Combined XAS and XRD Techniques in Physics, Chemistry and Material Science.

Contacts with the IXS (International XAFS Society) will be tightened. A strong presence at the next International Conference on X-ray Absorption Fine Structure (XAFS XIII), which will be held in 2006 at SSRL in Stanford, CA, USA, will be a good opportunity for this. B. Hedman is both a member of the IXS Executive Committee and Co-Chair of XAFS XIII.

A. M. Molenbroek, Chair

5. Appendix E: Committee on Electronic Publishing, Dissemination and Storage of Information

In the triennium, the Committee on Electronic Publishing, Dissemination and Storage of Information (CEP) constituted a small and very active working group. No changes to the membership of the Committee have occurred during the triennium.

Members of the CEP attended the following meetings in the triennium.

H. D. Flack gave a short presentation, FORTRAN Archaeology: an Issue for a Knowledge Organization like the IUCr?, to the Open Meeting of the Commission on Crystallographic Computing, The Problems Facing Crystallographic Computing, at the Geneva Congress in August 2002.

B. McMahon and H. D. Flack attended the 2nd Workshop on the Open Archives Initiative (OAI): Gaining Independence with e-prints Archives and OAI, 17–19 October 2002, CERN, Geneva, Switzerland.

H. D. Flack attended the discussion meeting organized by ICSTI entitled Open Access to Scientific and Technical Information: State of the Art and Future Trends, 23–24 January 2003, Paris, France.

H. D. Flack visited the IUCr editorial offices in Chester, UK, 28–30 April 2003. On this occasion D. Russon, representing ICSTI, and S. Parsons also visited Chester. An outcome of this meeting was the undertaking by the IUCr of a study into the long-term preservation of the digital records of the science of crystallography, described further in the report of the ICSTI representative.

H. D. Flack visited the IUCr editorial offices in Chester, UK, 20–22 October 2003.

H. D. Flack, as special representative of ICSTI, attended the meeting The Role of Science in the Information Society (RSIS), Geneva, Switzerland, 8–9 December 2003; RSIS was a satellite meeting organized by CERN to the World Summit on the Information Society, Geneva, Switzerland, 10–12 December 2003, organized by the United Nations Organization.

H. D. Flack attended the third workshop on the Open Archives Initiative (OAI3), CERN, Geneva, Switzerland, 12–14 February 2004, where he was an invited participant at the discussion panel on 14 February.

H. D. Flack visited the IUCr editorial offices in Chester, UK, 18–20 October 2004.

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.

5.1. Information services

The CEP has continued its task as editorial body for the online information services of the IUCr. The task of day-to-day maintenance of **Crystallography Online** is performed under the responsibility of S. Parsons. Y. Epelboin continues his good work on the maintenance of the list of software of interest for crystallography. Action has been taken on the restyling and restructuring of **Crystallography Online**. This activity concerns the functionality, the stylistic attributes and the technical specifications of a revamped IUCr information service. Particular attention was paid to the ease of use and integration of the several components of the IUCr information services. The voluntarily maintained mirror sites within the existing system have been phased out to allow future development of more centralized web services. Owing to the heavy workload in the editorial offices in Chester, progress on re-engineering the IUCr web site has been slower than hoped.

On 10 December 2003, the Science and Technology Committee of the United Kingdom House of Commons (UK national parliament) issued invitations for evidence to support its inquiry into scientific publications. M. H. Dacombe, J. R. Helliwell, H. D. Flack, P. R. Strickland and B. McMahon submitted written evidence to the Committee on 9 February, on behalf of the IUCr, entitled 'Publishing Crystallography Journals in the Electronic Environment: The Experience of a Specialist Learned-Society Publisher'. The report highlighted that real value to scientific literature has enormously increased in the past decade through technical innovations and that the IUCr has worked hard to provide added value in the field of crystallography. It was stressed that finite acquisition budgets may leave libraries unable to afford IUCr journals and that any economic restructuring of the scientific journals market (*e.g.* to promote open access) must guarantee its quality and longevity. Further, for the

assessment, selection and improvement of the content of scientific articles it was considered that peer review must remain paramount in future developments of scientific journals. The problem of the preservation and archiving of primary journals published in electronic format was also highlighted.

5.2. World Directory of Crystallographers (WDC)

Despite the use of the online interface to update entries on individuals, the coverage and completeness remains unsatisfactory. At present, the WDC is not integrated with the journals electronic submission procedure, which would ensure more regular and reliable updating. Yet more publicity is necessary to encourage crystallographers to keep their own record up-to-date. Of course, spam, 'phishing' and other abuses of openly available contact information act as a major discouragement for making personal data available online or otherwise.

5.3. NeXus CD-ROM

Under the continued leadership of L. M. D. Cranswick, 1,000 copies of new versions of the Xtal NeXus: Virtual Crystallographic Internet on CD-ROM versions 8.56 and 8.57 were produced in November 2002 and June 2003 in time to be distributed at the Asian and European Crystallographic Association meetings in Broome, Australia, and Durban, South Africa, respectively. All of these CD-ROMs have now been distributed and at present individual CD-ROMs are being made on request. The CD-ROM is made available to laboratories and scientists with an interest in crystallography lacking adequate connection to the internet. The CD-ROMs contain public domain software and copies of web sites of interest to crystallographers. The CD-ROMs were publicized through many channels in a way such that scientists have to apply to receive a copy. The CEP intends to continue with the NeXus project in the coming triennium. Indeed, flyers and NeXus CD-ROMs are being prepared for distribution at the Florence Congress.

5.4. Crystallography Journals Online

The CEP is particularly attentive to developments in the scientific community at large concerned with access to scientific literature and data. The CEP devoted considerable time and effort in the management of open-access initiatives related to crystallographic publications and data. This activity resulted in the production of position papers on open access and the subsequent introduction in January 2004 of an open-access option for contributors to IUCr journals on the principle of the 'author-pays' model. The IUCr applied for and won funding for a one-year contract to allow papers submitted from authors in the UK to become open access; this funding was subsequently renewed for a further one-year period. The CEP has been collaborating with the e-Bank project involving the UK National Crystallography Service at Southampton University. This project provides access to experimental records and observations associated with crystal structure determinations carried out by the Service. It provides original data suitable for harvesting by databases and linking from publications, and aims also to place in the public domain scientific results that do not find their way into formal published literature. This is one of a small but growing number of initiatives to provide data repositories and bridge the gap between data processing and publication for routine structures, a development that the IUCr is following with attention. The CEP has also been involved (through the Chester editorial office) in a collaboration with P. Murray-Rust of Cambridge University to derive chemical representations of molecules from published crystal structures, an initiative

that also has relevance for the work of COMCIFS in developing formal descriptions of chemical properties.

5.5. International Tables for Crystallography

Activity commenced late in 2003 and principally in the editorial office around the specification of new business and functional models for electronic versions of the information contained in *International Tables for Crystallography*. Subsequently a working group was appointed by the Executive Committee to deal with the specific needs of *International Tables* online. A report of the discussions of this group has been prepared by its Chair (S. R. Hall).

The CEP has a continuing role to play within the IUCr. It is of the greatest use that the IUCr's representatives to CODATA and ICSTI are members of the CEP and we recommend that this practice be continued.

H. D. Flack, Chair

6. Appendix F: Committee for the Maintenance of the CIF Standard

6.1. Membership

COMCIFS is a Committee appointed by the Executive Committee of the IUCr. It is charged with the supervision of the Union's Crystallographic Information File (CIF) project. The current voting members of COMCIFS, those whose votes are required for approval of COMCIFS policy, are: I. D. Brown (Chair), H. M. Berman, H. J. Bernstein, R. Grosse-Kunstleve, S. R. Hall, G. Madariaga, B. McMahon and J. D. Westbrook.

In addition to the voting members, there are many others who have joined the COMCIFS discussion list but do not vote. Except for meetings held during the IUCr Congresses, COMCIFS conducts all its business by e-mail.

6.2. General

It is fifteen years since CIF was adopted by the IUCr and CIF is now in regular use by the major crystallographic journals and structural databases. While CIF was at the forefront of information technology when it was adopted, it is now facing competition in the form of the industry standard XML. CIF's well developed and integrated suite of dictionaries is better adapted than XML to a mature discipline such as crystallography, but XML has many more software tools available, and in some situations its greater flexibility is seen as an advantage. COMCIFS needs to assess how CIF fits into the current state of information technology and to chart a course for its development over the next decade. This report outlines the changes that have occurred in CIF during the last triennium and the challenges that face it in the next.

6.3. Formal description of CIF

CIF is defined by the STAR file structure standard, the Dictionary Definition Language and the various CIF dictionaries, but some conventions are not covered by these sources. In response to requests from software writers, COMCIFS formalized these conventions in the CIF Specification 1.1 written using a machine-readable Backus-Naur Format (<http://www.iucr.org/iucr-top/cif/spec/version1.1/>).

6.4. Dictionary Definition Languages (DDL)

For valid reasons, the suite of CIF dictionaries has been developed using two different (though similar) dictionary definition languages,

DDL1 and DDL2. DDL1 was used for dictionaries describing the structures of small-cell crystals and DDL2 for large-cell crystals. As interest has focused on the interactions between small and large molecules, there is an urgent need to create a seamless join between these two sets of dictionaries. Possible remedies that COMCIFS will examine are encouraging the writing of programs that can read CIFs written in either language and making changes to the dictionaries to minimize the differences in the CIFs they describe.

6.5. Software

The lack of open-source software tools for CIF makes XML, with its wide range of available tools, an attractive alternative for those writing information-handling routines. The IUCr is encouraging the development of standards-based open-source utilities and each year sees a few more independently developed applications added to the collection (<http://www.iucr.org/iucr-top/cif/software/>). Most of these tools are able to validate CIFs against the machine-readable dictionaries, which is a major feature that adds to CIF's adaptability and robustness. However, many of the widely used crystallographic applications do not make use of this feature but have the CIF data names written into the program code. Such applications can only manipulate CIFs written using one version of the dictionary; they are unable to follow the dictionaries as they evolve to reflect the changes in both crystallography and information science.

Among the CIF software projects completed or under way is H. J. Bernstein's IUCr-sponsored upgrading of a number of standard CIF utilities, many of which are used in the publication of IUCr journals. The aim is to ensure that they are compatible with the CIF 1.1 specification and with both DDL1 and DDL2. A new version of *Rasmol* has been released that will display RCSB PDB mmCIFs in the same way it currently displays pdb2cif mmCIFs. Other programs recently released include B. Toby's *pdCIFplot*, which is designed for reviewing Rietveld refinements of powder diffraction patterns stored as pdCIFs. Two CIF browser–editors have also been released: *enCIFer* by the Cambridge Crystallographic Data Centre and *CIFEDIT* by B. Toby. These applications read in the appropriate dictionary when reading or writing a CIF, putting the user just a mouse-click away from all the information included in the dictionary. These browser–editors can be used with any dictionary and do not have to be revised as each new dictionary version is released. References to these programs can be found at <http://www.iucr.org/iucr-top/cif/software/>.

6.6. Dictionaries

COMCIFS approved a new dictionary for reporting electron densities (cif_rho_1.0) and following usual practice appointed a Dictionary Maintenance Group charged with recommending changes and additions to rhoCIF. The members of this Committee drawn from the electron-density community are: P. D. Mallinson (Chair), L. Farrugia, N. Hansen, C. Jelsch, T. Koritsanszky, P. Macchi, H. Sørensen and A. Volkov.

Dictionary Maintenance Groups were also appointed for the Modulated Structure (msCIF) and Symmetry (symCIF) dictionaries approved in the previous triennium. Modulated Structures: G. Madariaga (Chair), G. Chapuis, V. Petricek, M. Onada and J. Zuñiga; Symmetry: I. D. Brown (Chair), M. Aroyo, R. Grosse-Kunstleve, V. Kopsky, D. B. Litvin and G. Madariaga.

Approval was given to a minor revision of the Image CIF dictionary (cif_img_1.3.1), which includes modifications that were found necessary during the preparation of software to read and write imgCIFs. At the same time, a new version of CBFlib was released.

The magnetic and small-angle scattering CIF dictionaries are still in development and COMCIFS is awaiting their formal submission for approval.

After more than a decade of use, the coreCIF dictionary is currently the subject of a major review. The first part of this review led to the approval of version 2.3, which, in addition to incorporating part of the symCIF dictionary, includes a number of minor additions and changes. More extensive changes are being planned, including providing for the description of extended scattering density, twinning and a description of the chemical, as opposed to the crystallographic, structure. This latter feature will allow users to describe the properties of the individual molecules present in the crystal.

6.7. mmCIF

The macromolecular CIF dictionary forms the basis of the data-storage model used by the RCSB Protein Data Bank for depositing three-dimensional protein and nucleic-acid structures. Local extensions have been developed in the past three years to form an extensive PDB exchange dictionary, which includes several new items describing phasing strategies, crystallization and protein production. These items have been developed in collaboration with the structural genomics community. They will be used to capture information during the deposit of structures in the PDB and to integrate such deposits with publication of macromolecular structure reports in *Acta Crystallographica*. The mmCIF data model has been successfully converted to an exchange XML format in use by the worldwide PDB (wwPDB) consortium, and a set of CORBA objects for middleware-based interoperability within the broader life sciences community.

6.8. Applications of CIF

COMCIFS has been busy preparing Volume G of *International Tables for Crystallography*, the volume that will contain a comprehensive account of the CIF project with publication expected in 2005. It will be accompanied by a CD-ROM containing machine-readable versions of all the CIF dictionaries and much of the software available for manipulating CIFs.

The IUCr is also planning to make other volumes in the series *International Tables* available online with information on symmetry available for downloading in CIF format. This is likely to result in (or require) the development of a new and enlarged version of the symmetry CIF dictionary.

Nicola Ashcroft of the IUCr editorial office has, with advice from B. Toby, been developing a new set of web pages offering guidelines for authors submitting structures determined from powder patterns. Mike Hoyland of the IUCr office has modified *checkcif* to run appropriate tests.

6.9. Publicity

The IUCr maintains a comprehensive description of CIF, including archival versions of all the CIF dictionaries, on its web site at <http://www.iucr.org>. The IUCr also maintains a series of internet discussion groups for those working on different aspects of CIF. Occasional columns on CIF also appear in the *IUCr Newsletter*.

6.10. Meetings

COMCIFS held both open and closed meetings at the Geneva Congress in 2002. Those attending the Open Meeting heard about the 'methods' extensions that we hope eventually to incorporate into the CIF dictionary language, as well as several assessments of the tech-

nical problems of interfacing CIF and XML. Similar meetings are planned for the Florence Congress.

6.11. The future of CIF

The development of XML has stimulated an interest in the development of computer languages used for manipulating and archiving digital information, making it urgent that COMCIFS define the role of CIF and develop a clear policy for future development. CIF can learn from its fifteen years of experience and must evolve to meet the expectations of the community for a transparent information handling system. To avoid making *ad hoc* changes to the dictionaries in a manner that could unnecessarily complicate further evolution, COMCIFS will develop a plan for the future development of CIF.

6.12. Acknowledgements

While the CIF standard is now widely adopted by the crystallographic community, extending it, keeping it up to date and supplying it with software requires considerable effort. COMCIFS is much indebted to the many volunteers who contribute to this work and who help to chart the future course of CIF.

I. D. Brown, Chair

7. Appendix G: Committee on Crystallographic Databases

The role of the Committee is to keep the Executive Committee informed of developments connected with the crystallographic databases. Members of the Committee have met informally at a number of meetings throughout the triennium. Information relating to the Committee, including current membership and links to crystallographic information sources, is available *via* the IUCr web pages (<http://www.iucr.org/>).

Issues of note during the triennium have been:

The continued rapid increase in the numbers of structures recorded in the structural databases. During 2004, this total exceeded half a million for the first time, and had reached 531,000 by the end of the year. The number of accessions expected during 2005 is certain to exceed 40,000 across all databases.

The PDB has seen the most rapid development of all of the databases, with the number of entries increasing by approximately 40% during the triennium, reaching a total of 31,219 early in 2005. By comparison, the CSD increased by about 76,000 entries in 2002–2004, an increase of approximately 30%, with similar rates exhibited by the other databases.

Deployment of the PDB *via* the web has developed and improved significantly during the past three years. Software access to the other databases has also seen improvements, and the CSD System has been enhanced by the addition of Mogul, a knowledge base of intramolecular geometry.

All of the databases have entered into discussions with the IUCr concerning the Crystallography Open Database, and the CCDC has met with the IUCr Executive Committee to discuss academic access to the CSD System in particular (now at 65 countries worldwide). They have informed the Committee about provision in developing countries, where access is heavily subsidized or completely free.

In 2002, the Committee helped write or commission 18 papers that appeared in a 'databases' Special Issue of *Acta Crystallographica* Section B (jointly with Section D). It is pleasing to report that several of those papers have achieved high citation rates during this triennium, and this has made a contribution to the improved impact factor for the journal.

There are concerns about the large numbers of structures that remain unpublished, especially in the non-macromolecular area. This problem is being addressed *via* a number of e-science initiatives involving crystallography laboratories, with which the databases have close contact. Deposition of unpublished data directly with some of the databases is also increasing.

F. H. Allen, Chair

8. Appendix H: IUCr Newsletter

The *IUCr Newsletter* continues to be a vehicle for broadcasting and promoting the interests and activities of the IUCr and its Commissions. It also strives to enhance communication within the global community of crystallographers. Special effort is made to promote meetings and publications sponsored by the IUCr.

This report will cover 12 issues (Vol. 10, Nos. 1–4 in 2002, Vol. 11, Nos. 1–4 in 2003 and Vol. 12, Nos. 1–4 in 2004). In the first three issues of 2002 the President's column was written by H. Schenk and the editorial by W. L. Duax. Starting with the third issue of 2002, J. L. Flippin-Anderson replaced W. L. Duax as *Newsletter* Editor. W. L. Duax then began penning the President's column. J. L. Flippin-Anderson wrote the editorial for that issue and a number of highly regarded crystallographers were invited to write guest editorials for later issues. Guest editorials were written by J. R. Helliwell, M. G. Rossmann, C. Mealli, H. Fuess, Y. Ossipyan and J. M. Guss.

Each issue also contained news of various IUCr Commissions, notices of elections, awards to crystallographers, and information on web sites, resources and other activities of interest to crystallographic practitioners. The fourth issue in 2004 contained a report on the highlights of the Executive Committee meeting in Budapest. Contributions are received from crystallographers in many countries and other material is gathered from the Newsletters of crystallographic associations and science news magazines. Almost all submitted contributions are published and all material is edited to varying degrees.

Each issue contained highlights from selected articles in IUCr journals and, starting with the first issue of 2003, at least two pages have been devoted to highlighting one article from each of the IUCr journals, including *Acta F*, which made its debut in this feature in the last issue of 2004 (Vol. 12, No. 4).

Reports of 49 meetings on crystallographic topics in 25 countries (from North and South America, Europe, Russia, Australia, New Zealand, Asia and South Africa) were published. The reports included reviews of the meetings of national crystallographic associations as well as the IUCr Regional Associates and extensive coverage of the Geneva Congress. In addition, the reports covered topics such as high-throughput protein crystallography, materials microstructure, radiation damage, crystals in art and science, crystal growth, synchrotron updates, structural genomics, methods, supramolecular chemistry, small molecules, biomaterials, electron crystallography, applied crystallography, high-pressure studies, new materials and aperiodic crystals. School and commemorative meetings were also highlighted, *e.g.* Braggs, Chemistry and Leeds; 50 Years of Collagen Triple Helix, a tribute to G. N. Ramachandran; and coverage of activities highlighting the 50th anniversary of DNA.

IUCr Regional Associates took advantage of the *Newsletter* to advertise their upcoming meetings and in 2004 the ECM used the *Newsletter* to publish its second circular containing registration information. In addition, a calendar of future meetings throughout

the world was published in every issue and, sadly, obituaries of 17 prominent crystallographers were reported during the triennium.

Covers highlighted both the Geneva and Florence Congresses, logos of the various national crystallographic associations, the six volumes of *International Tables*, the arrival of *Acta F*, the Indaba Workshop, art in crystallography and maps of the countries featured in the 'national' issues.

The 'national' issue is a new feature that was introduced during this triennium. Various countries/regions have been invited to contribute articles summarizing the crystallographic research being conducted in their geographic area. The first such issue was published in the third issue of 2003 and covered crystallography in Latin America. The material for this issue was collected by I. Torriani. Crystallography in Italy, organized by D. Viterbo, followed in the first issue of 2004. Crystallography in Russia, organized by L. A. Aslanov, appeared in two issues (Nos. 2 and 4 of 2004). Several other national issues are planned and articles on crystallography in Japan, organized by Y. Ohashi, and crystallography in Australia, organized by J. Martin, are already in hand.

Nine of the twelve issues published in the triennium contained 32 pages, two had 24 pages and one had 24 pages plus a 28 page insert that served as the second circular for the Florence Congress. This amounted to a total of 388 pages, which was essentially equivalent to the 372 pages for the twelve issues in the previous triennium.

A significant portion of the support for the publication and distribution of the *Newsletter* comes from advertising revenue. The average number of pages of advertising per issue for this triennium was 17.5 compared to a 15.5 page average in 2001.

The staff of the editorial office in Buffalo, NY, USA, is responsible for the desk-top preparation of all copy, all negotiations with the printer, postal authorities, and distribution houses, maintenance and production of the mailing list and solicitation and handling of all advertising. They also handle a large part of the correspondence with contributors.

J. L. Flippen-Anderson, Editor

9. Appendix I: IUCr/Oxford University Press Book Series

In the reporting period, the following books were published in cooperation with OUP:

In the series *IUCr Texts on Crystallography*:

Crystal Structure Analysis: Principles and Practice, by W. Clegg, A. J. Blake, R. O. Gould and P. Main (2001).

Fundamentals of Crystallography by C. Giacovazzo, H. L. Monaco, G. Artioli, D. Viterbo, G. Ferraris, G. Gilli and others, second edition (2002).

In the Series *IUCr Monographs on Crystallography*:

Structure Determination from Powder Diffraction Data, edited by W. I. F. David, K. Shankland, L. B. McCusker and Ch. Baerlocher (2002).

Polymorphism in Molecular Crystals by J. Bernstein (2002).

Dynamical Theory of X-ray Diffraction by A. Authier (2003).

Crystallography of Modular Materials by G. Ferraris, E. Makovicky and S. Merlino (2004).

Diffuse X-ray Scattering and Models of Disorder by T. R. Welberry (2004).

Crystallography of the Polymethylene Chain – an Inquiry into the Structure of Waxes by D. L. Dorset (2005).

These all concern important topics in crystallography and represent the high professional standards adhered to in the IUCr/OUP Book Series.

It may be expected that in the coming triennium a similar number of new books with equally attractive titles will appear on the basis of the present number of proposals of potential authors under consideration. The Committee will be pleased to receive suggestions about possible titles and authors from the crystallographic community.

Throughout the whole period the cooperation with the Science Editor of OUP has been excellent.

H. Schenk, Chair

10. Appendix J: Sponsorship of meetings: Sub-committee on the Union Calendar

The composition of the Sub-committee for the past three years was decided at the first meeting of the Executive Committee elected at the last General Assembly and comprised: L. B. McCusker (Switzerland), G. Díaz de Delgado (Venezuela), L. T. J. Delbaere (Canada), M. Vijayan (India), R. O. Gould (UK), with Chair M. A. Carrondo (Portugal). The Sub-committee members, including the Chair, for the next triennium will be decided in Florence.

The guidelines for applicants were updated and published on the IUCr web site. The main innovations include the establishment of four deadlines over each year for the evaluation of the submitted proposals: end of March, June, September and December. However, and as before, applications for sponsorship were only considered if they were submitted at least nine months in advance of the date of the meeting. Restrictions on applications for meetings planned to occur close in time to the Regional Associate meetings were introduced following previous restrictions for meetings close to an IUCr Congress. Furthermore, and with the exception of special cases, IUCr funds should not be granted to sponsor more than one event per year in the same location. Explicit support from the relevant IUCr Commission(s) is now strongly recommended for any meeting. All applications should use USD as the currency for the requested funds. The successful applicants are requested to prepare a scientific report as well as a financial report. A template form is now provided for reporting on the use of money from the IUCr and applications from organizers who fail to provide the required reports within one year after the meeting will not be considered in the future.

During the past three years, the Sub-committee has considered and analysed many requests for sponsorship and financial support by the IUCr, and subsequently has made recommendations to the Executive Committee. The main policy consists of giving financial support to help young scientists, meaning graduate students, post-graduate students or post-doctoral fellows, with a maximum age of 30 years. Additional financial support for organizational expenses was considered by the Executive Committee whenever necessary and justified. Special attention was given to applications from regions where crystallography is less developed, such as African or South American countries. The entire procedure, from the submission of proposals to the final decision by the Executive Committee, was carried out by e-mail. The evaluation process was very efficiently conducted by e-mail discussions involving all members of the Sub-committee.

The total amount used for sponsoring the participation of young scientists in meetings in 2002 was CHF 111,983 in 2003 CHF 146,873 and in 2004 CHF 119,382.

The following meetings received support during this three-year period:

International School on Crystal Growth of Technologically Important Electronic Materials, Mysore, India, 20–27 January 2003.

VI Latin-American Workshop on Magnetism, Magnetic Materials and their Applications, Chihuahua, Mexico, 7–11 April 2003.

BCA/CCG 9th Intensive Course in X-ray Structure Analysis, Durham, UK, 7–14 April 2003.

School on X-ray Charge Density Analysis and the *XD* Programming Package, Buffalo, USA, 13–17 May 2003.

Third National Crystal Chemical Conference, Chernogolovka, Russia, 19–23 May 2003.

School on High Pressure Crystallography, Erice, Italy, 4–15 June 2003.

International School on Electron Crystallography, Moscow, Russia, 23–27 June 2003.

Third European Charge Density Meeting, Aarhus, Denmark, 24–29 June 2003.

ACA Annual Meeting, Covington, Kentucky, USA, 26–31 July 2003.

ACA Summer Course in Small Molecule Crystallography, Indiana, USA, 3–13 August 2003.

AsCA '03 and Crystal-23 Combined Conference, Biological Structure Workshop and Sagamore XIV Meeting on Charge, Spin and Momentum Densities, Broome, Australia, 10–18 August 2003.

21st European Crystallographic Meeting (ECM-21), Durban, South Africa, African Neutron Diffraction Meeting (satellite to ECM-21), Pelindaba, South Africa, and Indaba 4 (satellite to ECM-21), Kruger National Park, South Africa, 17–29 August 2003.

XIX Conference on Applied Crystallography, Kraków, Poland, 1–4 September 2003.

Summer School on Polycrystalline Structure Determination by Direct Methods, Kraków, Poland, 4–7 September 2003.

International Conference on Aperiodic Crystals, Belo Horizonte, Brazil, 8–13 September 2003.

Conference on Structure Solution from Powder Diffraction Data, Stara Lesna, Slovak Republic, 14–19 September 2003.

XV International Conference on X-ray Analysis and Crystal Chemistry of Minerals, St Petersburg, Russia, 15–19 September 2003.

XIIth International Symposium on Supramolecular Chemistry (ISSC-XII), Eilat, Israel, 6–11 October 2003.

First Workshop on Radiation Based Analytical Techniques and 9th Symposium of International Radiation Physics Society, Cape Town, South Africa, 24–31 October 2003.

IV National Conference on Application of X-ray, Synchrotron Radiation, Neutrons and Electrons for Material Characterization, Moscow, Russia, 17–23 November 2003.

Workshop on High Pressure Structure and Reactivity: The Science of Change, Berkeley, USA, 4–7 December 2003.

Anniversary Fedorov Session 2003, St Petersburg, Russia, 9–10 December 2003.

International School on Crystal Growth, Characterization and Applications, La Pedera, Uruguay, 9–13 December 2003.

Latin-American Course of Macromolecular Crystallography: From Crystal to Structure to Biological Function, Buenos Aires, Argentina, 30 March–2 April 2004.

Second Moroccan School of Crystallography, El Jadida, Morocco, 10–14 May 2004.

School on Diversity amidst Similarity: A Multidisciplinary Approach to Polymorphs, Solvates and Phase Relationships, Erice, Italy, 9–20 June 2004.

School on Electron Crystallography: Novel Approaches to Structure Determination of Nano-Sized Materials, Erice, Italy, 9–20 June 2004.

AsCA '04, Hong Kong, People's Republic of China, 27–30 June 2004.

XVI International School on Physics and Chemistry of Condensed Matter, Bialowieza, Poland, 1–10 July 2004.

Gordon Conference: Electron Distributions and Chemical Bonding, South Hadley, USA, 4–9 July 2004.

ACA Annual Meeting, Chicago, USA, 17–22 July 2004.

Twelfth International Summer School on Crystal Growth, Berlin, Germany, 1–7 August 2004.

ICCG-14 and ICVGE-12, Grenoble, France, 9–13 August 2004.

Crystallography at High Pressure, Saskatoon, Canada, 18–21 August 2004.

22nd European Crystallographic Meeting (ECM-22); Crystallography at the Start of the 21st Century: Mathematical and Symmetry Aspects (satellite of ECM-22), Budapest, Hungary, 22–31 August 2004.

EPDIC IX, Prague, Czech Republic, 2–5 September 2004.

7th Biennial Conference on High Resolution X-ray Diffraction and Imaging (XTOP 2004), Prahonice, Czech Republic, 7–10 September 2004.

International Workshop on Nanomagnetism, Havana, Cuba, 15–19 November 2004.

Course on Fundamentals of Modern Methods in Biocrystallography (BioCrys2004), Oeiras, Portugal, 19–26 November 2004.

Recent Advances in X-ray Powder Diffraction, Cairo, Egypt, 27 November–2 December 2004.

Regional School of Crystallography and Diffraction, Havana, Cuba, 4–9 December 2004.

Micro- and Mesoporous Mineral Phases: Mineralogical, Crystallographic and Technological Aspects, Rome, Italy, 6–7 December 2004.

International School on Crystal Growth: Fundamentals, Methods and Applications to Biological and Nano Crystals, Puebla, Mexico, 7–11 March 2005.

BCA/CCG 10th Intensive Course in X-ray Structure Analysis, Durham, UK, 4–11 April 2005.

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

Evolving Methods for Macromolecular Crystallography, Erice, Italy, 19–29 May 2005.

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

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 2005.

11. Appendix K: Reports of Representatives on Regional and Scientific Associates

11.1. American Crystallographic Association (ACA)

During the last three years, the excellently structured organization of the ACA has continued to work for the advancement of crystallography in the American continent and abroad through the action of its Officers, Standing Committees and Special Interest Groups (SIGs). The membership list of the ACA contains 2,200 members and most of the SIGs organize one or more sessions at the Annual Meetings. The *ACA Newsletter*, published four times a year, provides an efficient forum for news, events and information.

The 2003 Annual Meeting took place in Northern Kentucky (26–31 July). Three workshops were offered on Twinning and Crystals, Data Processing and Crystal Growth, and Macromolecules. Thirty-eight parallel sessions covered subjects related to all the SIGs. Poster sessions had more than 250 contributions. Prizes were offered for the

best posters. The *Transactions Symposium* was dedicated to Biological Neutron Diffraction. The Buerger Award was presented to J. A. Ibers and the Warren Award was presented to T. Egami. The Margaret C. Etter Early Career Award was granted to J. Chan. The total attendance was more than 900 participants.

In 2004, the ACA Annual meeting was organized in Chicago, Illinois. This meeting had a record attendance of 1,213 participants. Four workshops were organized, including one special visit to the APS/IPNS synchrotron facilities. Thirty-two parallel sessions were organized by the SIGs and 272 poster contributions were presented during three poster sessions. The *Transactions Symposium* dealt with the topic Crystals in Supramolecular Chemistry. The Fankuchen Award was presented to A. McPherson and the Trueblood Award was presented to R. E. Marsh. The Margaret C. Etter Early Career Award was granted to L. MacGillivray.

The 2005 ACA Spring Meeting was held in Orlando, Florida (28 May–2 June). It was preceded by four one-day workshops (27 May). The A. L. Patterson Award was granted to T. A. Jones (University of Uppsala, Sweden) and the Margaret C. Etter Early Career Award was presented to J. 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 discussing 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.

It is important to note the special effort on the part of the organizers of all the ACA Annual Meetings in obtaining funds to offer travel awards to students and young scientists, to make their participation possible.

ACA Summer Courses were organized at Indiana University of Pennsylvania by B. M. Craven and C. H. Lake in 2003, 2004 and 2005. The ten-day intensive course is offered to young crystallographers interested in learning theory and practice of single crystal and powder diffraction. Candidates from the USA and several Latin-American countries have been awarded scholarships to attend these courses, which are mainly financed by the ACA, the US National Committee for Crystallography and some commercial firms. These courses represent a remarkable educational effort.

In 2004, the ACA established a new category of membership, the Latin-American Country Membership. The rules, requirements and benefits of the membership were sent to the National Committees of all the countries in Central America, South America and Mexico. This was a very important step in the direction of establishing a more effective regional interaction. In early 2005, membership requests were submitted by Argentina and Brazil.

As regards publications, on-line versions of Volumes 36 (Los Angeles), 37 (Kentucky) and 38 (Chicago) of the *Transactions* are reported to be under way.

The next ACA Annual Meeting is scheduled for 22–27 July 2006 in Honolulu, Hawaii.

I. Torriani, Representative

11.2. Asian Crystallographic Association (AsCA)

In the tenth Council meeting of AsCA held 10 August 2002, during the Geneva Congress, the issue of the timing of the election of the office bearers of AsCA, discussed earlier in the ninth Council meeting at Bangalore, India, was settled. It was decided that the office bearers would henceforth be elected at the Council meeting held during triennial AsCA meetings instead of those held during the

IUCr Congresses. The constitution was appropriately amended. The Council elected the following office bearers: President Y. Wang, Vice-President M. Vijayan, Secretary/Treasurer B. Skelton. They would serve until the 2004 meeting of AsCA. The Council confirmed Hong Kong, People's Republic of China, as the venue for the 2004 meeting with I. D. Williams as the Chair of the Organizing Committee and M. Sakata as the Chair of the Programme Committee.

In pursuance of the decision of the ninth Council meeting at Bangalore in 2001 to hold joint meetings of AsCA and national crystallographic societies in the region in the years when regular triennial AsCA meetings and IUCr Congresses do not take place, the first such meeting jointly sponsored by AsCA and the Society of Crystallographers in Australia and New Zealand (SCANZ) took place 10–13 August 2003 in Broome, Western Australia. The meeting was attended by 240 full registrants, 60 student registrants and 40 accompanying members. The IUCr was represented by its President, W. L. Duax. 15 travel scholarships were awarded to Australian students by SCANZ while 15 were awarded using IUCr support to young scientists from other parts of the region. The conference consisted of 6 plenary talks, 56 oral presentations, 136 poster presentations and 3 specialized workshops. The preparations for the Hong Kong AsCA meeting were reported in the eleventh Council meeting held at Broome on 12 August 2003. It was decided that the next joint meeting would be held in Japan in 2006 in association with the Crystallographic Society of Japan.

AsCA '04 was held in Hong Kong 27–30 June 2004. There were more than 300 registered participants including young scientists supported by the IUCr and Rigaku. There were 6 plenary lectures, 70 oral presentations distributed in 15 Microsymposia and about 200 poster presentations. The IUCr was again represented by W. L. Duax. The twelfth Council meeting took place 29 June 2004. The following office bearers were elected for the next triennium: President M. Vijayan, Vice-President J. M. Guss, Secretary/Treasurer I. Williams. S. R. Hall, the Trustee, reported that the financial position of AsCA was healthy. It was confirmed that the joint meeting of AsCA and the Crystallographic Society of Japan would be held at Tsukuba, Japan, in November 2006. The proposal to hold the triennial meeting in Taiwan in 2007 was accepted.

Y. Ohashi, Representative

11.3. European Crystallographic Association (ECA)

In 2002, the main activity was the preparation of the European Crystallographic Meeting, ECM-21, to be held in Durban, South Africa, in August 2003, in strict collaboration with the local coordinators A. Roodt and D. C. Levendis. It was decided that the meeting would last four full days with 8 plenary lectures, 40 parallel oral sessions and two poster sessions. The topic of the satellite Indaba IV workshop 'Patterns in Nature', was also approved.

The ECA Council and Executive Committee met in Geneva, Switzerland, during the Congress. The membership of Morocco was approved, while the candidatures of Tunisia and Algeria were announced. The importance of holding ECM-21 in South Africa as a way of contacting all crystallographic activities in Africa and expanding both ECA and IUCr memberships was recognized. Preliminary steps for the organization of ECM-22 in August 2004 in Budapest, Hungary, were discussed and it was decided to hold ECM-23 in 2006 in Leuven, Belgium. Two new Special Interest Groups (SIG) on Extreme Conditions (SIG11) and Material Science (SIG12) were proposed and approved and the preliminary steps for the approval of a SIG on Molecular Structures and Chemical Properties

were undertaken. Finally, the announcement of the Third ECA Prize, to be presented in Durban, was prepared and publicized.

In 2003, the most important activity was the 21st European Crystallographic Meeting, ECM-21, held in Durban, South Africa, 24–29 August 2003, with A. Roodt as Chair of the Local Organizing Committee and J. C. A. Boeyens as Chair of the Programme Committee. Almost 500 people attended the meeting. The meeting was preceded by the Indaba IV workshop on Patterns in Nature and by a satellite meeting on Neutron Diffraction.

The ECA Council and Executive Committee met in Durban. The new SIG on Molecular Structures and Chemical Properties was approved. The new elected Executive Committee comprised H. Fuess as President, M. Jaskolski as Vice-President and A. Liljas, A. Roodt and C. C. Wilson as members, while G. Filippini and T. Duarte were confirmed as Secretary and Treasurer and C. Lecomte remained as Past President. L. Fábíán gave a detailed description of the arrangements for ECM-22 to be held in Budapest, Hungary, 26–30 August 2004. Preliminary steps for the organization of ECM-23 in August 2006 in Leuven, Belgium, were discussed. The site for ECM-24 in 2007 was chosen to be Marrakesh, Morocco.

The Third ECA Prize was awarded in Durban to C. Giacobozzo for his major theoretical and practical contributions to the solution of the phase problem in a wide spectrum of applications.

In 2004, the 22nd European Crystallographic Meeting, ECM-22, was held in Budapest, Hungary, 26–31 August 2004, with A. Kálmán as Chair of the Organizing and of the Programme Committees. The number of registered participants was over 600. A satellite meeting on Crystallography at the Start of the 21st Century: Mathematical and Symmetry Aspects was held before the ECM.

The ECA Council and Executive Committee met in Budapest. The membership application from Algeria was approved, while contacts with Tunisia continued and preliminary contacts with Belarus and Moldova were established. The return of Ukraine into the ECA was welcomed and that of Bulgaria encouraged. Reports of the activities of the 13 SIGs were presented. A permanent contribution from the ECA in the *IUCr Newsletter* was arranged. L. Van Meervelt gave a detailed description of the arrangements for ECM-23 to be held in Leuven, Belgium, 6–11 August 2006. Preliminary steps for the organization of ECM-24 in Marrakesh, Morocco, were discussed.

The Executive Committee decided to give the ECA Prize the name of Max Perutz and in Budapest the first Max Perutz Prize was conferred on G. M. Sheldrick 'for seminal contributions to the development of direct methods and for converting the theory into straightforward procedures for solving small and large crystal structures'.

D. Viterbo, Representative

11.4. International Centre for Diffraction Data (ICDD)

As in previous years, R. L. Snyder represented the ICDD at the Commission on Powder Diffraction (CPD) meetings, and now also the International X-ray Analysis Society (IXAS). A main target of the Commission on Powder Diffraction is to maintain active collaborations and good relationships with these organizations.

R. Dinnebier, Representative

11.5. International Organization of Crystal Growth (IOCG)

The triennial Congress that took place in Grenoble, France, 9–13 August 2004 (<http://iccg14.inpg.fr>), and the triennial Summer School on Crystal Growth that was held in Berlin, Germany, 1–8 August (<http://isscg12.ikz-berlin.de/index.phtml>), are certainly the events

that most heavily characterized the life of the IOCG during the last triennium. Several members and consultants of IUCr Commissions were involved in both events as main organizers, lecturers or session Chairs.

As usual, several prizes were awarded to outstanding scientists for their contribution to the development of crystal growth theory and technology. The prizes were awarded during a ceremony at the ICCG-14 banquet on 12 August 2004: the IOCG Frank Prize was awarded to G. Comsa, Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany, for quantitative studies of crystal growth far from equilibrium; the IOCG Laudise Prize was awarded to T. Nishinaga, President, Toyohashi University of Technology, Toyohashi, Japan, for research on epitaxial growth of semiconductors; the Scheiber Prize was awarded to J. Boniakowski, Groupe de Physique des Solides, Paris, France, for his work on electronic and energetic trends for transition metals adsorbed on large gap oxides.

During the Executive Committee meeting in Grenoble, France, G. Stringfellow presented an update of plans to host ICCG-15 in Salt Lake City, Utah, USA, 5–10 August 2007, with G. Stringfellow and R. Feigelson as Co-Chairs. The associated ISSCG-13 is planned to be held the previous week in nearby Park City, Utah, with C. Wang and J. De Yoreo as Co-Chairs. The Council approved these plans for ICCG-15 and ISSCG-13. It was also decided that in 2010 both school and conference will be held in the People's Republic of China.

The Ukrainian Crystal Growth Society requested membership of the IOCG. This request was unanimously recommended by the Executive Committee and approved by the Council.

An IOCG policy of not endorsing international conferences that compete with ICCG and ISSCG meetings was discussed. A policy of not endorsing competing international crystal growth conferences or schools that are held during the period six months before and four months after an ICCG was approved.

Elected Officers and Executive Committee Members of the IOCG (2004–2007): President: R. F. Sekerka (USA); Vice-Presidents: J. P. Van der Eerden (The Netherlands), T. Ohachi (Japan); Secretary: T. F. Kuech (USA); Treasurer: T. Duffar (France); Past President: T. Nishinaga (Japan); Honorary Principal Founder IOCG: M. Schieber (Israel); Executive Committee (eight elected for 2004–2007): G. Mueller (Germany), J. N. Sherwood (UK), K. Kakimoto (Japan), J. Derby (USA), R. Fornari (Italy), Jiang Min-Hua (China), E. Zharikov (Russia) (replacing V. Osiko who declined to serve), M. Heuken (Germany).

A new web site was arranged during the last triennium (<http://www.iocg.org/>), which provides useful information about the Organization, its officers and its history as well as a number of useful links to national crystal growth organizations. A new logo was selected during the conference at Grenoble.

R. Fornari, Representative

12. Appendix L: Reports of Representatives on Bodies not belonging to the Union

12.1. Interdivisional Committee on Terminology, Nomenclature and Symbols of the International Union of Pure and Applied Chemistry (IUPAC ICTNS)

The IUCr is one of seven international organizations, which include the Bureau International des Poids et Mesures and the International Organization for Standardization (ISO), that are represented on ICTNS, the Committee charged by the International Union of Pure and Applied Chemistry (IUPAC) with responsibility

for ensuring that all recommendations concerned with terminology, nomenclature and symbols made in its name are consistent with IUPAC and other international standards. ICTNS experienced a major reorganization at the beginning of this triennium, with responsibility for terminology added to the Committee's charge as J. W. Lorimer became its new Chair and B. J. Herold its new Secretary.

Matters of interest to IUCr include IUPAC-NIST's Chemical Identifier (InChI) project, now available as InChI version 1 at: <http://www.iupac.org/inchi>. The software produces a unique alphanumeric string representation for any chemical compound and provides a means of communicating inorganic or molecular structures electronically without the need to use a registry or database system. A report of the IUCr Working Group on Crystal Phase Identifiers, under review by the Commission on Crystallographic Nomenclature, is fully consistent with InChI. IUPAC's Committee on Printed and Electronic Publications has made good progress in translating existing IUPAC standard terminologies and related information to data dictionaries in eXtensible Markup Language (XML) format for primary use in web publication.

Revisions to the guidelines for drafting IUPAC technical reports and recommendations were completed and appear in *IUPAC Handbook 2004–2005*. The 3rd edition of *Quantities, Units and Symbols in Physical Chemistry* is expected to become available soon. An abbreviated and very useful list of these quantities, units and symbols is freely accessible at: <http://www.iupac.org/reports/1993/homann/index.html> and a Periodic Table of the elements dated 2005 at: http://www.iupac.org/reports/periodic_table.

The Comité Consultatif des Unités (CCU) introduced the Dalton, symbol Da, into Table 7 of its brochure entitled *The International System of Units*, 8th edition, according it equal status with the unified atomic mass unit [where 'unified' refers to the agreement between physicists and chemists to change the previous definition to $m(^{12}\text{C}/12)$]. The rules for printing numbers were clarified by the Conférence Générale des Poids et Mesures so that the decimal marker shall be either a comma on the line or a point (*i.e.* a dot) on the line.

The question of whether or not to insert a space between numerical values and their unit symbol, *e.g.* between '2.5' and 'Å' or between a value and its uncertainty within parentheses, has again arisen. The current ISO standard 31-0 requires a thin (half) space; however, the draft ISO/IEC 80000 follows CODATA style and has no space. Another proposal concerns the use of the name 'uno', symbol U, for the unit one so that dimensionless numbers may be treated in the same way as all other SI units. Thus, a second phase in a material detected at a 15 µg/kg level, for example, would be expressed as 15 nU (15 nanouno) of that phase. Among other advantages, the proposed unit eliminates the present widespread and sometimes ambiguous use of abbreviations such as p.p.m. (for the number 10^{-6}), p.p.b. (for the number 10^{-9} in the USA and UK, 10^{-12} in continental Europe). CCU had proposed the name uno in 1999 but no action was taken at that time by the Comité International des Poids et Mesures. All Directors of National Institutes of Metrology and other relevant institutions have been canvassed for the widest views on the proposal. Dissatisfaction with the continued definition of a base unit of the International System of Units in terms of a material artefact (the mass of the international prototype of the kilogram in the form of a 90% Pt, 10% Ir cylinder kept in a vault in Sèvres, France) has led to the proposal of new definitions for the kilogram [I. M. Mills, P. J. Mohr, T. J. Quinn, B. N. Taylor & E. R. Williams (2005). *Metrologia*, **42**, 71–80]. ICTNS is now engaged in discussions of this proposal.

S. C. Abrahams, Representative 2002–2004

12.2. International Council for Science (ICSU)

The IUCr was represented at the 27th ICSU General Assembly in Rio de Janeiro, Brazil, in September 2002 and at the meeting of International Union Presidents in Paris, France, in February 2004. The latter meeting is of crucial importance for the interactions of ICSU with its Union members, as the ICSU General Assembly numbers more than 120 members, Unions and countries.

For the activities of ICSU I refer to the website (<http://www.icsu.org>), which has been renewed in the last period and is now very informative giving many details. In particular, the 'resource centre' presents a great deal of information.

One of the main decisions of the General Assembly was the establishment of a new regional structure. As a result, the first ICSU Regional Meeting for Africa was hosted by the Research Council of Zimbabwe in Harare, 9–11 October 2004. D. C. Leventis represented the IUCr at this meeting, at which the decision was taken to open a Regional Office for Africa in Pretoria, South Africa, the host being the National Research Foundation. The ICSU Regional Office will be responsible for the promotion of increased participation of scientists from Sub-Saharan Africa in ICSU programmes and activities. Other regions will follow.

Another important point is that ICSU focuses its limited funds on visible and relevant projects in which many Unions and country members are involved. Traditionally the proposals of the IUCr were focused on crystallographic aspects alone.

Our input in various sections of ICSU is greatly appreciated, particularly in the IT area. The next ICSU General Assembly will be held in Shanghai and Suzhou, People's Republic of China, 17–21 October 2005.

H. Schenk, Representative

12.2.1. ICSU Committee on Data for Science and Technology (CODATA). CODATA is the interdisciplinary Committee on Data for Science and Technology of the International Council for Science (ICSU). It is currently a worldwide network of 23 national data committees, 15 international scientific unions, 4 co-opted delegates, and 20 supporting organizations from industry, government and academia, which define and lead its scientific programme. It is concerned with collection, management, manipulation, access to and exploitation of quantitative data in science and technology. Specific projects are addressed by Task Groups answerable to the CODATA General Assembly, by Working Groups, by themed workshops or conferences, and by publications on specific aspects of data handling or data compilation, including conference proceedings.

The major activities of CODATA in the past triennium were as follows:

Biennial conferences were held in Montreal, Canada, September/October 2002, and in Berlin, Germany, November 2004. The Montreal meeting was entitled *Frontiers of Scientific and Technical Data*, and the Berlin meeting was entitled *The Information Society: New Horizons for Science*. Both were very well attended and offered rich overviews of new technologies in data science, interoperability initiatives, scientific data for economic development, data access and preservation, intellectual property rights concerns, and the increasingly important role of scientific data within the broader concerns of society. The IUCr representative presented a paper on the handling of crystallographic data at the Montreal meeting. Full meeting reports are available at <http://www.iucr.org/iucr-top/data/docs/>.

CODATA has been heavily involved in preparations for the intergovernmental World Summit on the Information Society (WSIS). Phase One of WSIS culminated in a Summit at Geneva,

Switzerland, in December 2003. CODATA developed with UNESCO an Agenda for Action, which was largely incorporated into the formal Summit Plan for Action. CODATA was also a co-organizer of the pre-Summit scientific conference in Geneva on the Role of Science in the Information Society. In preparation for the Second Phase of the WSIS in Tunis in November 2005, CODATA hosted a one-day Workshop during the CODATA 2004 meeting at which further areas of concern were identified. This is also reported in detail at <http://www.iucr.org/iucr-top/data/docs/>.

CODATA's relationship with ICSU, and its strategic role in managing international and interdisciplinary initiatives in scientific data management, were scrutinized by the ICSU Priority Area Assessment panel on data and information. A CODATA sub-committee welcomed the ICSU review and encouraged CODATA to formulate a strategic plan consonant with ICSU's vision of the management of scientific data and information in the next decade. This initiative may strongly influence the direction in which CODATA moves, and could result in closer collaboration with the other members of the ICSU family of organizations in formulating coherent long-range non-governmental science policies.

CODATA retained active involvement with large-scale biodiversity and taxonomy projects, such as the Global Biodiversity Information Facility (GBIF); with Earth Sciences projects (including endorsement of the forthcoming Electronic Geophysical Year, and coordination of worldwide gas hydrates research); and with numerous scientific data initiatives in the developing world. The valuable interdisciplinary *Data Science Journal* continues as an open-access online publication

In the course of this triennium, many CODATA activities have become even more relevant to the work of the IUCr in the areas of data management, access, interoperability, intellectual property rights and archiving, and I endorse the IUCr's continuing membership of CODATA.

The CODATA web site is at <http://www.codata.org>.

B. McMahon, Representative

12.2.2. ICSU Committee on Science and Technology in Developing Countries – Incorporating International Biosciences and Other Scientific Networks (COSTED-IBN). COSTED-IBN was dissolved at the 27th General Assembly of ICSU held in Rio de Janeiro, Brazil, 20–28 September 2002.

12.2.3. ICSU Committee on Space Research (COSPAR). The most important event for COSPAR in 2002 was the 34th General Assembly and 2nd World Space Congress, which took place in Houston, USA, 10–19 October 2002. The following new Bureau was elected by the General Assembly: President: R. M. Bonnet (France); Vice-Presidents: W. Hermsen (The Netherlands), E. C. Stone (USA); Bureau members: J. Audouze (France), G. Horneck (Germany), T. Kosugi (Japan), M. E. Machado (Argentina), G. G. Shepherd (Canada), J. B. Zielinski (Poland); Finance Committee: D. Kendall (Canada, Chair), L. Sehnal (Czech Republic), E. V. Thrane (Norway).

The 65th COSPAR Bureau meeting was held in Paris, France, 20 March 2003. There were several meetings and workshops co-sponsored by COSPAR but none were related to subjects close to crystallography or crystal growth.

A new COSPAR Publications Committee was appointed for 2002–2006, chaired by W. Hermsen, with the main goal to increase the impact and the speed of publication of *Advances in Space Research*, the main journal supported by COSPAR. The Publications Committee enthusiastically endorsed the proposal for typesetting

made by Elsevier. It was also agreed to change the format of the *COSPAR Information Bulletin*.

The 35th COSPAR Scientific Assembly took place on 18 July 2004. The Scientific Commission on Materials Science in Space was chaired by R. Narayanan, A. Cröll and H. Kawamura. Only one session was devoted to materials science while origins of life, extraterrestrial life and obviously space exploration were much more represented.

The 68th COSPAR Bureau Meeting was held in Paris, France, 21–24 March 2005. The main issue was a comprehensive list of recommendations of all the task groups involved in the reflection on the future of COSPAR, including interfaces with other organizations (particularly ICSU). The next Bureau meeting will be held in the week of 20 March 2006.

The activities of COSPAR were mainly concerned with traditional space topics such as new satellites, climate studies, new pulsars, gravitational lensing *etc.* rather than with materials science in space research. However, the new field of space exploration and the possibilities to send elsewhere X-ray diffraction machines for mineral analysis open interesting possibilities for applied crystallography.

The 36th COSPAR Scientific Assembly will be held in Beijing, People's Republic of China, 16–23 July 2006, while Canada has issued an invitation to organize COSPAR 2008. Italy has also issued an informal invitation to host COSPAR for the same year, or 2010.

J. M. Garcia-Ruiz, Representative

12.2.4. ICSU Programme on Capacity Building in Science (PCBS).

The 27th General Assembly (GA) of ICSU, held in September 2002, endorsed the recommendation of the Committee on Scientific Planning and Review (CSPR) to carry out a Priority Area Assessment (PAA) on Capacity Building as part of ICSU's overall strategy development process. An independent *ad hoc* expert panel has been established to carry out this assessment.

The PAA will help define ICSU's role and future strategy in the broad area of capacity building, with a particular focus on the needs of developing countries.

The immediate outcome of the PAA will be a report and key recommendations that will be published and widely disseminated. This report will form the basis for future actions by ICSU and ICSU family members and partners, including the potential development of new programmes, the development of policy initiatives and definition of priorities for the ICSU grants programme.

P. Spadon, Representative

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

The IUCr representative attended the following ICSTI meetings in the triennium 2002–2004:

Annual ICSTI meeting held in the Royal Institute of Technology Library, Stockholm, Sweden, 15–19 June 2002. This included a one-day public conference entitled Scientific Information: the Challenges of Creating and Maintaining Access.

Annual ICSTI meeting held in London, UK, 13–17 May 2004. This meeting was hosted by INSPEC. The main discussion session was entitled Technical and Economic Challenges of Scientific Information (STM Content Access, Linking and Archiving).

In addition, the IUCr was represented by H. D. Flack at the following ICSTI meetings:

Winter committee and discussion meeting held at ICSU, Paris, France, 16–17 February 2002.

ICSTI Seminar on Digital Preservation of the Record of Science – State of the Art, UNESCO, Paris, France, 14–15 February 2003.

Winter committee meeting and discussion meeting on Open Access to Scientific and Technical Information: State of the Art and Future Trends, Paris, France, 23–26 February 2003.

Winter committee meeting and discussion meeting on Economic Models for Scientific Information, Production and Distribution, Paris, France, 15–18 January 2004.

No representative of the IUCr was present at the annual meeting in Ottawa, Canada, 8–12 May 2003.

A major preoccupation of ICSTI is the archiving and preservation of digital information. At the winter 2003 meeting of ICSTI, it was suggested that the IUCr might undertake 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. In May 2003, the IUCr agreed in principle to undertake the survey and it was recognized that there should be two separate survey questionnaires: (a) for individuals who publish crystallographic information and (b) for organizations that publish crystallographic information. Initial drafts of survey questionnaires were discussed at a second meeting held in August 2003. Subsequent to this meeting, the questionnaires were further refined and comments sought from a number of crystallographers. This led to final drafts of the questionnaires in November 2003. The final drafts were then tested by a number of volunteers. During 2004, the survey questionnaires were sent out. The survey focused on formal refereed journal articles, informal publications, theses, published and unpublished data, and personal archives. A report of the findings and recommendations for action will be published during 2005.

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). A distribution list operates where the ICSTI Executive Director distributes news clips and other information.

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, Representative

13. Appendix M: Budget estimates for period to Twenty-First General Assembly: determination of unit contribution

13.1. Budget estimates

The estimated budget for the General Fund is set out below, for the period until the next General Assembly. Since the budget estimates had to be prepared at a time when the decisions on many activities were still to be made, these estimates should be considered with due reserve. With this proviso, and in accordance with Statute 9.3, the Executive Committee presents to the General Assembly the following estimates for the three-year period 1 January 2005–31 December 2007.

	CHF	CHF
Income		
Subscriptions from Adhering Bodies	465,000	
Yield from investments and banking accounts	450,000	915,000
Expenditure		
Administration	1,011,000	
Subscriptions to ICSU and bodies of ICSU	33,000	
Administrative meetings	252,000	
Scientific meetings	137,000	1,433,000
Estimated profit or deficit		–518,000

13.2. Unit Contribution

According to Statute 5.10(k), the General Assembly has to determine the Unit Contribution to be paid by the Adhering Bodies for the period to the next General Assembly. The Executive Committee recommends to the General Assembly that the Unit Contribution should remain at its present level of CHF 1,000 (set at the Beijing Congress in 1993) for the years 2006–2008.