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Annex I
Appendices to the Agenda of the Nineteenth General Assembly

1. Appendix A: Report of the Executive Committee

1.1. Executive Committee and Finance Committee meetings

The Executive Committee met in Glasgow, Scotland, in July/August 1999 before and during the General Assembly, in Nancy, France, in August 2000 at the time of the Nineteenth European Crystallographic Meeting and in Los Angeles, USA, in July 2001 at the time of the American Crystallographic Association annual meeting. The Finance Committee met in March 1999, July 1999, March 2000, August 2000 and March 2001, 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 at these meetings, and in postal ballots between meetings, were:

(1) editorial policy, pricing policy and subscription rates, consideration of appointment of new Editors for *Acta Cryst.* Sections A, B, D and E and the *Journal of Synchrotron Radiation*, approval of appointments of Co-editors, electronic publishing, Special Issues, digitization of back issues and other matters concerning the IUCr journals;

(2) launch of *Acta Cryst.* Section E *Structure Reports Online*;

(3) review of *Journal of Synchrotron Radiation*;

(4) review of contract with Munksgaard;

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

(6) approval of the audited accounts;

(7) the 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, establishment of Journal Grants Fund;

(10) sponsorship and financial support for meetings, including young scientists' support;

(11) cooperation with databases, including relations between the IUCr and the Cambridge Crystallographic Data Centre and between the IUCr and the Fachinformationszentrum Karlsruhe and NIST;

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

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

(14) appointment of the Selection Committee for the sixth Ewald Prize;

(15) change of venue of the 19th General Assembly and Congress from Jerusalem, Israel, to Geneva, Switzerland;

(16) discussion of the arrangements for the Geneva Congress;

(17) approval of the membership of the Programme Committee for the Geneva Congress;

(18) level of financial support for the Geneva Congress;

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

Other items dealt with in this way were:

(20) the 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;

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

(22) crystallography in Africa;

(23) use of financial support through ICSU;

(24) review of the activities of Commissions;

(25) review of the activities of Regional Associates;

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

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

(28) work of Inter-Union Bioinformatics Group.

Items concerning the Chester office were:

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

(30) upgrading of office technology in the IUCr office in Chester, provision of internet services, upgrade of internet connection, establishment of mirror sites.

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 1999, 2000 and 2001 were:

	1999	2000	2001
Acta Crystallographica Section A	1,073	649	803
Acta Crystallographica Section B	1,128	1,127	877
Acta Crystallographica Section C	2,192	2,179	1,504
Acta Crystallographica Section D	2,079	1,723	1,980
Acta Crystallographica Section E	-	-	1,998
Journal of Applied Crystallography	1,208	1,468	798
Journal of Synchrotron Radiation	1,209	419	1,255
Total	8,889	7,565	9,215

In 1999, *JSR* contained 686 pages of papers presented at the Tenth International Conference on XAFS, Chicago, USA, 10–14 August 1998; and *Acta Cryst.* Section D contained 142 pages of the Proceedings of the 1999 CCP4 Study Weekend on Data Collection and Processing. In 2000, *JAC* contained 441 pages of papers presented at the Eleventh International Conference on Small-Angle Scattering, Brookhaven, USA, 17–20 May 1999; and *Acta Cryst.* Section D contained 152 pages of the Proceedings of the 2000 CCP4 Study Weekend on Low Resolution Phasing. In 2001, *JSR* contained 992 pages of papers presented at the Eleventh International Conference on XAFS, Ako, Japan, 26–31 July 2000; and *Acta Cryst.*

Section D contained 136 pages of the Proceedings of the 2001 CCP4 Study Weekend on Molecular Replacement and its Relatives.

The **Crystallography Journals Online** service was announced at the Glasgow Congress and became fully operational at that time. All the IUCr journals are available electronically through this service, including all back issues of the journals from 1948.

In 2001, the fully electronic *Acta Cryst.* Section E: *Structure Reports Online* was launched in close collaboration with the Cambridge Crystallographic Data Centre. It is an online-only journal and is available free of charge to subscribers to Section C.

The IUCr home page on the web continues to expand and the main site in Chester, UK, is currently mirrored in Australia, France, Israel, Japan, Russia, South Africa, Sweden, Switzerland and the USA. 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 50,000 from about 5,000 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 has recently undergone major development to provide increased functionality and to allow online amendments and additions to be made by individual crystallographers. All entrants have been contacted to ensure that data contained in the Database is current. Those not replying have been removed. The Eleventh Edition of the *World Directory of Crystallographers* will be produced from this Database once the update is complete.

The *IUCr Newsletter* is distributed free of charge to 587 libraries and 15,000 crystallographers and other interested individuals in 39 countries. W. L. Duax 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 I to the Agenda.

The IUCr/OUP Book Series continues to be successful. Details are given in Appendix J to the Agenda.

1.3. Sponsorship of meetings

The Executive Committee has established a Sub-committee on the Union Calendar to consider and to advise the Executive Committee on requests for IUCr sponsorship and financial support of meetings. The Chair of the Sub-committee has been H. Fuess in this triennium. A list of IUCr-sponsored meetings is given in Appendix K to the Agenda.

Applications for sponsorship and financial support are considered if they are submitted at least nine months in advance of the date of the meeting. 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.

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 meetings seeking IUCr sponsorship or support must assure the Calendar Sub-committee that the authorities of the country in which the meeting is to take place guarantee free entrance of *bona fide* scientists from all countries.

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), A. Cawley and M. J. Robinson (Administrative Assistants 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, N. J. Ashcroft, A. Weight, S. Froggatt, S. Glynn, L. Stephenson and D. L. M. Williams (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 Israel Crystallographic Society for the invitation to hold the Nineteenth General Assembly and International Congress of Crystallography in Geneva. It particularly wishes to thank the Chair of the Programme Committee, M. Kaftory, and the Chair of the Organizing Committee, J. Bernstein.

On behalf of the IUCr, the Executive Committee wishes to thank the support of the Swiss National Committee for Crystallography and all our Swiss colleagues for their full understanding and support concerning the change of venue of the present Congress from Jerusalem, Israel, to Geneva, Switzerland. The present Congress will be considered as being sited in Israel and not Switzerland when future venues are considered.

The support shown by UNESCO in the form of its annual subvention received by the IUCr through ICSU in 1999 and 2000, and the support of ICSU itself, is gratefully acknowledged.

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 1999, 2000 and 2001 have been published [*Acta Cryst.* (2000), A**56**, 609–642; (2002), A**58**, 80–116; (2003), A**59**, 66–102]. The accounts for the three years 1999,

2000 and 2001 are summarized in Tables 1–14. 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 1,362,492 from CHF 6,916,067 to CHF 5,553,575, or 20%, over the triennium. It should be noted that these figures include the fluctuations in exchange rates. If the exchange-rate fluctuations are disregarded, the total assets decreased by CHF 1,300,806 from CHF 7,234,810 to CHF 5,934,004, or 18%, 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 2001 is CHF 4,772,261 at market value, as shown in Table 2, of which 35% is held by Merrill Lynch, 57% by Foreign & Colonial and 8% is held in UK Treasury Gilts. 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.

2.2. General Fund

Table 3 shows the accounts for the General Fund (GF) and Table 4 compares these accounts for the triennium with the budget approved by the Glasgow 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 income from investments and bank accounts. The subscriptions from Adhering Bodies are based on the unit contribution, which was CHF 1,000 for 1999, 2000 and 2001. The total number of membership units was 152 for each year. The yield from investments is less than the budgeted amount by CHF 323,538. This is because this figure includes losses that were realized when some investments that were doing poorly during the significant market decline in 2000 and 2001 were sold to avoid greater losses in the long term. The decline in the world markets adversely affected the assets of the IUCr during the triennium. However, it should be noted that the investments are held primarily for long-term gain and although the performance in the last triennium was poor, over a ten-year period the return has been between 5 and 7% per annum. During the triennium, the assets were also drawn upon to fund the development of the **Crystallography Journals Online** service, the digitization of all back issues of the journals and the production of new and revised volumes of *International Tables for Crystallography*.

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

	31 December 1998	Fluctuations in rates of exchange	31 December 2001
General Fund	3,059,757	854,738	2,253,503
President's Fund	58,947	1,042	56,803
Acta Crystallographica	1,583,252	26,142	810,560
Journal of Applied Crystallography	152,033	2,759	202,815
Journal of Synchrotron Radiation	19,391	−144	103,877
International Tables	195,270	2,116	−2,025
Book Fund	25,600	612	−31,489
Publications and Journals Development Fund	457,847	9,722	567,419
Research and Education Fund	886,870	19,823	959,904
Ewald Fund	419,858	9,562	483,945
Newsletter Fund	57,242	2,931	148,263
Total accumulated balance	6,916,067	929,303	5,553,575

Table 2
Balance sheet, Assets (Swiss Francs).

	31 December 1998		31 December 2001	
Fixed assets				
Tangible fixed assets		130,413		97,216
Current assets				
Stock		26,061		77,359
Cash at banks and in hand				
Current accounts	19,765		62,708	
Deposit and savings accounts	421,499		244,167	
Cash with Union officials	30,763	472,027	29,466	336,341
Investments at market value		6,163,824		4,772,261
Debtors		293,490		450,736
Subscriptions due		60,000		23,874
Total current assets		7,015,402		5,660,571
Deduct Creditors and accrued charges		−229,748		−204,212
Net current assets		6,785,654		5,456,359
Total assets		6,916,067		5,553,575

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 two meetings in each of 1999 and 2000 and one in 2001. The cost of these meetings varies, as seen from Table 3, depending on the location and the circumstances. In Table 4, 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 4 include the travel grants and other expenses for the Glasgow Congress in 1999, the cost of the 2001 meeting of the Programme Committee for the Geneva Congress, the expenses of the non-publishing Commissions, financial support to meetings and schools (including a refund from the Glasgow Congress), 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 12.

Table 3
General Fund (Swiss Francs).

	1999		2000		2001	
Income						
Subscriptions from Adhering Bodies	144,930		152,316		164,998	
Yield from investments and bank accounts (including profit/loss on disposal of investments)	272,054		228,564		−74,156	
Grants from UNESCO/ICSU	10,544		12,493		8,656	
Amount charged to other Funds:						
Acta Crystallographica	121,491		139,793		127,294	
Journal of Applied Crystallography	21,635		38,831		19,727	
Journal of Synchrotron Radiation	23,300	593,954	11,549	583,546	30,863	277,382
Expenditure						
Administration	380,136		433,818		405,597	
Subscriptions to ICSU/ICSU bodies	10,098		9,707		10,568	
Executive Committee	103,729		18,084		54,892	
Finance Committee	25,532		18,518		12,854	
18th General Assembly and Congress expenses	47,963		1,315		–	
19th General Assembly and Congress expenses	–		–		6,620	
19th General Assembly and Congress Programme Committee	–		–		34,777	
IUCr Representatives on other bodies	4,231		6,276		3,840	
Expenses of Commissions	12,075		–		10,315	
Sponsorship of meetings (including refund from 17 GAC)	−36,692		4,426		1,824	
President's secretarial	7,910		10,000		10,000	
IUCr/FIZ Agreement	−8,759		−7,960		−8,353	
Bad debts – subscriptions	5,000		4,000		8,000	
Promotion	–		–		14,048	
Programming and development costs	53,980	605,203	61,494	559,678	42,361	607,343
Excess of income over expenditure		−11,249		23,868		−329,961
Transfers to other Funds:						
Newsletter Fund	−25,000		−25,000		−25,000	
Ewald Fund	−25,000	−50,000	–	−25,000	–	−25,000
Fluctuations in rates of exchange		838,607		405,151		−389,020
Movement in market value		182,734		−863,121		−563,263
Accumulated balance at end of year		4,019,849		3,560,747		2,253,503

Table 4
General Fund. Comparison of budget and accounts for the years 1999–2001 inclusive (Swiss Francs).

	Budget		Accounts		Difference	
Income						
Subscriptions from Adhering Bodies	456,000		462,244		6,244	
Yield from investments and bank accounts (including profit/loss on disposal of investments)	750,000		426,462		−323,538	
Grants from UNESCO/ICSU	60,000	1,266,000	31,693	920,399	−28,307	−345,601
Expenditure						
Administration (net)	783,000		901,861		118,861	
Subscriptions to ICSU/ICSU bodies	30,000		30,373		373	
Administrative meetings	255,000		247,956		−7,044	
Scientific meetings	194,000		57,551		−136,449	
Transfers to other Funds	100,000	1,362,000	100,000	1,337,741	–	−24,259
Unfavourable variant from budget						−321,342
Estimated profit or deficit		−96,000				−96,000
Deficit of income over expenditure				−417,342		−417,342

Table 5
President's Fund (Swiss Francs).

	1999	2000	2001
Income			
Donations, transfers and interest	2,244	2,164	3,207
Expenditure			
Grants	21,542	4,063	5,196
Excess of income over expenditure	−19,298	−1,899	−1,989
Transfers from other Funds:			
Acta Crystallographica	–	20,000	–
Fluctuations in rates of exchange	474	420	148
Accumulated balance at end of year	40,123	58,644	56,803

In Table 4, the unfavourable deviation from budget of CHF 321,342 is almost entirely accounted for by the low income from investments (including loss on disposal) mentioned above. Overall expenditure over the triennium was less than predicted.

2.3. President's Fund

Table 5 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 problems to take part in the activities of the IUCr.

2.4. Journals Funds

Tables 6, 7 and 8 give the accounts for *Acta Crystallographica* (AC), the *Journal of Applied Crystallography* (JAC) and the *Journal of Synchrotron Radiation* (JSR). In view of the significant costs involved in publishing Special Issues, the difference between the actual costs incurred and the contribution received from the conference organizers is charged to the Publications and Journals Development Fund. During the triennium, 584 pages of Special Issues on special topics in crystallography were published as fully technically edited issues of the journals and 2,119 pages of Conference Proceedings were published as camera-ready submissions. The total number of pages printed for AC, JAC and JSR were 8,889, 7,565 and 9,215 in 1999, 2000 and 2001, respectively. The Finance Committee (FC) and the Executive Committee (EC) have monitored the financial development for all journals very closely. The total number of subscriptions (including full and reduced-rate) decreased by about 10% for AC, 6% for JAC and 7% for JSR 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 5,000 unique hosts and receives on average about 50,000 requests per day. The online-only *Acta Cryst.* Section E *Structure Reports Online* was launched at the beginning of 2001 and is accessible free of charge to subscribers to AC Section C. 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 9. The costs of printing and reprinting the various volumes are charged to the appropriate years. Volume A was out of print in 2000 and 2001 [a revised edition has been printed in 2002]. Volume F on Biological Crystallography was published in July 2001, only five years after its inception – all concerned are to be congratulated on this achievement. 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 10 gives the accounts of the Book Fund. The accumulated balance of this fund became negative during 2001 as a result of the large amount of work involved with updating and restructuring the World Database of Crystallographers, which will be used to produce the next edition of the *World Directory of Crystallographers*.

2.7. Publications and Journals Development Fund

Table 11 shows the accounts of the Publications and Journals Development Fund (PJDF). This fund was established in 1984 and has been built up through transfers from other funds, such as AC. In order to build up the fund further and in a systematic way, with the goal to make it self-supporting, in 1989 the EC decided to increase its balance by crediting it with interest currently calculated as 6% of the balance of the fund, as shown in Table 11. 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 and Special Issue costs (see Journals Funds above). It remains the EC's policy 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), STAR/CIF expenses and support for the Journal Grants Fund. As the programming and development activities underpin much of the Union's activity, in 1997 the EC decided that the associated costs should be assigned to the Journals Funds, the *International Tables* Fund and the General Fund, in proportions based on the annual expenditure in these funds. In 2001, this principle was extended to the promotion expenses.

2.8. Research and Education Fund

Table 12 shows the accounts of the Research and Education Fund, REF. The fund was also established in 1984 and, like the PJDF, has been built up through transfers from other funds. As for the PJDF, this fund is currently increased by 6% per year, taken from the interest income, with the goal to make it self-supporting. CHF 321,449 was given as young scientists' support during the triennium.

2.9. Ewald Fund

The accounts of the Ewald Fund are given in Table 13. The interest on the capital is intended to cover the costs of the Prize. It is calculated as 6% 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 PJDF and the REF. The balance of the interest from the investments is credited to the GF. An additional CHF 25,072 has been transferred to the fund during the triennium.

2.10. Newsletter Fund

Table 14 shows the accounts of the Newsletter Fund (NF). The fund was established in 1994 following the successful launch of the

Table 6
Acta Crystallographica (Swiss Francs).

	1999		2000		2001	
Income						
Subscriptions	2,623,639		2,591,111		2,580,225	
Sale of back numbers and single issues	19,594		26,122		18,612	
Distribution costs charged to subscribers	100,368		109,046		105,510	
Profit/loss on offprints	−34,581		2,751		28,732	
Special issue income	27,976		30,761		30,316	
Royalties, copyright fees	12,133		9,018		11,164	
Pay per view and secondary services (net)	–	2,749,129	–	2,768,809	4,803	2,779,362
Less Publisher's commission	−185,021		−183,888		−185,612	
Yield from advertisements	6,820		4,735		3,214	
Recharge/Recredit to Publications and Journals Development Fund for Special Issues	41,340	2,612,268	28,585	2,618,241	−11,943	2,585,021
Expenditure						
Printing and binding	680,929		523,715		507,782	
Distribution and postage	137,240		119,722		86,147	
Annual index/other incidental costs	9,222		–		–	
Special Issue costs	69,316		59,346		18,373	
Editorial expenses, including promotion	928,237		1,305,185		1,255,330	
Programming and development	196,380		224,413		169,449	
Administration expenses	121,491	2,142,815	139,793	2,372,174	127,294	2,164,375
Excess of income over expenditure		469,453		246,067		420,646
Transfers to other Funds:						
President's Fund	–		−20,000		–	
International Tables	−200,000		−250,000		−200,000	
Publications and Journals Development Fund	−200,000		−200,000		−200,000	
Journal of Synchrotron Radiation	−100,000		−150,000		−75,000	
Research and Education Fund	−70,000		−70,000		−100,000	
Newsletter Fund	−50,000	−620,000	−50,000	−740,000	–	−575,000
Fluctuations in rates of exchange		17,139		6,893		2,110
Accumulated balance at end of year		1,449,844		962,804		810,560

IUCr Newsletter in 1993 (when the expenses were charged to the GF). 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 86,232 in 1999, CHF 53,561 in 2000 and CHF 36,429 in 2001.

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, his family informed the President that Professor Ewald had wished to make a 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 Professor J. M. Cowley and Dr A. F. Moodie. The second Prize was presented during the Bordeaux Congress to Professor B. K. Vainshtein. The third Prize was presented during the Beijing Congress to Professor N. Kato. The fourth Prize was presented during the Seattle Congress to Professor M. G. Rossmann.

In March 2002, it was announced that the sixth Ewald Prize had been awarded to Professor M. M. Woolfson for his exceptional contributions in developing the conceptual and theoretical framework of direct methods along with the algorithm design and computer programs for automatic solutions that changed the face of structural science and for his contributions to crystallographic education and international collaboration, which have strengthened the intellectual development of crystallographers world wide.

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

Table 7
Journal of Applied Crystallography (Swiss Francs).

	1999		2000		2001	
Income						
Subscriptions	363,383		391,819		384,698	
Sale of back numbers and single issues	12,314		3,556		4,852	
Distribution costs charged to subscribers	16,052		30,165		28,889	
Profit/loss on offprints	−2,595		2,605		4,563	
Special issue income	–		56,606		–	
Royalties, copyright fees	3,369	392,523	2,368	487,119	2,120	425,122
Less Publisher's commission	−26,299		−28,184		−27,703	
Yield from advertisements	734		3,388		702	
Recharge/Recredit to Publications and Journals Development Fund for Special Issues	–	366,958	−6,016	456,307	–	398,121
Expenditure						
Printing and binding	124,763		114,624		68,595	
Distribution and postage	24,303		30,927		11,726	
Special Issue costs	–		50,590		–	
Editorial expenses, including promotion	209,314		159,981		180,237	
Programming and development	33,953		32,059		26,688	
Administration expenses	21,635	413,968	39,241	427,422	19,727	306,973
Excess of income over expenditure		−47,010		28,885		91,148
Transfers to other Funds: *Newsletter* Fund	–	0	–	0	−25,000	−25,000
Fluctuations in rates of exchange		1,256		975		528
Accumulated balance at end of year		106,279		136,139		202,815

4. Appendix D: Reports of Commissions of the Union

4.1. Commission on Journals

4.1.1. Overview. The triennium 1999–2001 saw the publication of 25,669 pages and 6,121 articles compared with 21,947 pages and 5,196 articles in the period 1996–1998.

Milestones accomplished in the triennium were the launch of *Acta Crystallographica* Section E in January 2001 and the completion of the 50-year digitization project in November 2001. In both these projects, we witness again the electronic revolution. With *Acta Cryst*. Section E, we have a very fast mechanism for publication of chemical crystal structures in electronic form. With the full archive of papers now digitized, we have complete access at the click of a mouse to all articles for our subscribers back to 1948. In the accompanying reports there are very buoyant trends in numbers of articles with *Acta Cryst*. Sections D and E, and a level number for *Acta Cryst*. Sections B and C and *Journal of Applied Crystallography* (*JAC*). *Acta Cryst*. Section A started the triennium with some concerns over the number of submissions but *via* fast handling and new Co-editor appointments to reflect new fields it has been able to return to expected levels. The *Journal of Synchrotron Radiation* (*JSR*) has been subject again to considerable variations in the number of published pages between Conference Proceedings (XAFS X and XI) and issues containing regular articles. Indeed, the number of regular articles in *JSR* is causing increasing concern. Discussions have started to evaluate what benchmarks represent a 'minimum viability' and of ideas for broadening its scope.

Journal article highlighting has continued and been well received. The close collaboration with the *IUCr Newsletter* and its Editor W. L. Duax is gratefully acknowledged. The Journals Working Group has produced a number of general promotional leaflets for the journals, as well as leaflets for *Acta Cryst*. Section E and *JAC*, and a joint marketing leaflet for *Acta Cryst*. Section D and *International Tables*. This involved working closely with the Promotion Committee (Chair A. M. Glazer, whose collaboration is also gratefully acknowledged).

The fruits of 'staying at the forefront' of publishing for our subscribers are twofold. Firstly, readers and authors are ever more sophisticated in their expectations. Secondly we also hope to improve the subscriptions situation where, although our losses year on year are better than the journal publishing average, the number has still gone down over the last 20 years. In addition to new projects, referred to above, we have, *via* the Journals Working Group, been able to undertake analyses of our subscriber and author base, and trends. This has informed the Finance Committee in its deliberations. Finally, let me especially thank the following retiring Section and Main Editors for their major commitment to serving the IUCr Journals, namely A. Authier (Section Editor of *Acta Cryst.* Section A), F. H. Allen (Section Editor of *Acta Cryst.* Section B), and S. S. Hasnain and H. Kamitsubo (two of the Main Editors of *JSR*). Their successors will be formally appointed at the upcoming Geneva General Assembly.

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

4.1.2. *Acta Crystallographica* Section A. In the triennium, Section A has published 18 bimonthly issues and a Special Issue dedicated to A. F. Moodie, which appeared in March 1999. The total number of pages was 2,525, corresponding to 245 Research Papers, including 18 papers in the Special Issue, and 20 Short Communications. There was a decrease in the number of papers published in 2000, but this number picked up again in 2001. The average reviewing time has been reduced from more than four months to 2.8 months.

Table 8
Journal of Synchrotron Radiation (Swiss Francs).

	1999		2000		2001	
Income						
Subscriptions	134,075		134,396		163,649	
Sale of back numbers and single issues	5,050		1,442		4,407	
Distribution costs charged to subscribers	11,299		5,160		5,143	
Profit/loss on offprints	−478		−4,052		8,771	
Special issue income	64,993		3,081		125,058	
Royalties, copyright fees	540	215,479	724	140,751	1,397	308,425
Less Publisher's commission	−9,698		−10,723		−12,528	
Yield from advertisements	11,297		7,365		5,099	
Recharge/Recredit to Publications and Journals Development Fund for Special Issues	19,139	236,217	17,216	154,609	−5,389	295,607
Expenditure						
Printing and binding	80,115		43,679		44,276	
Distribution and postage	19,156		5,452		4,560	
Special Issue costs	84,132		20,297		119,669	
Editorial expenses, including promotion	156,049		109,071		76,519	
Programming and development	38,542		49,831		9,743	
Administration expenses	23,300	401,294	11,549	239,879	30,863	285,630
Excess/Deficit of income over expenditure		−165,077		−85,270		9,977
Transfers from other Funds: *Acta Crystallographica*	100,000	100,000	150,000	150,000	75,000	75,000
Fluctuations in rates of exchange		−547		133		270
Accumulated balance at end of year		−46,233		18,630		103,877

Table 9
International Tables (Swiss Francs).

	1999		2000		2001	
Income						
Sales:						
Volume A	52,633		−503		811	
Volume A Teaching Edition	6,200		3,671		116	
Volume B	23,582		22,250		67,989	
Volume C	95,974		68,056		45,091	
Volume F	–		–		112,122	
Volumes II, III and IV	86		96		–	
Less Publisher's commission	−46,067	132,408	−25,768	67,802	−58,423	167,706
Donation	–	132,408	14,806	82,608	–	167,706
Expenditure						
Production Volume A	19,329		30,287		–	
Production Volume A Teaching Edition	5,448		4,811		–	
Production Volume B	4,952		33,027		30,036	
Production Volume C	61,611		10,830		5,569	
Production Volume D	–		1,536		1,507	
Production Volume E	–		3,651		–	
Production Volume F	351		7,874		57,307	
Editorial expenses	262,974		267,524		215,907	
Promotion	–		–		14,048	
Programming and development	37,012	391,677	42,164	401,704	114,378	438,752
Deficit of income over expenditure		−259,269		−319,096		−271,046
Transfers from other Funds: *Acta Crystallographica*	200,000	200,000	250,000	250,000	200,000	200,000
Fluctuations in rates of exchange		1,627		494		−5
Accumulated balance at end of year		137,628		69,026		−2,025

Table 10
Book Fund (Swiss Francs).

	1999		2000		2001	
Income						
Sales:						
Historical Atlas of Crystallography	178		296		140	
World Directory of Crystallographers	6,222		1,830		900	
Escher *Kaleidozyklen*	159		–		127	
Structure Reports	1,305		4,005		393	
Sundry publications	164		–		–	
Royalties						
IUCr/OUP Book Series	1,358	9,386	3,593	9,724	2,595	4,155
Expenditure						
World Directory of Crystallographers	1,776		2,160		1,980	
Programming and development	–		–		61,002	
Promotion	–	1,776	–	2,160	14,048	77,030
Excess/Deficit of income over expenditure		7,610		7,564		−72,875
Fluctuations in rates of exchange		397		297		−82
Accumulated balance at end of year		33,607		41,468		−31,489

Table 11
Publication and Journals Development Fund (Swiss Francs).

	1999		2000		2001	
Income						
Investment income		13,686		11,916		20,714
Expenditure						
Computer expenses:						
Purchase of computer equipment and software	37,517		50,308		9,207	
Programming and development	359,857		409,961		414,414	
Programming and development recharged to other Funds	−359,857		−409,961		−423,621	
Electronic Publishing Committee/Section Editors' meeting	1,183		2,765		10,676	
STAR/CIF	7,170		1,319		556	
Promotions Representative	107,416		137,922		126,560	
Promotions Representative recharged to other Funds	–		–		−126,560	
Web input	3,892		1,502		626	
Special Issue costs (surplus) recharged to (from) other Funds	60,479		39,785		−17,331	
Journal Grants Fund subsidies	–		–		968	
Digitization project	–		–		32,928	
Crystallographic neXus	–		2,774		2,244	
Depreciation of computer equipment	12,097	229,754	12,097	248,472	37,573	68,240
Excess/Deficit of income over expenditure		−216,068		−236,556		−47,526
Transfers from other Funds:						
Acta Crystallographica	200,000	200,000	200,000	200,000	200,000	200,000
Fluctuations in rates of exchange		5,285		2,960		1,477
Accumulated balance at end of year		447,064		413,468		567,419

A highlight of 1999 was the Special Issue dedicated to A. F. Moodie on the occasion of his 75th birthday. Its Guest Editors were J. C. H. Spence and J. Etheridge. More such Special Issues would be very welcome.

A. Authier, Editor

4.1.3. *Acta Crystallographica* Section B. In the triennium 1999–2001, Section B published 3,132 pages, comprising 332 full Research Papers, 10 Short Communications, 3 Topical Reviews and 2 Lead Articles. The number of pages published exceeds that for 1996–1998, despite the fact that atomic coordinate tables no longer appear in the printed journal from 2001 onwards. In line with the international aims of the IUCr, authors from 31 countries were represented in Section B during 2000 and from 28 countries in 2001. There is a healthy stream of new submissions, and a joint Special Issue with Section D on Crystallographic Databases is due for publication in mid-2002.

The chemical balance of papers is almost equally divided between organic (48%) and inorganic (52%) topics, a slight swing from the 40:60 split in the previous triennium. Across these chemical categories, Section B continues to serve the needs of those working on charge-density studies, neutron and powder diffraction, structural

Table 12
Research and Education Fund (Swiss Francs).

	1999		2000		2001	
Income						
Investment income	47,069		47,366		48,532	
Refund of Congress income	–	47,069	–	47,366	29,556	78,088
Expenditure						
Young scientist support	82,157		112,200		127,092	
Visiting Professorship Programme	20,226	102,383	10,700	122,900	6,937	134,029
Deficit of income over expenditure		−55,314		−75,534		−55,941
Transfers from other Funds:						
Acta Crystallographica	70,000	70,000	70,000	70,000	100,000	100,000
Fluctuations in rates of exchange		10,785		6,539		2,499
Accumulated balance at end of year		912,341		913,346		959,904

Table 13
Ewald Fund (Swiss Francs).

	1999		2000		2001	
Income						
Investment income	22,442		25,591		27,322	
Bequest	72	22,514	–	25,591	–	27,322
Expenditure						
Ewald Prize		45,902		–		–
Excess/Deficit of income over expenditure		−23,388		25,591		27,322
Transfers from other Funds:						
General Fund	25,000	25,000	–	–	–	–
Fluctuations in rates of exchange		5,042		3,260		1,260
Accumulated balance at end of year		426,512		455,363		483,945

systematics from the inorganic and small-molecule databases, studies of polymorphs and phase transitions, and computational methodologies, including *ab initio* crystal structure prediction. It is pleasing to note that the impact factor of Section B continues to rise, from 1.463 in 1997 to 1.734 in 2000 (the most recent available data).

There have been significant changes in manuscript handling and in-house procedures. CIF submission is now mandatory, and in-house typesetting from electronic author manuscripts is now the norm, with proof delivery and online journal availability *via* the web. There have been very significant improvements in processing times, with much shorter times permitted for author revisions.

In my final report as Editor of Section B, it is a pleasure to record thanks to the authorship for quality input, to all referees (without whom no journal can flourish and aspire to high standards), and particularly to the IUCr office staff in Chester. Their innovative and responsive approach to journal editing, production and presentation has been much appreciated over the past nine years.

F. H. Allen, Editor

4.1.4. *Acta Crystallographica* Section C. During the Commission meetings in the summer of 1999, the decision was made to require that Full-Paper submissions to *Acta Cryst.* Section C should have a significant structural-comment section. Submissions that had a minimal *Comment* section (as decided by Co-editors and referees) were thereafter recommended for transfer to the CIF-Access publication stream introduced in 1997. Authors always had the option of improving their structural comment significantly and continuing with a Section C Full-Paper publication. It was anticipated that the number of CIF-Access papers (later called electronic papers) would increase with time as authors realized the benefits of this publication mode and the ease of reprint preparation *via* the (then) new IUCr **Crystallography Journals Online** web site. The electronic paper option proved to be very popular and it was decided to transfer all electronic papers from Section C to a new IUCr journal, *Acta Crystallographica* Section E, which started electronic publication in January 2001.

With the January 2000 issue of Section C, a new format was adopted for all papers, with each one starting on a new larger page. Authors are now asked to collect their proofs electronically *via* the **Crystallography Journals Online** web site and this has been working very well. Authors are also able to download reprints of their papers from the **Crystallography Journals Online** web site. As Editor, I am also able to download and review all Section C proof pages from the

Table 14
Newsletter Fund (Swiss Francs).

	1999		2000		2001	
Income						
Advertisements	139,475		173,980		174,692	
Reimbursement of 19GAC circular	–	139,475	–	173,980	14,331	189,023
Expenditure						
Editorial honoraria	6,732		7,920		7,260	
Editorial expenses	80,710		51,862		65,915	
Printing and distribution	103,398		124,264		108,604	
Advertising costs	34,867	225,707	43,495	227,541	43,673	225,452
Deficit of income over expenditure		−86,232		−53,561		−36,429
Transfers from other Funds:						
Acta Crystallographica	50,000		50,000		–	
Journal of Applied Crystallography	–		–		25,000	
General Fund	25,000	75,000	25,000	75,000	25,000	50,000
Accumulated underspend in prior years not previously recognised		86,312		−22,000		–
Fluctuations in rates of exchange		1,583		962		386
Accumulated balance at end of year		133,905		134,306		148,263

web site at the same time as the authors. This has allowed any of my comments on the proofs to be acted upon in a timely manner with no significant delays to the publication process.

Significant changes have been made to the appearance of author proofs; these now contain the artwork within the body of the paper so that the proofs are very much closer to the final appearance of the published paper.

Starting with the January 2002 issue, papers are now posted on the web on a regular basis. These papers receive an online publication date when they appear on the web site. At the end of a month, the online papers are collected and published as the next month's issue of Section C. These changes, coupled with a faster turn around at the typesetters, have reduced publication times considerably.

Over the last three years, the data-validation suite of programs has been revised and updated as the need arose and as required by changes in the Notes for Authors. In this regard, I am indebted to A. L. Spek for his invaluable work on the *PLATON* checking suite of programs. Authors are required to pre-check their CIFs prior to submission. The introduction of notes to the pre-check output explaining concisely what problems have been detected has been much appreciated by authors.

As noted in previous reports, the changes to Section C in this present triennium continue to provide a faster more efficient publication mode for delivering structural information, and ensure a consistently high standard of publication through explicit acceptance criteria. The high standard of Section C papers is due in no small part to the careful work of Co-editors, referees and the Chester staff; once again I very much appreciate the fine work done by these colleagues.

G. Ferguson, Editor

4.1.5. *Acta Crystallographica* Section D. Section D, devoted to any aspect of biological crystallography, has been a monthly journal since January 1999. The number of submitted articles has justified the changeover from a journal that previously had appeared only every two months. The journal publishes Research Papers, Topical Reviews, Short Communications, Crystallization Papers, Book Reviews and Letters. The annual content has remained rather constant with about 170 Research Papers (including Short Communications) together with 200 Crystallization Papers annually. A strong and welcome component is the addition of the Proceedings of CCP4 (Collaborative Computational Project, Number 4) Study Weekends that have been published each year.

The published articles demonstrate how much macromolecular structure determination has advanced during the three-year period. Larger structures are now described in more detail and at higher resolution. Crystallization techniques involving more sophisticated protocols are now being introduced. Methods for solving the phase problem are improved, and structure refinement is reported in more cases. This means that analyses of structural results have a firmer and more extensive basis. The informational crystallographic databases are expanding rapidly with fine data from such structure reports.

Research Papers cover a wide variety of subjects from details of the growth of crystals and effects of microgravity to new methods of data collection or structure determination and methods for assessing the accuracy of the results to full reports of structures, often with deductions on the biological modes of action of the molecule or molecules under consideration. Each of these adds to the value of this journal.

Figures in colour are provided free of charge, but only when the colour adds to the scientific content of the article. The journal continues to have excellent illustrations and authors are generally delighted when their work is chosen for the monthly cover. All authors are asked to sign a form attesting to the fact that they have seen the final manuscript. Section D requires that, for publication (as stated in the Notes for Authors), all crystallographic data on biological macromolecules (atomic coordinates and structure factors) be deposited in the Protein Data Bank or the Nucleic Acid Database. This means that the crystallographic data are then available for inspection and, if necessary, re-refinement. In this context, we are endeavouring to ensure that structure factors as well as atomic coordinates are deposited in the Protein Data Bank. If a small molecule is involved, the coordinate and structure-factor data must be deposited as for Section C of *Acta Cryst.* The database reference

codes are published in Section D. The following table lists a summary of depositions with the PDB and NDB during the triennium:

	1999		2000		2001	
	A	*B*	*A*	*B*	*A*	*B*
0.6–1.0 Å	3	2	2	1	9	14
1.0–1.5 Å	13	18	13	20	20	25
1.5–2.0 Å	24	40	31	51	46	81
2.0–2.5 Å	23	24	15	19	33	47
2.5–3.0 Å	19	15	8	8	11	19
3.0 Å and lower	7	5	6	5	5	3
Totals	89	104	75	104	124	189
Totals 1999–2001					288	397

A = number of macromolecules described; *B* = number of PDB and NDB depositions.

Full lists of structures published in Section D in 2000 and 2001 may be found in the Annual Reports of the Executive Committee for those years.

Crystallization Papers continue to provide important and useful information on what people are working on. For some authors, they are a prelude to a structure determination (which may even have been completed) but represent experimental challenges. For others, they are the result of much effort and structural studies will follow in the future. The dissemination of crystallization data is still of importance to the international scientific community that we serve. A list of appropriate data for such papers is described in Notes for Authors. The three Crystallization Co-editors – N. Chayen, A. Zagari and M. Pusey – handle most of the Crystallization Papers, and it is planned to have them eventually deal with all articles in this category. These three Co-editors deserve our thanks for streamlining the publication of such articles. We envision the possible eventual publication of an electronic version of this part of the journal.

We were delighted to be able to publish the Proceedings of CCP4 Study Weekends in Section D in each of the three years reported on here. Previous Proceedings of CCP4 Study Weekends have been published as Daresbury Laboratory technical reports, but it was felt that Section D would reach a wider audience. Single copies of each issue can be purchased by interested scientists. In 1999, the focus was on Data Collection and Processing. The issue contains 18 articles on sources, detectors, optics systems, data collection strategies, cryodata, MAD data, and data from twinned crystals. At the end there is a useful listing by P. Evans of recommendations on choices that have to be made during data collection. The organizers were S. Bailey, A. Ashton, P. Broadhurst and D. Brown. The subject for 2000 was Low-Resolution Phasing. J. Wilson, H. Saibel and J. Grimes were the Guest Editors for this issue of 17 articles. The proceedings of the CCP4 Study Weekend on Molecular Replacement and its Relatives, held 3–9 January 2001 at York University, and organized by K. Cowtan, J. Naismith, A. Ashton, D. Brown, P. Broadhurst and M. H. Eales, were published in Section D in October 2001. K. Cowtan and J. Naismith were the Guest Editors for this. It includes an introduction to the method by P. Evans, a historical account by M. G. Rossmann, and 17 other articles. Therefore it should be very useful for all, and extra copies of this issue can be purchased. The extra thickness of the November 2001 issue of Section D (the issue after the CCP4 issue) indicates the good general influx of manuscripts.

Now that we are entering the area of 'high throughput' macromolecular crystallography, it is necessary to consider the impact of such results on Section D. Crystallization papers may eventually be published in an electronic subsection and we are considering an electronic only structural genomics subsection. We welcome J. M. Guss as a Co-editor helping us with this.

My sincere thanks to the many members of the crystallographic community who have served as reviewers of submitted papers and ensure that this is a high-quality journal, and to the staff at Chester, particularly L. E. Jones, who have done an excellent job in shepherding the articles to the publishers. The Co-editors are also deserving of our thanks; they oversee the publication fate of a large proportion of the submitted manuscripts. I thank J. R. Helliwell, the Editor-in-Chief, and P. R. Strickland, the Managing Editor, and S. Glynn in Chester, and E. Pytko, A. Katz and C. Afshar in Philadelphia for their continued assistance in ensuring the quality of the journal.

J. P. Glusker, Editor

4.1.6. *Acta Crystallographica* Section E. In early 2000, the IUCr decided to establish a new section of *Acta Crystallographica*, namely Section E: *Structure Reports Online* – a purely electronic journal. During 2000, planning sessions took place, Notes for Authors were drafted and a team of nine Co-editors assembled. Crucial to this initiative was the decision to terminate the publication of electronic papers in Section C, with effect from January 2001. Thus, starting in October/November 2000, electronic papers originally destined for Section C were diverted towards Section E, thereby ensuring a good number of articles for the launch of the new Section.

The first issue of Section E duly appeared in the first week of 2001, with 68 papers in the issue. This new and rapid means of publication has been welcomed and embraced by a growing number of authors. In its first year of operation, a total of some 800 papers, one crystal structure per paper, were published, corresponding to almost 2,000 pages in PDF format.

Authors are reminded that all submissions should be checked, and preferably read in preprint form, before they are uploaded through the journals web site for review and publication; the checkcif and printcif facilities are available through the same web site for this purpose. To help authors produce a suitable CIF submission, a model CIF is provided on the web site, generously annotated with explanations and comments on the important features.

In collaboration with the Cambridge Crystallographic Data Centre (CCDC), screening of all organic and metal-organic structures is carried out against the Cambridge Structural Database (CSD). This reveals whether or not the structure has been previously published. The results of this process are of considerable help to the Co-editors in deciding whether or not to accept a paper for publication. A similar screening has been put in place for inorganic structures, using the facilities of Fachinformationszentrum Karlsruhe where the Inorganic Crystal Structure Database is produced.

Although there is a formal publication date each month, individual articles are made available on the web as soon as proofs have been corrected, and this may be within a few days of receipt of the original CIF through the journals electronic submission procedure. The average time from receipt to publication is about four weeks, and this is one of the major attractions of *Structure Reports Online*.

Accreditation of the journal by the Institute for Scientific Information, leading to inclusion of articles in the *Science Citation Index*, was granted during 2001. This is a significant recognition of the journal's importance and relevance, and adds to its attraction as a publication medium.

All published articles are available in HTML and PDF formats, and free reprints are made available to authors electronically. A range of supplementary material is provided. This includes the output of the checkcif process and any associated responses from authors. Throughout the year, there has been a steady increase in the number

of submissions and it will probably not be long before we have 100 articles in a single monthly issue. In anticipation of this, another five Co-editors have been appointed and another three to four may be needed by mid-2002.

During 2001, 795 papers were accepted, 24 rejected and 53 withdrawn. The average review time was 0.6 month and the average editing time 0.4 month. Of the 795 published papers, 48 correspond to inorganic structures, 229 to metal-organic and 518 to organic. The distribution of papers by country is rather skewed. Thus with 30 or more papers we have Australia, Canada, People's Republic of China, Germany, India, Japan, UK and USA. However, within this group, the People's Republic of China accounts for 8% of the total, India for 8.3% and the USA for only 9.7%.

D. G. Watson and **W. Clegg**, Editors

4.1.7. *Journal of Applied Crystallography*. *JAC* published 1,208 pages in 1999, 1,020 pages in 2000 (plus 448 pages of Conference Proceedings of the 11th International Conference on Small-Angle Scattering) and 798 pages in 2001. The new format and layout of the journal were rather well received by the community. The decline in the number of pages published is related primarily to a reduced number of submissions and not to a dramatic increase in rejection/withdrawal rates. While Co-editors in Europe received fewer manuscripts, the numbers received in Asia and North America remained low. A new promotional leaflet prepared in late 2001 should re-orient some of the groups working with or on crystallographic methods towards *JAC*.

G. Kostorz, Editor

4.1.8. *Journal of Synchrotron Radiation*. *JSR* celebrated its eighth year of existence in 2001. During the last triennium (1999–2001), two major Conference Proceedings were published, the International Conferences on X-ray Absorption Fine Structure, XAFS X in 1999 and XAFS XI in 2001. These two Proceedings contributed 686 and 968 pages, respectively, to the overall total of 2,883 published pages.

The turnaround time for papers has continued to fall, with average publication times of around 6 months. The financial situation of the journal has also improved during the triennium.

We are currently working to put together a Special Issue devoted to accelerator challenges and potential science for the next level of enhancements of synchrotron-radiation production, namely energy recover linacs (ERLs) and X-ray free electron lasers (XFELs). In summary, *JSR* remains the pre-eminent journal dedicated to reporting scientific and instrument advancements in the ever-expanding field of synchrotron-radiation research.

S. S. Hasnain, **H. Kamitsubo** and **D. M. Mills**, Editors

4.2. Commission on *International Tables*

During the Glasgow Congress, the Commission held one Open Meeting and one closed meeting, in addition to numerous personal contacts between volume editors, technical editors and authors. The Open Commission Meeting featured eight lectures on the status of the various *International Tables* volumes. Reports about this meeting are available on the internet as part of the IUCr home page (see below) and in the Newsletter of the British Crystallographic Association (September 2000, No. 74, pp. 20–22). Reports on the status of the different volumes of *International Tables* are given below. Details of the scope and the contents of these volumes may be found at the home page of the Commission (see below) and in the Triennial Report for 1996–1998 [*Acta Cryst.* (2001), A**57**, 758–761].

Detailed reports of sales and stock figures for the individual volumes of *International Tables*, published up to 31 December 2001 and currently active, are given below:

Volume	A	Brief A	B	C	F
Date of publication	1983	1985	1993	1992	2001
Dates of reprinting	1984	1988	1996	1995	–
	1987	1989	2001	1999	–
	1989	1993	–	–	–
	1992	1996	–	–	–
	1995	–	–	–	–
	1996	–	–	–	–
	1998	–	–	–	–
Number of copies sold					
up to end 1998	7,861	5,034	1,926	2,379	0
in 1999	284	249	152	307	0
in 2000	0	149	116	306	0
in 2001	0	0	337	209	484
up to end 2001	8,145	5,432	2,531	3,201	484
Stock at end of 2001	0	0	932	331	1,516

The web site containing the home page of the Commission is maintained by U. Shmueli at Tel Aviv University, Israel (http://crystal.tau.ac.il/xtal/comit/index.html). The home page is frequently retrieved by the IUCr office at Chester (http://www.iucr.org/iucr-top/welcome.html) and distributed among several mirror sites, to ensure timely communication of the updates.

Apart from some minor updates introduced during 2001, the descriptions of Volumes B and F – published during this year – were removed from the home page of the Commission and transferred to the publication page, which is maintained in Chester, along with the relevant publication data (http://www.iucr.org/iucr-top/it/index.html).

4.2.1. Volume A. *Space-Group Symmetry*; Editor Th. Hahn. The preparation of the LaTeX files of the space-group tables for the Fifth, Revised Edition of Volume A by M. Aroyo and P. Konstantinovic in Sofia, Bulgaria, was completed by the end of 1998, the revisions and updating of the text sections by the end of 1999.

The years 1999–2001 were spent with incorporation of all space-group diagrams, checking of the LaTeX files and fixing the overall layout of the space-group tables. The text sections were converted to SGML and checked in up to three proof stages.

Both processes were completed by the end of 2001. Publication of the volume is expected for the spring of 2002. Shortly afterwards the Fifth, Revised Edition of the *Brief Teaching Edition of Volume A* will appear.

4.2.2. Volume B. *Reciprocal Space*; Editor U. Shmueli. Although all manuscripts for the Second Edition of Volume B were available for technical editing at the beginning 1997, it was not until April 1999 that this process could be started. This delay was caused by the decision to translate all the material to SGML (Standard Generalized Markup Language) and to ensure thereby fully computerized typesetting from SGML files as well as to enable storage of Volume B on other media. This procedure is applied to all Volumes of *International Tables* that are being prepared; it is expected that this will lead to cheaper and faster implementation of future corrections and production of new editions.

The extensive work on the preparation of the manuscripts for the production of galley proofs was commenced after the Glasgow Congress in 1999. This Congress, as many of the previous ones, was a fine opportunity for informal meetings with the technical editors and many authors. The rest of 1999 and most of 2000 was dedicated to the production, correction and reviewing of the galley proofs of all chapters and sections. This work was accompanied by extensive correspondence between the Editor, the Technical Editor and the authors; the collaboration between these three parties was remark-

able. The effort invested in this careful examination of the galley proofs and an expert implementation of the corrections turned out to lead to a very small number of corrections in the page proofs, which were prepared and distributed towards the end of 2000.

The first few months of 2001 were still devoted to final correspondence with authors and the Technical Editor, regarding minor corrections of the page proofs. The volume was then sent to press and was published in April 2001.

The description of the Second Edition of Volume B and a table of its contents are available at the following URLs: http://crystal.tau.ac.il/xtal/comit/promot.html and http://www.iucr.ac.uk/iucr-top/it/index.html.

4.2.3. Volume C. *Mathematical, Physical and Chemical Tables*; Editor E. Prince. The publication of the Second Edition of Volume C in June of 1999 substantially completed the project of replacing all of the outdated information that had been carried over from the earlier series of the *International Tables* because of the need to publish the first edition without further delay. In July of 2001 it appeared that the stock of the Second Edition would run out early in 2003. Because the entire contents of the Second Edition exist as computer files, it is possible to make fairly extensive revisions at minimal cost. A memorandum was therefore sent to all authors asking whether developments in their fields would require significant revisions to their respective chapters. About ten of the authors replied to this memorandum indicating some need for correction or revision. These authors have been advised that revisions must be in the hands of the editor by 31 July 2002, and that anything beyond simple corrections of typographical errors should be in a machine readable form suitable for importing into the printers' system.

4.2.4. Volume D. *Physical Properties of Crystals*; Editor A. Authier. Volume D comprises three parts, *Tensorial Aspects of Physical Properties*; *Symmetry Aspects of Excitations*; and *Symmetry Aspects of Structural Phase Transitions and Twinning and Domain Structures*, and will be accompanied by a CD-ROM containing two software packages, one on Tensors and Irreducible Representations, the other on Phase Transitions. All manuscripts of the three parts and the final versions of the two software packages have now been received. It is expected that the volume will be printed in 2002/2003.

4.2.5. Volume E. *Subperiodic Groups*; Editors V. Kopsky and D. B. Litvin. Volume E is being prepared for publication in 2002.

4.2.6. Volume F. *Macromolecular Crystallography*; Editors M. G. Rossmann and E. A. Arnold. Volume F was published in July 2001. It comprises 26 chapters and a total of 72 articles written by 156 authors. 561 copies have been sold as of the end of February 2002, already exceeding the first-year sales projection of 450. A very favourable review of the volume has been published in the March issue of *Structure* (2002), **10**, 289. The contents and further description of the volume can be found at the IUCr web site: http://www.iucr.org/iucr-top/it/itf/itf.html.

Volume F is the first *International Tables* volume devoted to macromolecular crystallography. The inception and creation of this book reflects the acceleration of activity and interest in structural biology and also recognizes the extraordinary contribution that knowledge of macromolecular structure has made, and will make, to the analysis of biological systems, from enzyme catalysis to the workings of whole cells, and to the rapidly growing field of structural genomics. The volume covers all stages of a crystallographic analysis, including the preparation of samples using the techniques of molecular biology, crystallization, diffraction data collection, phase determination, structure validation and structure analysis. There are chapters on the fundamentals, history and current perspectives of macromolecular crystallography, as well as the availability of useful programs and databases, including the Protein Data Bank.

We thank the authors for their many excellent contributions and for maintaining good humour about the project despite many deadline reminders. We are grateful for the continual help and support of the IUCr editorial staff, our own administrative staffs, the IUCr Executive Committee, and the IUCr Commission on *International Tables* in making the project possible. We also greatly appreciate the help and support of many friends and colleagues, including the volume's Advisory Board members and authors, for input and feedback on the design of the volume. Now that Volume F has been published in print version, it is important to consider different possible modes of electronic access. We suggest that the IUCr might consider making a version available on the internet, accessible to those who have either purchased the volume or who have paid for a password. A CD-ROM version of Volume F would also be a valuable and easily portable resource. This CD-ROM version could be sold separately, perhaps at a very substantial discount for owners or new buyers of the volume.

4.2.7. Volume G. *Crystallographic Information*; Editors B. McMahon and S. R. Hall. Volume G is intended as a reference handbook for crystallographic information, and specifically in its early editions as a documentation of the Crystallographic Information File (CIF) project. The volume will include the definitions of public data names maintained by the IUCr (data dictionaries), and will also document the file structure and formal grammar of CIF, and the techniques and software libraries available for creating, editing and reading CIFs.

Since the Volume was first commissioned, the initial dictionaries covering small-molecule single-crystal studies, powder diffraction experiments, and macromolecular structure determinations have been complemented by dictionaries covering the storage and interpretation of image-plate data, and the refinement and interpretation of incommensurate modulated structures. A new dictionary has also been developed to clarify and extend the treatment of symmetry in the original core dictionary. These developments have contributed to a delay in producing the Volume, which is now expected to be published in late 2002 or early 2003.

4.2.8. Volume A1. *Maximal Subgroups of Space and Plane Groups*; Editor H. Wondratschek. Volume A1 was approved by the Executive Committee in August 1995. The data on subgroups of space groups had been derived and typed by hand. Meanwhile, they have been checked several times by different methods. In 2000 it was decided to expand the contents of this volume by the data on the relations between the Wyckoff positions of group–subgroup pairs of space groups. These data had been derived and typed by U. Müller.

Volume A1 will now have two editors and will consist of three parts:

Part 1: *Introduction* (to Parts 1 and 2)

Part 2: *Maximal subgroups of space groups*

Part 3: *Splitting of Wyckoff positions*.

Regrettably, because of illness the publication of this volume has been considerably delayed.

Th. Hahn, Chair

4.3. Commission on Aperiodic Crystals

Many Commission members had the opportunity to meet during various international conferences. The most important event was the Aperiodic 2000 meeting, which took place in July 2000 in Nijmegen, The Netherlands. Commission members met during the Glasgow

Congress to discuss activities. The General Assembly reappointed the Commission including several new members.

The activities of the Commission were focused on the organization of international conferences and the coordination of acivities between the different communities working on quasicrystals and incommensurate structures. The work on the establishment of a CIF standard for incommensurately modulated structures was completed, and an internet site with information on aperiodic crystals was created.

The International Conference on Aperiodic Crystals, Aperiodic 2000, took place 5–8 July 2000 in Nijmegen and was organized by T. Janssen from the University of Nijmegen. Aperiodic 2000 was the seventh in a series of conferences on Modulated Structures, Polytypes and Quasicrystals, that started as MOSPOQ in 1984 in Marseille, France. There were 139 participants from 25 different countries. As compared to previous meetings, the number of contributions related to quasicrystals and composite crystals increased, while the number of contributions on modulated structures decreased. The proceedings of Aperiodic 2000 have been published as Volume 250, Numbers 1–4 of the journal *Ferroelectrics* (publication date February 2001) with A. Fasolina and T. Janssen as guest editors. A complete report on this meeting may be found at the web pages of the Commission. The Commission has asked N. Speziali to organize Aperiodic 2003, to be held in Belo Horizonte, Brazil, in September 2003. Information may be found at the Commission's web pages or at http://www.fisica.ufmg.br/~ap2003/.

The Commission continued to promote activities on the crystallography of aperiodic crystals at national and international meetings. Members of the Commission were actively involved in the organization of microsymposia at the Glasgow Congress, at the European Crystallographic Meetings ECM-19 in August 2000 in Nancy, France, and ECM-20 in August 2001 in Krakow, Poland, and at the fourth meeting of the Asian Crystallographic Association AsCA '01 in November 2001 in Bangalore, India. A satellite meeting to the International Congress on Quasicrystals was organized by W. Steurer (Zürich, Switzerland) on the topic Quasicrystal Structure Analysis (24–25 September 1999, Stuttgart, Germany). The Chair of the Commission organized a Workshop on the Structural Analysis of Aperiodic Crystals in Bayreuth, Germany, 5–6 March 1999. In addition to a series of lectures, the participants could study the crystallography of incommensurately modulated structures and composite crystals using a script on a series of worked-out examples together with the computer program *JANA*. A second Workshop of this kind was held 1–4 March 2000.

Following previous work, the CIF dictionary for modulated structures was almost completed (final version 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 (COMCIFS). 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.

A database on quasicrystals was developed at the Laboratory of Crystallography at ETH Zürich, Switzerland (W. Steurer). It contains an extensive database on the literature on quasicrystals (5,712 entries on 1 January 2002) as well as databases on data sets and materials. It is available at http://www.kristall.ethz.ch/QDB/.

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 may be found at http://www-xray.fzu.cz/sgip/aphome.html.

S. van Smaalen, Chair

4.4. Commission on Biological Macromolecules

In the past three years, the Commission has undertaken a limited number of wide-ranging and diverse activities. For a Commission that covers what is arguably the most active and vigorous scientific community within the IUCr, it may therefore seem incongruous that the Commission undertakes relatively few independent activities. An explanation may lie in the fact that the scientific outlets for the macromolecular community are so diverse and numerous and relatively well supported by other bodies including industry that little call is placed by this community on this Commission of the IUCr. Macromolecular crystallography is strongly represented at meetings of the Regional Associates of the IUCr, namely the American Crystallographic Association (ACA), the Asian Crystallographic Association (AsCA) and the European Crystallographic Association (ECA), as well as at meetings of national crystallographic societies. Vigorous representation at these meetings is sometimes even mistaken for dominance by other members of the crystallographic community. In addition, there are many specialized workshops and schools held regularly that cater for the macromolecular crystallography community including those at Cold Spring Harbor (USA), Erice (Italy), Uppsala (Sweden) and the CCP4 (UK) study weekends.

In 2001, the Commission supported an International Symposium on Crystallography and Bioinformatics held in November 2001 in Bangalore, India. The Symposium immediately followed an extremely successful meeting of AsCA held in the same location. The organization of the meeting, the venue and the gracious support of the Indian Institute of Science can only be described as superb. The meetings honoured two distinguished members of the international macromolecular community, S. Ramaseshan and M. Vijayan on the occasion of his birthday. The Symposium showcased the range and depth of biomolecular crystallography in India as well as keynote talks from both Indian and foreign attendees. The enthusiastic participation by so many students was extremely pleasing.

Major changes in the rapidity of structure determination and the throughput of macromolecular crystallography in the last few years has prompted a number of initiatives of the Commission, particularly in the areas of data deposition and rapid publication. The first act of the Commission during this triennium was to finalize the statement on the submission of crystallographic data for biological macromolecular structures. The starting point for the discussion by the Commission was the previously published statement, which comprehensively argued the various options [Baker & Saenger (1999). *Acta Cryst.* D**55**, 2–3]. The opinions expressed by the community at an Open Meeting of the Commission at the Glasgow Congress were considered. It was ultimately agreed to make a number of changes to the previously decreed criteria. These included equal treatment of coordinates and measured structure-factor amplitudes and a recommendation that the data be made available on publication of the work. Provision is included for a maximum hold period of six months. A full statement of the new deposition requirements for IUCr journals has been published [Commission on Biological Macromolecules (2000). *Acta Cryst.* D**56**, 2]. The Commission Chair wrote to the editors of all journals that routinely publish papers describing macromolecular structures, acquainting them with the revised guidelines and asking that they be adopted as minimum standards. Most responded in a positive vein but several of

the most high profile journals were clearly concerned about losing a competitive advantage should they insist on conditions for publication not imposed by their rivals. The Commission strongly encourages individual scientists to deposit all their data in order that they are properly curated and not lost for future generations. In order that the IUCr establish a formal link with the principal repository of macromolecular structural data, the IUCr Executive Committee approved a suggestion from the Commission to nominate a representative on the Protein Data Bank Advisory Committee (PDBAC) following an invitation from the Director of the Protein Data Bank. The Commission's nominee, E. N. Baker, has been appointed to the PDBAC as the first nominee of the IUCr.

The Commission is aware of changes to the field of macromolecular crystallography that may result from recent initiatives to fund large-scale projects in the area of structural genomics. As well as benefits that will flow to the entire community from the development of more efficient procedures for all steps of a structure analysis from cloning and expression to refinement and interpretation, there will be the need for changes to the publication and validation of data. The Chair of the Commission is a member of one of the teams examining these issues. Close contact is being maintained with the Protein Data Bank and the IUCr journals.

The need to cater for the high-throughput needs of the structural genomics community has been recognized by editors of *Acta Crystallographica* Section D with the foreshadowed inclusion of a new category of contribution [*Acta Cryst*. (2002), D**58**, 189]. This category will provide rapid reporting of structural genomics research and other areas requiring rapid publication of short papers for structural biology. In order to acquaint the community with the new opportunities and challenges associated with this initiative, a joint meeting of the Commissions on Biological Macromolecules and on Journals is scheduled to be held 9 August 2002 during the Geneva Congress.

J. M. Guss, Chair

4.5. Commission on Charge, Spin and Momentum Densities

4.5.1. Meetings, workshops and schools. Bringing together scientists from different disciplines is a key objective of the Commission, and meetings play a major role in its activities. As usual, several have been organized either under close guidance from the Commission, such as the Sagamore meetings, or in the form of cooperation, such as the Gordon Conferences, or as microsymposia within the IUCr Congresses and other major meetings.

Glasgow Congress, August 1999

In addition to a Key Lecture by Yu Wang (Taiwan), two microsymposia were directly relevant to the Commission's interests:

6C: Chemical Insights from Charge Density Analysis. The idea for this microsymposium arose from the recognition that a great deal of chemically meaningful information is now being derived from careful charge-density studies of X-ray data. However, in many instances, this is not being conveyed to the wider chemical community. The invited speakers were asked to focus, as much as possible, on the chemical outcomes of their studies.

9D: Synchrotrons and Charge Density Analysis. The increasing use of synchrotrons for collection of precision diffraction data for charge-density analysis indicated that a session devoted to just these studies would be timely.

Both microsymposia proved to be extremely popular, with lecture halls filled to capacity, and feedback indicates that they were very well received by charge-density practitioners as well as the wider chemical community. Nearly 50 poster presentations were also made in topics related to these microsymposia.

Second European Charge Density Meeting (ECDM), Sitges, Spain, September 1999

These meetings fill the gap between the Sagamore and Gordon Conferences on charge, momentum and spin densities. ECDMs are growing, both in attendees (more than 70 on this occasion) and interest, and they are being established as a new meeting point between the other two conferences. Scientific sessions were devoted to three main subjects: Intermolecular Interactions; Modelling Spin and Momentum Densities; and X-ray Diffraction under External Perturbations. The organizers tried to cover much of the charge, momentum and spin density community, and theorists and experimentalists were involved together in both sessions and discussions.

Nineteenth European Crystallographic Meeting, Nancy, France, August 2000

This meeting featured three sessions relevant to the Commission's activities, and coordinated by P. Becker: Applications to Materials Science, New Developments, and Crystallography of Excited States. The coverage of charge-density studies at this meeting, combined with the many and varied poster presentations, underlines the increasing importance and relevance of charge-density research in modern crystallography.

Sagamore XIII, Stare Jablonki, Poland, September 2000

The Sagamore meetings remain the most important 'outcome' of the Commission, and this particular meeting was an outstanding success. The 13th in this series of triennial meetings took place at Hotel Anders, in the Taborskie Woods beside the wonderful Lake Szelag Maly in the Mazurian lakes and woods region of north-eastern Poland. The Sagamore meetings focus on aspects of charge, spin and momentum distributions, their determination from a wide variety of experimental techniques, and their detailed analysis and comparison with theory, and have a considerable history, recently documented by M. J. Cooper (http://alpha.uwb.edu.pl/sagamore/page_history.html). The meeting attracted just over 100 participants, with nearly 50% of those in attendance from either France or Poland. L. Dobrzynski and his Local Committee did a truly superb job of organizing the meeting, impressing all with their warm hospitality. As expected, the oral and poster presentations contained more physics than chemistry, but that did not distract from some wonderfully lively discussions, even if there was always the perception that most present worked and thought in either direct space or momentum space and had some difficulty traversing the landscape in between! Many presentations dealt with the use of synchrotron radiation in various forms, and this was reflected in the large number of participants from ESRF and Japan. However, there was a disappointing turnout from the charge-density, neutron and electron diffraction communities, and the discussions could have benefited from a few more theoreticians. A number of talks described quite substantial and dramatic improvements in methods and measurements (shorter times and increased accuracy and precision), and it was clear that maximum-entropy methods are being employed to great effect in all aspects of charge, spin and momentum density research. Proceedings of Sagamore XIII have been published as a special issue of *J. Phys. Chem. Solids* [(2001), **62**(12), 2095–2256.]

Gordon Research Conference on Electron Distributions and Chemical Bonding, South Hadley, USA, July 2001

Chaired by C. Lecomte and J. C. H. Spence, this meeting attracted 95 attendees, a considerable increase on previous meetings, and most pleasingly over 50% of attendees were under 40. The scientific

programme was designed to bring together experimentalists and theoreticians, X-ray and electron diffraction experts, crystallographers, physicists, materials scientists and chemists, and resulted in very stimulating and interesting discussions. The conference was a success owing to the quality of lecturers, discussion leaders and poster sessions (which always lasted very late into the night). Support from the Gordon Research Conferences, IUCr, NSF, Oxford Cryosystems, Bruker Nonius Molecular Structure Corporation and JEOL allowed 65 conferees to be partly or fully sponsored. The meeting demonstrated that charge-density-related research is entering a new and very alive period, attracting more and more new communities of physicists, chemists and material scientists.

*IXS*2001 – *Fourth International Conference on Inelastic X-ray Scattering, Haikko, Finland, August* 2001

Also organized under the auspices of the Commission, and chaired by K. Hämäläinen, S. Manninen and P. Suortti, this was the fourth conference in the series (previous meetings being in Montauk, USA, 1998, Tokyo, Japan, 1995 and Krakow, Poland, 1993). The main emphasis of the meeting was on the application of inelastic X-ray scattering in the study of electronic structure and dynamics, as well as in many-body phenomena. The purpose of the meeting was to bring together specialists to discuss both the experimental advances accomplished at various synchrotron-radiation sources, and the theoretical and computational challenges that have been overcome, and those that are to be met. The scientific programme was designed to encourage dialogue between theory and experiment. Participants numbered 70, and the conference was truly international, with the greatest representation coming from outside Europe. Inelastic X-ray scattering has recently demonstrated tremendous breakthroughs owing to the advent of third-generation synchrotron sources. Besides very strong fundamental research, real applications in materials science, chemistry and even in biology have started to appear. Highlights included work on high-resolution X-ray spectroscopy on biomaterials, especially on photosynthesis, several resonant scattering studies on high-T_c cuprates, studies under high pressure, and impressive theoretical progress on understanding the electron–hole interaction. The conference was funded mainly through registration fees, with some sponsorship received from the IUCr, the University of Helsinki, the Academy of Finland, and private foundations and companies. The next meeting will be organized by APS 'somewhere close to Chicago' (to be chaired by E. Alp) in 2004. This is very timely because at that time several IXS-capable beamlines under construction at APS will have begun to produce new results.

Future meetings

Planning for Sagamore XIV, the next triennial conference on charge, spin and momentum densities, is well under way. The meeting is being organized by M. A. Spackman and will be held 14–18 August 2003 in Broome, Western Australia, following a joint meeting of the Society of Crystallographers in Australia and New Zealand and the Asian Crystallographic Association at the same venue. Preliminary details may be found at http://www.crystal.uwa.edu.au/CrystalsDownUnder. As always, the Gordon Research Conference was evaluated, and a future meeting has been approved for 2004 (Chair, J. C. H. Spence).

Commission meetings

The Commission held open and closed meetings during the Glasgow Congress (1999) and during the Sagamore XIII Meeting on Charge, Spin and Momentum Densities (Stare Jablonki, Poland, September 2000). Major topics of discussion at the meetings were planning for forthcoming meetings and especially progress on Commission projects. Increasingly, the business of the Commission is being conducted most efficiently by e-mail correspondence.

4.5.2. Projects. Several projects have been supported by the Commission in recent years and its meetings have elicited some vigorous debate on their continuation. Projects on Density Matrices (W. Weyrich) and Fermiology (A. Bansil) have been active for some time; W. Weyrich is keen to return to activity on the Density Matrix project, and is planning to involve a number of new participants, while interest and participation in the Fermiology project is increasing rather than decreasing according to A. Bansil. The Maximum Entropy project (M. Sakata) is still active, and current details may be found at http://www.mcr.nuap.nagoya-u.ac.jp/mem/index.html; M. Sakata would like to see some interaction between the MEM and Multipole Refinement projects, and is keen for others to look at the standard data sets. The project on Multipole Refinement (C. Lecomte) is in progress, with analyses completed of both experimental and theoretical data for corundum. According to C. Lecomte, there were a disappointing number of takers for this project, but S. Pillet has recently analysed all data sets and this work has been submitted for publication. An important Commission project, on developing a Multipole Refinement Program (T. Koritsanszky), has essentially been completed, and *XD* now has over 70 subscribers world wide, and has quickly become the package of choice for multipole refinement and subsequent estimation of properties based on the charge distribution. P. Mallinson has attended recent COMCIFS meetings, and is now actively seeking input from the charge-density community, particularly *XD* users, in order to refine further a CIF dictionary (rhoCIF) for charge-density analysis. V. Tsirelson proposed a project on Topological Features, and this was considered best as part of the Multipole Refinement project.

M. A. Spackman, 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) International School on Crystal Growth and Advanced Materials, Campinas, Brazil, 18–24 July 1999, chaired by H. Klapper and R. Caram. This School was attended by about 90 participants, mostly from Brazil and other Latin American countries. Three members of the Commission were involved as lecturers at the school. The lecture notes were collected in a volume edited by S. Baldochi and R. Caram and delivered to the students at the beginning of the school. The School was sponsored and supported by the IUCr by the grant of two Visiting Professorships.

(2) The Commission contributed to the programme of the Glasgow Congress by establishing and chairing two microsymposia on crystal growth: Bulk Single Crystal Growth and Surface Phenomena (Chair L. Smolsky, Russia) and Growth of Mesoscopic Crystals (Chair Naiben Ming, People's Republic of China).

(3) International School on Crystal Growth of Materials for Energy Production and Energy-Saving Applications, Trieste, Italy, 5–10 March 2001. This school was entirely organized by the Commission, under the auspices of the International Organization for Crystal Growth (IOCG) and directed by R. Fornari. Three more members from the Commission were involved as lecturers. The School was held at the Abdus Salam International Centre for Theoretical Physics (ICTP) and sponsored by the IUCr through

awards for young scientists. It was specifically aimed at young researchers, PhD and Masters students working in materials science. Three main classes of materials were considered: materials for energy conversion (terrestrial and space solar cells, thermo-photovoltaic converters), for energy storage (carbon nanotubes and superconductors) and for energy saving (superconductors, soft magnets for low-loss transformers, nitrides for visible and white light LEDs). Some lectures on structural and electrical characterisation were also included. The School was attended by 40 participants (15 from Italy, 15 from Eastern and Western Europe, 4 from northern Africa and the others from South America and Asia). In addition to registered participants, several ICTP guests could follow the lectures.

(4) International Workshop on Preparation and Characterization of Technologically Important Single Crystals, National Physical Laboratory, New Delhi, India, 26–28 February 2001. The workshop was sponsored by the IUCr through awards for young scientists. Four members of the Commission were involved in the organization of this meeting, either as members of the International Advisory Committee or as lecturers. The Workshop dealt with growth and characterization of single crystals (in particular, oxides) but also served to celebrate the 60th birthday of K. Lal, an eminent scientist who has contributed for more than three decades to the development of new crystallographic methods for the characterization of defects in crystalline materials. He was also a member of the Commission for three triennia between 1987 and 1996. Nearly 150 abstracts of contributed papers were accepted. The Proceedings, containing 17 invited and 119 contributed papers, were distributed to over 180 delegates, including 20 from outside India, representing countries such as USA, UK, Germany, Japan, Russia, Bangladesh *etc*.

(5) 11th International Summer School on Crystal Growth, Doshisha, Japan, 24–29 July 2001. This school is held every three years and it is certainly the most important school organized by the IOCG. This Commission contributed to the Japanese edition with many suggestions and by supporting the sponsorship application presented by the Chair K. Sato. 25 lectures were presented, ranging from theory of crystal pattern formation to nanocrystal formation. The level of the lectures was in most cases tutorial but some high-level seminars regarding advanced fields were also included (blue light emitters, high-efficiency solar cells, quantum structures, superlattices *etc.*). The school was successful and attracted a large number of students, particularly from the crystal growth community of Japan.

(6) International Conference on Crystallogenesis and Mineralogy, Department of Crystallography, Saint Petersburg State University, Russia, 17–21 September 2001. This conference focused on the development of fundamental crystallogenesis in mineralogy: modelling of mineral formation processes; analysis of the genetic character of crystal morphology and crystal chemistry of minerals; and studies of aggregate structures. These subjects also included some applied aspects of crystallogenesis in multicomponent media: synthesis of minerals and other crystalline materials, crystallization in glasses and adhesive crystalline materials, and treatment of mineral resources. The Conference was timed to coincide with a centenary celebration of the birthday of G. G. Laemmlein (23 August 1901 – 15 November 1962), an outstanding crystallographer and mineralogist and one of the founders of modern crystallogenesis and of crystallogenic modelling of mineral formation. The conference was chaired by A. E. Glikin and two members of the Commission served on the Programme Committee. This event was also sponsored by the IUCr.

R. Fornari, Chair

4.7. Commission on Crystallographic Computing

The last three years have been rather disappointing for the Commission. With a few notable exceptions, most of the members have been unable to find time to join in active participation of any initiatives. This raises a number of issues:

(1) The growing divide between large- and small-molecule crystallographers, and the growing specialization within small-molecule crystallography. Powder people are no more enthusiastic to hear about incommensurate modulations than incommensurate people want to hear about MIR. Hybrid microsymposia are almost inevitably disrupted by the shuffling of chairs whenever there is a substantial change in topic. In reality, each fragment of the community is happy to organize its own symposia in its own way, without reference to other computing crystallographers.

(2) The escalating costs of meetings and schools. The drift away from campus to commercial venues has greatly raised the cost of meetings, and while this may not have a serious impact on groups with large industrial collaborations, it is very serious elsewhere.

(3) Is there still a role for the Computing Commission? Except for exotic machines for special purposes, the choice of hardware for most crystallographers has reduced to a handful of actual or generic systems. Adequate crystallographic software is available for day-to-day work on most of the machines. The growth of service crystallography, and the need to maintain high throughput, has also had an impact upon software innovation. In small-molecule crystallography, the tightening grip of checkCIF has made research-to-recipe the norm. The incentive to develop new software is diminished by the cost of compilers for stand-alone machines, by the need for new software to have sophisticated user interfaces if it is to be distributed, and by a growing reluctance for the crystallographic community to experiment with software with which they are not accustomed. Excellent software is still being developed, but it is usually written in response to a closely defined need, and workers outside that field are unlikely to have a real interest in it. Perhaps the former role of this Commission has now been taken over by active groups within other Commissions or by other autonomous groups (*e.g.* CCP4).

(4) The growing importance of national and regional associations. The ACA, BCA, ECA *etc*. are now immensely successful. They provide a local forum for the exchange of ideas, which, coupled with the growth of web-based communications, means that research groups are now less isolated than formerly. The establishment of a Special Interest Group for computing within the ECA has helped provide coherence for European programmers.

I believe that there is a way ahead, and I suggest that a re-structuring of the Commission is needed. Firstly, it is clear that a smaller Commission could function just as well. Secondly, the Commission needs focused roles. Amongst these, the organization of schools must be the most important. The Bricogne–Bloomer school at Hixton, UK, in 1999 sets a style for future schools, although the organizers declined offers of assistance from the Commission.

Activities

There was a brief period of high activity as the Commission tried to implement its long-standing aim to establish a database of experimental data to be used for teaching or program validation. Many interesting contributions were located, but it became evident that there were very few people wishing to make use of these data. The project was put on hold.

In year two, we were instrumental in setting up the ECA Computing SIG, with help from C. Lecomte and C. Giacovazzo. This has been extremely successful, and was able to organize four microsymposia at the last European Crystallographic Meeting.

The Commission's web activities are still organized by L. M. D. Cranswick, who was reappointed to run the EPSRC CCP14 project for a further five years. His unbounded enthusiasm is having a good impact on small-molecule computing.

Members of the Commission have chaired or spoken at sessions in many major meetings, including the 1999 Glasgow Congress, the 1999 Ecole Thématique: Analyse Structural par Diffraction des Rayons X (Toulouse, France), the 2000 ECM (Nancy, France), the 2001 ACA (Los Angeles, USA) and the 2001 ECM (Krakow, Poland).

The Open Meeting at the Geneva Congress will be devoted to issues related to intellectual property, funding software research and maintenance, and software diversity. These issues have become more important as institutions discovered both the cost and the value of novel software.

D. J. Watkin, Chair

4.8. Commission on Crystallographic Nomenclature

The Commission met in closed session during the Glasgow Congress, all other internal discussions during the triennium having been conducted electronically. The nomenclature of phase transitions together with the nomenclature of crystallography in *n* dimensions remained the Commission's primary concerns. The only new nomenclature matter, arising at the end of the triennium, was the possibility of assigning identifiers to crystalline phases for use in databases.

The first Report of the Working Group on Phase Transition Nomenclature entitled *Structural Phase Transition Nomenclature* was published in *Acta Cryst*. (1998), A**54**, 1028–1033. The renewed Working Group, with J.-C. Tolédano continuing as Chair and P. J. Brown, A. M. Glazer, R. S. Roth, R. S. Berry, R. Metselaar, D. Pandey, M. Perez-Mato and S. C. Abrahams appointed members, was charged with extending the recommended structural phase-transition nomenclature to other classes of phase transition. Following a planning meeting of Working Group members present at the Glasgow Congress, it was determined that the six-field notation of the first Report was fully applicable to the more complex nomenclature of transitions involving magnetic phases, incommensurate phases and transitions that occur as a function of composition change. The notation also proved fully applicable to a series of other phase types, including polytype, radiation-induced, other transient and quasi-crystalline phases and their transitions. The conditions for phase stability in the latter series of phases are ill defined, hence the nomenclature recommended for them is necessarily tentative. It was found possible to recommend a uniform notation for translational periodicity, propagation vectors or wavevectors in magnetic and/or incommensurate substances. The notation adopted for incommensurate phases, which relies in part on the existence of an average structure, also proved consistent with that for a sequence of commensurate phases. In the case of polytypes and transient phases, the sixth field of the nomenclature is used to emphasize special features. Illustrative examples of the recommended nomenclature are provided for each category of phase sequence. The second Report, as accepted by the Commission, appeared in *Acta Cryst.* (2001), A**57**, 614–626; six printing errors were corrected in *Acta Cryst*. (2002), A**58**, 79.

The first Report of the Sub-committee on the Nomenclature of *n*-Dimensional Crystallography, entitled I. *Symbols for Point Group Transformations, Families, Systems and Geometric Classes*, appeared in *Acta Cryst*. (1999), A**55**, 761–782. The renewed Sub-committee, with T. Janssen continuing as Chair and J. L. Birman, F. Denoyer, V. Kopsky, V. A. Koptsik, W. Steurer, D. Weigel, J.-L. Verger-Gaugry, A. Yamamoto and S. C. Abrahams appointed members, was charged with proposing a set of recommendations to supplement those contained in the first Report, thereby completing the recommended nomenclature and symbolism for use in *n*-dimensional crystallography. Sub-committee members in Glasgow for the Congress and advisor G. Chapuis met to discuss future progress. Following extensive discussion throughout the triennium, a zeroth draft of Report II with recommended symbols for arithmetic crystal classes, Bravais classes and space groups in four, five and six dimensions was circulated in the second week of 2002. The final Report is expected to be ready for review by the Commission before the next Congress in Geneva.

An *ad hoc* group appointed by the Commission to consider both an ambiguity in the definition of 'symmetry element', as presented in the Commission report of 1989 entitled *Definition of Symmetry Elements in Space Groups and Point Groups*, and the completeness of Fig. 3 in the 1992 Commission Report entitled *Symbols for Symmetry Elements and Symmetry Operations*, removed the ambiguity by redefining the term 'geometric element'. Three new types of glide plane, in addition to the original 15 illustrated in the 1992 Report, were recognized in a report that appeared in *Acta Cryst*. (2000), A**56**, 96–98.

Late in the final year of the triennium, through the good offices of H. D. Flack, IUCr's Representative to ICSTI, several Commission members participated in a vigorous discussion concerning possible modification of the IUCr recommended phase nomenclature in order to meet the requirements of the joint IUPAC–CODATA–ICSTI Project on the Standardization of Physico-Chemical Property Electronic Datafiles. The structure of the recommended nomenclature is not presently suited to searching in computerized databases. A Commission-appointed group to study the definition of crystalline phase identifiers is under consideration.

Commission Observer to COMCIFS, A. Authier [see *Acta Cryst*. (1997), A**53**, 822], reported that Version 2 of the mmCIF (macromolecular) dictionary; the imgCIF/CBF dictionary designed for the transmission and archiving of images from array detectors and suitable for any multidimensional image; the msCIF dictionary of data names for the description of modulated incommensurate structures; and the dictionary of symmetry data names, cif_sym.dic, had been approved. These, along with the powder diffraction dictionary, which has been adopted as the standard of the powder diffraction file, show that a large number of IUCr Commissions have now adopted the CIF standard. Drafts of the sasCIF (small-angle scattering), rhoCIF (electron densities) and magCIF (magnetic structures) dictionaries have been prepared; the Observer emphasized that no nomenclature issues were in contention.

The name of each member, the IUCr office on which *ex officio* membership depends, and the titles of all published Commission Reports are listed on the Commission's home page at http://www.iucr.org/iucr-top/comm/cnom/index.html. The page presents information about the Commission, links both to each member and to the full online content of all Commission reports, and in addition provides links to a valuable group of sites containing nomenclature resources of interest to crystallographers.

S. C. Abrahams, Chair

4.9. Commission on Crystallographic Teaching

The principal concerns of the Commission during the triennium were concerned mainly with (1) how to develop and update the existing web site and (2) how to produce teaching materials, and in what form. The aim is to produce teaching materials not only for

crystallographers but also for school children and the general public and authorities. There have been considerable activities by the members and consultants of the Commission in the years following the Glasgow Congress. The Commission organized with the Egyptian Society of Crystallography and Application (ESCA) a Teaching School on the Structure and Characterization of Amorphous and Nanocrystalline Materials, Ismailia, Egypt, January 2000. The opening lecture of the School was given by the President of the IUCr, H. Schenk. The School covered a wide range of topics summarized in the following: (1) preparation and characterisation of nanoparticles by X-ray diffraction and electron microscopy; (2) neutron and X-ray amorphography; (3) models for interpreting small-angle neutron and X-ray scattering results; (4) synchrotron and method of X-ray absorption spectroscopy; (5) reverse Monte Carlo method; (6) combining the reverse Monte Carlo method and Rietveld methods for amorphous materials structure modelling; (7) substructure analysis by means of X-ray diffraction line broadening; and (8) molecular dynamic simulation of glasses. This school received IUCr sponsorship and financial support. All the previous lectures were published in a Proceedings.

The Commission also held two informal meetings, one at ECM-19 in Nancy, France, and the other at ECM-20, Krakow, Poland. The discussions at these Commission meetings were mainly centred on how to manage and update the teaching web site and to follow up the progress of the updating. The discussions were also about the formulation of the November 2001 workshop, which was planned to be organized in cooperation with the Egyptian National Committee for Crystallography. The title of the workshop was chosen to be: Computer-Based Crystallographic Teaching Materials. A discussion about this workshop continued for almost six months using the discussion list set up for the Commission on the Chester server.

At the Krakow meeting, the discussion was centred mainly on the teaching activities at the Geneva Congress. The Commission decided to have two sessions: (1) the usual microsymposium and (2) an Open Commission meeting allocated to one topic, which was chosen to be macromolecules. The November (2001) Workshop was, in fact, held in February (2002) at Ismailia, Egypt; four members of the Commission were involved as lecturers and seven were involved as members of the Scientific Programme Committee. The opening lecture was assigned to the teaching of crystallography to the general public and the authorities. The Workshop covered a wide range of topics in teaching: (1) crystal growth from melts by computer video simulation; (2) teaching diffraction using computer simulation over the internet; (3) the teaching of crystallography web-based module; (4) the power of powder diffraction in solving many problems in life sciences; (5) X-ray absorption as a complementary tool to X-ray diffraction for characterising local structures of materials; (6) teaching crystallography to pharmacists; (7) crystallography courseware; and (8) a school children session for three hours, designed in Arabic. The last session was successful, with about 20 school children aged 10–14 attending and happily interacting with the speakers. They had a two-hour practical in which they had fun in making their own models and learning symmetry through playing with a video game CD-ROM especially made for them.

Finally, the Commission has just finished the organization of the two sessions planned for the Geneva Congress.

K. El-Sayed, Chair

4.10. Commission on Electron Diffraction

There has been considerable activity by members of the Commission in the past three years. D. L. Dorset has replaced J. C. H. Spence as Co-editor of *Acta Crystallographica* Section A to represent the interests of electron diffraction and electron crystallography. Since D. L. Dorset has relocated to another workplace and will complete his term on the Commission in 2002, responsibility for the Commission web page has been taken over by the Secretary, S. Hovmöller, from his location at Stockholm University, Sweden.

Commission members have organized sessions/meetings or presented talks on themes related to electron crystallography or diffraction at crystallography or microscopy conferences. These include: 21st Meeting of the Society of Crystallographers in Australia, Thredbo, NSW, Australia (conference talk by D. L. Dorset); Microscopy 2000, Canberra, ACT, Australia (organized by R. Withers with presentations by J. C. H. Spence and D. L. Dorset); EUREM 2000, Brno, Czech Republic, July 2000 (Workshop on Electron Crystallography organized by I. G. Voigt-Martin and J. R. Fryer, contributions by H. Zandbergen, D. Van Dyck, J. Gjønnes, and D. L. Dorset); International Kunming Symposium on Microscopy, Kunming, People's Republic of China, July 2000 (entire meeting on electron diffraction and electron microscopy organized by Li Fang-hua); ECM-19, Nancy, France, August 2000 (session on electron crystallography organized by I. G. Voigt-Martin, contribution by J. Gjønnes); ECM-20, Krakow, Poland, August 2001 (session on new frontiers on electron crystallography organized by C. J. Gilmore and U. Kolb, contribution by H. Zandbergen). For the European Crystallographic Association, a special-interest group (SIG) on electron crystallography has been organized, initially chaired by S. Hovmöller and J. Gjønnes. A web site entitled 'The Electron Crystallography Forum' has been constructed for this SIG by T. Weirich, Darmstadt, Germany. A similar SIG is being considered by the American Crystallographic Association.

Education has always been a strong theme for the Commission, exemplified, for example, by the annual schools on electron crystallography organized by S. Hovmöller in Stockholm, Sweden, or at other sites in Europe, wherein other members of the Commission have been invited as lecturers. In the past two years there has been the Euro Summer School held in Aachen, Germany, in 2000, and in Barcelona, Spain, in 2001. These schools attract 50–60 students world wide. Future meetings are being planned for Tampere, Finland (S. Hovmöller), Moscow, Russia (A. Avilov) and Asia (Li Fang-hua). Additionally, small informal meetings on electron crystallography have been organized by H. Zandbergen at TU, Delft, The Netherlands, in December, for discussion of practical issues related to structure determination. The first was held in December 1998 and the most recent one was held in December 2001.

There will be three sessions in the Geneva Congress related to the activities of the Commission. One treats the combination of X-ray crystallography and electron microscopy, and is chaired by H. Saibil and A. Engel. Another, on electron diffraction, is chaired by H. Zandbergen and Li Fang-hua. Finally, a session on high-resolution electron microscopy is chaired by D. Van Dyck and Y. Matsui. D. L. Dorset will present a keynote address on electron diffraction.

Special journal issues have also been edited by Commission members. A special issue of *Zeitschrift für Kristallographie* on electron crystallography is in progress, edited by C. J. Gilmore and D. L. Dorset. J. C. H. Spence is editing a special issue of *Microscopy and Microanalysis* devoted to the quantitative electron microscopy of inorganic materials.

Finally, two Commission members have been honoured for their work in electron diffraction. D. Van Dyck, RUCA, Antwerp, Belgium, has been awarded the Franqui Chair by the University of Leuven, one of the highest scientific prizes in that country. D. L.

Dorset, the Commission Chair, has been given the 2002 A. L. Patterson Award by the American Crystallographic Association.

D. L. Dorset, Chair

4.11. Commission on High Pressure

This has been the second triennium for the Commission, following its creation at the Seattle Congress. A great deal of work was done in the first triennium by all members and consultants to establish the Commission, frame its Terms of Reference, and broaden its scope from that of the previously existing High Pressure Group within the Commission on Crystallographic Apparatus. In these special circumstances, it was agreed at the Glasgow Congress that all members should continue in office, and that the two consultants appointed after the Seattle Congress to assist in broadening the Commission's range of activity and expertise should become full members. After the Glasgow Congress, two new consultants, M. Kunz and J. Tse, were added to bring in new blood and a broader range of expertise without further increasing the formal membership. J. B. Parise and W. F. Kuhs were reappointed to continue to serve as Secretary and Treasurer, respectively. This present triennium has been a period of consolidation and continuing effort to strengthen the links between high-pressure crystallography and the wider field of high-pressure science, to disseminate information about high-pressure activities, methods and facilities, and to encourage and assist young scientists and others new to the field.

This triennium has seen further rapid progress and many new developments. Detailed structural studies are being taken to ever more extreme pressures and temperatures; high-pressure structural studies are also expanding increasingly into exciting new areas, such as proteins and fundamental chemical systems; more and more complex structures are being discovered under high pressure, in everything from metallic elements to simple molecular systems; structural complexity is now sometimes defeating powder diffraction methods, and a growing use of single-crystal samples, even at very high pressures, is emerging; at the same time, there has been a strong surge in work on liquid and amorphous materials, including melt structures at very high P–T; and a wide range of complementary studies – X-ray and neutron phonon measurements, optical spectroscopy, EXAFS, nuclear resonant scattering, NMR and many other probes – are being applied to an increasingly multitechnique approach to high-pressure science. This is all supported by developments in synchrotron and neutron facilities, improved detectors and pressure devices, and breakthroughs in materials (such as synthetic diamond), and by remarkable advances in *ab initio* computational and simulation techniques.

In view of this high level of progress and change, the Commission's principal activity has remained the organization of annual meetings to keep the community in touch with new science and techniques, and to provide regular opportunities to broaden the field and draw in new people. In addition, high priority is given to encouraging and supporting participation by young scientists, with the valuable assistance of generous funding by the IUCr.

4.11.1. Symposia and workshops. After the very successful six microsymposia, two keynote lectures and Open Commission Meeting at the Glasgow Congress, the first meeting of the triennium focused on the special topic of 'Crystallography at High Pressure and High Temperature using X-rays and Neutrons', and was held at the third-generation synchrotron facility SPring-8, Japan, 30 September–3 October 2000. This international workshop was jointly organized by the Commission, the SRRC Japan Atomic Energy Research Institute (JAERI), and the Japan Synchrotron Radiation Research Institute (JASRI), and the organizer was Commission member O. Shimomura. Topics included structures and transitions in molecular and elemental liquids; novel (and often complex) structures in simple systems – like lithium, oxygen and xenon; theoretical studies of liquid carbon, molecular hydrogen and alkali metals under pressure; a wide variety of geo-planetary science – mineral phases and equations of state, the Earth's lower mantle and core, and planetary ices; high P–T synthesis of new materials like cubic boron carbonitride and 3D polymerization of C_{60}; and high P–T experimental techniques using X-ray synchrotron and neutron sources. Nearly 80 high-pressure scientists from 13 countries took part, including 13 young scientists generously supported by both the IUCr and JAERI. Three young scientists were invited speakers. Considerable assistance with local arrangements was given by JAERI and JASRI staff.

In each triennium, the Commission holds one meeting that covers the full scope of its activities. This was arranged as an international workshop on 'Crystallography at High Pressures – 2001' held at Orsay, France, 4–8 September 2001, hosted by the French national neutron facility, Laboratoire Léon Brillouin (LLB). Commission member I. Goncharenko was the organizer. Topics ranged over pressure effects in proteins, membranes and polymers; liquid and amorphous systems, including supercritical fluids; structures and transitions in (complex) 'simple' fundamental systems like elemental metals and CO_2, and studies of minerals; highly unusual physical phenomena in magnetically unstable compounds, spin-ladders, intermediate valence systems, and organic superconductors, and the interaction of magnetism and superconductivity under high pressure; new structures in ices, gas hydrates and clathrates, including implications for sources of methane on Saturn's moon Titan; recent progress in inelastic X-ray scattering in geophysical materials under pressure, and chemical reactions and Fe compounds in planetary interiors; new materials and high-pressure synthesis, including a new polymer of C_{60} said to be harder than diamond, and quasicrystals and carbon nanotubes; new developments in X-ray synchrotron and neutron techniques and facilities, including remarkable advances in inelastic X-ray scattering; and the latest innovations in pressure cells and other high-pressure instrumentation. There were 115 participants from 15 countries, including 35 young scientists – two thirds of whom benefited from generous IUCr support for the meeting. Eleven of the invited talks were given by young scientists and three others received poster prizes. The meeting also benefited considerably from funding by the CEA, the CNRS and the French Ministry of Research, and much appreciated local support from facilities and staff at LLB and LURE.

Members have most recently put considerable effort into devising the Commission's programme for the Geneva Congress, particularly W. F. Kuhs who is a member of the Programme Committee. Several members and consultants are acting as Chairs or Co-Chairs of the planned four microsymposia, two Open Commission Meetings, and three keynote lectures, which together will form a focused 'workshop' over three days of the Congress.

4.11.2. Meetings of the Commission. The main meeting of Commission members and consultants was held during the Orsay workshop. Ten members and consultants were present. The principal items of business were: future membership of the Commission, plans for sessions at the Geneva Congress, the general issue of how the Commission should best participate in Congresses for the benefit of its very wide and to some extent 'non-crystallographic' community, and other future plans and activities.

4.11.3. Other events. The workshop at Orsay included a special session to celebrate the life and work of J. M. Besson, whose untimely death in early 2001 robbed the high-pressure community of one of its

great pioneers and leaders. Most of his working life had been spent in Paris and at LURE near the conference site. Four of his close colleagues gave talks on his seminal contributions to high-pressure science. The session was introduced and chaired by the Commission Chair, who had been a close collaborator of Michel Besson's over the past decade.

4.11.4. Future plans and activities. The Commission intends to organize workshops in 2003 and 2004, at venues yet to be finally agreed. Plans are now well advanced for the International School on High Pressure Crystallography to be held in Erice, Italy, 4–15 June 2003. Commission member A. Katrusiak is a Director of the School, with P. F. McMillan. This is a major and important first venture of its kind for the Commission, and is planned as a substantial contribution to the dissemination of high-pressure methods and science to which the Commission is committed, particularly for the benefit of younger scientists. Over this triennium, the Commission's web site has been developed to give information about forthcoming high-pressure meetings, and about high-pressure facilities on neutron and synchrotron sources. A directory of high-pressure crystallographers has also been compiled and is in regular use by the community. In these various ways, the Commission is actively implementing all its Terms of Reference. There is much yet to do in further expansion of the community, extending the reach of 'high-pressure crystallography', and encouraging new, and especially young, people to enter the field and flourish in it. A large change of membership is to be made at the Geneva Congress after six years of getting the Commission fully launched, and this should be timely refreshment for the many new challenges and opportunities that the coming triennium seems certain to bring.

R. J. Nelmes, Chair

4.12. Commission on Neutron Scattering

The triennium is ending with a mixture of sorrow and joy because of the sad and exciting news about neutron sources world wide. The former was the permanent shutdown of the High Flux Beam Reactor at Brookhaven National Laboratory (USA) in 1999 and the DR-3 reactor of Risø National Laboratory (Denmark) in 2001, both of which had always been in the forefront of neutron science, including crystallography, for more than three decades. The latter news was the start of the construction of two major MW-class spallation neutron sources: the Spallation Neutron Source at Oak Ridge National Laboratory (USA) in 2000 and the Japanese Spallation Neutron Source at the JAERI Tokai site in 2001. In addition, the new powerful FMR-II reactor at Munich (Germany) is now coming close to completion while in the Asia–Oceania Region several research reactors have been newly built or refurbished such as RRR of ANSTO (Australia), CARR of CIAE (People's Republic of China), TRR-II of INER (Taiwan) and one of OAEP (Thailand). The Commission has not been directly associated with these developments as a Commission but the standing of its members in their various communities is playing a major part in these developments.

On the occasion of the Fourth International Conference on Neutron Scattering (ICNS-2001), our Commission Business Meeting was formally held in Munich, Germany, on 11 September 2001, during which the shocking news on the World Trade Center tragedy in New York was heard. Some of the Commission members met briefly to exchange their opinions on the progress of the Commission's activities when other opportunities arose, such as the 1st IUPAP–ICFNS in Mito, Japan (1999), the 2nd ECNS in Budapest, Hungary (1999), the XV-ICANS in Tsukuba, Japan (2000), and the 4th AsCA in Bangalore, India (2001).

4.12.1. International meetings. The 2nd European Conference on Neutron Scattering (ECNS) hosted by the European Neutron Scattering Association (ENSA) was held in Budapest, Hungary, in September 1999 with 750 participants. It was very exciting to see the breadth of neutron scattering application over a wide variety of research fields ranging from fundamental science to industrial research. The XV-ICANS Meeting held in Tsukuba, Japan, in November 2000 focused on the state-of-the-art technology of the accelerator-based neutron source and instruments as traditionally operated. This time, however, it also encouraged participation by reactor-based neutron scientists especially from the Asia–Oceania region to promote neutron scattering activity in this region where a large number of neutron sources have been built/refurbished for neutron science. For five days in September 2001, nearly 1,000 participants met at ICNS-2001 in Munich, Germany, the quadrennial international festival for neutron scattering, where neutrons were found to be used more importantly and widely in research fields such as crystallography, physics, chemistry, polymer science, biology, pharmacy, materials science, fundamental and industrial applications. New and exciting technology was also reported on neutron sources, optical devices, detectors, data acquisition/analysis systems and ancillaries. One day was devoted to three parallel regional meetings (Europe, North America and Asia–Oceania) and the scientific tour to the brand new FMR-II reactor and the forefront instruments under construction at Garching Campus of Technische Universität München. During the conference, it was clearly seen that the neutron scattering community is still growing with active participation by a large number of young students/scientists, particularly in Europe and Asia–Oceania, and there is a strong demand for new neutron sources. The Neutron Scattering Society of America (NSSA) has shifted gear to promote its activity to hold the 1st Biennial Meeting at Knoxville in June 2002. The 4th Meeting of the Asian Crystallographic Association (AsCA) under the auspices of the IUCr was held at Bangalore, India, in November 2001. Many key persons representing the crystallographic community of each country/region showed their strong interest in our plan to form the Asia–Oceania Neutron Scattering Association (tentatively called) to complement the existing ENSA and NSSA. After the IUCr Executive Committee's decision to change the venue for the XIX IUCr General Assembly and Congress from Jerusalem to Geneva, the ILL and ESRF scientists, including our Commission member, proposed to welcome an IUCr satellite meeting at Grenoble, France, on neutron scattering and synchrotron radiation to be linked to the Geneva Congress. By taking such scientific and geographical advantages of Grenoble where the world top-class neutron and synchrotron facilities are located 150 km from Geneva, the Commission on Neutron Scattering decided to co-host it with the Commission on Synchrotron Radiation with generous support from ILL and ESRF. The satellite meeting is now entitled 'Crystal Chemistry of New Materials and Soft Matter – Studied by Synchrotron and Neutron Diffraction', 1–4 August 2002, which complements another satellite meeting 'Neutron and Synchrotron X-ray Scattering in Condensed Matter Research', 4–6 August at Villigen, Switzerland, to celebrate the new neutron source (PSI) and the Swiss synchrotron source, and several microsymposia on neutron and synchrotron science at the main Congress in Geneva.

4.12.2. Neutron sources – international cooperation. A large neutron source, either reactor or accelerator, cannot be built without international cooperation because of technological and/or financial constraints within a single country. In 1997, the Mega Science Forum of the Organization for Economic Cooperation and Development (OECD) recommended three major spallation neutron sources to be built in each of Europe, America and Asia. Since then a series of

meetings organized by the International Union of Pure and Applied Physics (IUPAP) have been held in Budapest, Hungary, in 1999 and in Mito, Japan, in 2000. The Commission Chair (Y. Fujii) was invited to both meetings, not explicitly as a Commission Chair but as President of the Neutron Scattering Association of Japan (now the Japanese Society for Neutron Science). In September 2001, the OECD Global Science Forum (GSF) transformed from the former Mega Science Forum (MSF) hosted its Workshop entitled 'Large Facilities for Studying Structure and Dynamics of Matter' in Copenhagen, Denmark. About half of the 75 participants were scientific experts while the others were policy makers of OECD countries responsible for funding scientific programmes. The large facilities chosen for this Workshop were a neutron source, a photon source (SR, FEL) and NMR. Its charge was to discuss scientific priorities and promising future lines of research, as well as to obtain information on the utility, feasibility, time-scale and cost of various types of research facilities and related infrastructures. The need for international cooperation was also discussed. The Commission Chair was invited to give a keynote lecture on the future of reactor-based neutron scattering as a large facility representative. Both representatives from IUPAP and IUPAC gave an invited talk on their Union's views on these issues. Thus both academic and governmental organizations have paid their strong attention to neutron sources. However, it must be emphasised that both reactor- and accelerator-based neutron sources must be well balanced because of their complementary role. The Report by this OECD-GSF will be available in April 2002.

After the recommendation by the OECD-MSF in 1997, the USA funded the 2 MW Spallation Neutron Source at Oak Ridge National Laboratory in 1999, now being built jointly by five National Laboratories, while Japan started construction of the 1 MW Japanese Spallation Neutron Source in 2000 under the joint project by KEK and JAERI, both of which will substantially exceed the currently most intense pulsed neutron source of ISIS in UK (0.16 MW). The European Spallation Source (ESS, now 10 MW planned) project has been well planned so that it should be started as soon as possible to minimize the 'neutron drought'.

4.12.3. Other activities. The Commission has taken part in the preparations for the formation of the Asia–Oceania Neutron Scattering Association (tentatively named), which was initiated by the former Chair, J. W. White, to complement ENSA in Europe and NSSA in North America for overarching the globe. By taking several opportunities, the present Chair has contacted key persons of each country/region who will recommend both user representatives and facility representatives. It has been agreed that both Japan and Australia, having already established strong users societies, would take an initiative in progressing the process toward its formation in a few years.

In order to pursue carefully the future of neutron sources, it is important to update the current status of existing and planned neutron sources all over the world. The Commission is now preparing for a compilation 'Catalogue of Neutron Sources', which collects specifications of source and instruments as well as user's programs for nearly 100 sources. However, this project will be carried over to the next triennium for completion.

The Commission on Neutron Scattering has been expected to play a more important role not only for promoting purely academic research/education but also for taking an initiative in global scientific programmes to widen the IUCr's contribution.

Y. Fujii, Chair

4.13. Commission on Powder Diffraction

The Commission carried out an ambitious programme, rich in events and projects. Most tasks were successfully concluded and new initiatives announced for the coming years. Important developments concern the Commission on Powder Diffraction (CPD) *Newsletter*. During the triennium, the mailing list expanded from about 1,300 in 1999 to over 2,000 today. Many more people freely download the electronic versions of the *Newsletter* from the CPD web site, so the actual number of readers is certainly larger than the current mailing list. The mailing list has expanded from just over 800 to 1,346, indicating strong and expanding worldwide interest. The *Newsletter* has become almost self-funding from advertising revenue, thus allowing the achievement of a high standard for graphical quality and extension, in addition to the increasing interest in the scientific themes discussed in each issue.

The CPD supported IUCr decisions concerning sponsorships and, in particular, the CPD recommended support for several workshops and schools to encourage world wide teaching of powder methods.

An important initiative supported by the CPD was the establishment of an ECA Special Interest Group (SIG) based on the Scientific Committee of the European Powder Diffraction Conference (EPDIC). This initiative improved connections between the powder diffraction (PD) community and the IUCr, especially concerning conference organization and decisions on event dates.

The CPD had a high profile in promoting a wide variety of workshops, tutorials and schools.

The Commission had an ambitious programme of events and projects during the triennium. The Commission has recommended support for a large number of workshops and schools to encourage worldwide teaching of powder methods. It has recommended that the powder community be re-integrated with the body of the crystallographic community for the Glasgow Congress. It was felt that the subject had made such progress in the last decade that it was now appropriate that this achievement be recognized by the mainstream crystallographic community. Led by Commission member L. B. McCusker on the Glasgow Programme Committee, the whole Commission has worked very hard on the programme for Glasgow. A major point of emphasis here was the collaboration with other Commissions. This has been especially successful with the Commissions on Electron Diffraction, XAFS, Small-Angle Scattering and Synchrotron Radiation (*via* a satellite meeting). The result has been an unprecedented expansion in the microsymposia dedicated to materials science and powder methods. The establishment of the ECA and associated Special Interest Groups (SIGs) has raised interesting new ways of interacting with the European powder community. A committee has been formed to represent the EPDIC series of meetings. At least four Commission members, including the Chair, now sit on that committee to ensure maximum co-operation and dialogue between EPDIC and the Commission.

4.13.1. Meetings/workshops/schools. The main event of 1999 was the Glasgow Congress, a real success in terms of attendance and scientific quality. The programme was exceptional for PD, with at least 16 microsymposia (MS) concerning PD and many others on related subjects. The CPD, led by L. B. McCusker (on the Glasgow Programme Committee) and the former Chair R. J. Cernik, sponsored and organized the following MS: 30 years of Rietveld Refinement; Optimization Methods; Challenging Rietveld Refinements; Industrial On-line Analysis; *In Situ* Studies using PD; Thick Coatings; Line Broadening; Non-structural Aspects of Rietveld Refinement; Microporous Materials; Structure Solution from Powder Data; Molecular Compounds; Structure Solution from Inorganic Materials;

Combined PD, XAFS and DAFS; Combination of Electron and Powder Diffraction; and *Ab Initio* Structure Prediction.

Other meetings of interest for the CPD chiefly include the European Powder Diffraction Conference series. Started in Munich, Germany, in 1991, EPDIC has now reached the 8th in the series. During the triennium, the conference took place in Barcelona, Spain (May 2000, Chair J. Rius) and in Uppsala, Sweden (May 2002, Chair R. Tellgren). Following the tradition of the previous successful meetings, the programme included the most relevant topics of PD in crystallography, materials science and technological applications: structure solution and refinement from powder data; quantitative phase analysis (QPA); *in situ* kinetics and non-ambient studies; nanocrystalline materials and catalysts; disordered structures; instrumental developments; line profile analysis for the study of domain size and lattice distortion effects (size–strain); accuracy and standards; phase identification (search–match); thin films and coatings; residual stress and texture analysis; and general materials. After the establishment of the EPDIC committee ECA SIG, the CPD takes part in the planning activity for the EPDIC conference, also through the CPD Chair (*ex officio* member).

As a further involvement in conference programmes and organization, CPD members took part in the European Crystallography Meeting (ECM-19) in Nancy, France, in 2000 (two PD-dedicated sessions). Moreover, the CPD gave ample logistic support to the organization of Accuracy in Powder Diffraction III (APD3), held in Gaithersburg, Maryland, USA, in April 2001, and to the third Size–Strain Conference (SS-III), held in Trento, Italy, in December 2001. APD is a historical conference in the PD field. Started in the late 1970s, it was repeated after nearly ten years, always with considerable success. APD3 was also the site of the CPD meeting for 2001. Several CPD members were involved in the programmes of both events and/or participated as speakers and session Chairs. SS-III was the third conference of the Size–Strain series, initiated in 1995 at Liptosky Mikulas, Slovakia, and continued in Freiberg, Germany, in 1998. The conference was endorsed by the CPD and financially supported by the IUCr.

Several schools and workshops were given support and were endorsed by the CPD. These included a powder workshop organized by Shao Fan Lin at Kunming, People's Republic of China, in 1999, the International Workshop on the Rietveld Method (RW2000-PL), Wisla, Poland, 7–10 September 2000, and the Workshop on Powder Diffraction, Bayreuth, Germany, 4–8 October 2000. Finally, the CPD gave support to the II International School on Powder Diffraction, organized by S. Sen Gupta at the Indian Association for the Cultivation of Science (Jadavpur, Calcutta, India). The school was scheduled for 2001, but for political reasons was moved to January 2002.

4.13.2. Projects. *Rietveld guidelines*. The CPD project directed by L. B. McCusker was concluded in 1999, with the publication of a paper in *Journal of Applied Crystallography* [McCusker, Cox, Von Dreele, Louer & Scardi (1999). *J. Appl. Cryst*. **32**, 36–50] that contains advice and guidelines for Rietveld refinement. A large number of reprints were purchased by the Commission and distributed together with the spring 1999 *Newsletter* (No. 21) to over 1,400 scientists.

Quantitative phase analysis. The project started in 1997 and was carried out by several scientists coordinated by I. C. Madsen. Briefly, four samples of carefully constituted multiple composition were distributed to those people who volunteered for the study. There was an excellent response to the original request for participants, with distribution of 140 questionnaires. The samples were: (1) corundum + zincite + fluorite; (2) as (1) but with preferred orientation and brucite; (3) as (1) but with amorphous glass; and (4) corundum + magnetite + zircon. During 2001, the results obtained during the previous years were published by I. C. Madsen and co-workers in an important publication entitled *Outcomes of the International Union of Crystallography Commission on Powder Diffraction Round Robin on Quantitative Phase Analysis: Samples 1a to 1h* [Madsen, Scarlett, Cranswick & Lwin (2001). *J. Appl. Cryst*. **34**, 409–426]. Free reprints were distributed as an annex to *Newsletter* No. 25. A special budget was allocated thanks to the generous contribution of the commercial sponsors advertising in the *Newsletter*. Copies of the article may also be freely downloaded from **Crystallography Journals Online** and are also available through the CPD web site. The activity continues with the preparation of a second part of the round robin results, accepted for publication in *Journal of Applied Crystallography*.

Round robin: size–strain analysis. This project was mostly carried out during the last two years. During 2001, the promoter, CPD member D. Balzar, produced a detailed report on the results, which should appear soon as a publication in an IUCr journal. All the data are still available *via* the internet for free download. Several scientists have studied the data sets provided by the round robin and the results are now appearing in various publications. Specific presentations were given at the last SS-III conference on this subject.

CPD Newsletters on CD-ROM. This project, started during 2001, should be completed by summer 2002 in order to be presented at the Geneva Congress. The goal is to transfer all CPD *Newsletters* from paper to electronic format (most probably as PDF files), to be distributed on CD-ROMs. Beyond the historical value as a rather peculiar perspective of PD development in the last twenty years, the CD-ROM collection can be a valuable support to many powder diffractionists. In fact, articles appearing in the CPD *Newsletters* (now officially registered as a periodical with ISSN) are increasingly cited in the PD literature.

Newsletters. There have been five *Newsletters* published in this period. They were edited by CPD members R. B. von Dreele, D. Balzar, W. I. F. David, R. E. Dinnebier, and by R. J Cernik and I. C. Madsen. Forthcoming (2002) issues will be edited by G. J. Kruger (No. 27, spring) and P. Scardi (No. 28, fall). One of these issues will include as an annex the second paper of the QPA round robin edited by I. C. Madsen and co-workers, and a final report on the size–strain round robin.

All editions are available on the CPD web site: http://www.iucr.ac.uk/iucr-top/comm/cpd/index.html. CPD *Newsletter* No. 22, (fall 1999), edited by R. B. von Dreele, was aimed at showing neutron diffraction developments in the field of PD. Starting with this issue, the structure of the *Newsletter* was established in a stable way, always including Chair communications, guest editor remarks, round robin activity reports, a group of contributed papers addressing a main topic (the core of the *Newsletter*), computer software pages (edited by L. M. D. Cranswick), and information on schools, workshops, congresses and other events. In addition, ICDD and, recently, IXAS, have been given a page to report the many activities and news of interest to the PD community.

The spring 2000 issue (No. 23) was edited by R. J. Cernik and I. C. Madsen and focused on synchrotron radiation PD and non-ambient techniques; it also contained an extended report on the first part of the round robin on quantitative phase analysis. The fall 2000 *Newsletter* (No. 24), edited by D. Balzar, addressed the study of materials' microstructure by PD, and reported several contributions on line profile analysis and full information on forthcoming events for 2001.

The ISSN first appeared on No. 23. For the official record, the ISSN is 1591-9552. The summer 2001 issue (No. 25) was edited by W. I. F. David and was entitled *Structure Determination from Powder Diffraction Data*, whereas the following fall issue (No. 26) was edited

by R. E. Dinnebier and focused on *Rietveld Refinement from Powder Diffraction Data*. These two issues can be considered as particularly important references for the state of the art in PD. *Newsletter* No. 25 included as an annex the paper on the QPA round robin.

The *Newsletter* has grown considerably during the past six years. The number of pages is now nearly a constant at 40 pages. The overall trend can be appreciated from Fig. 1.

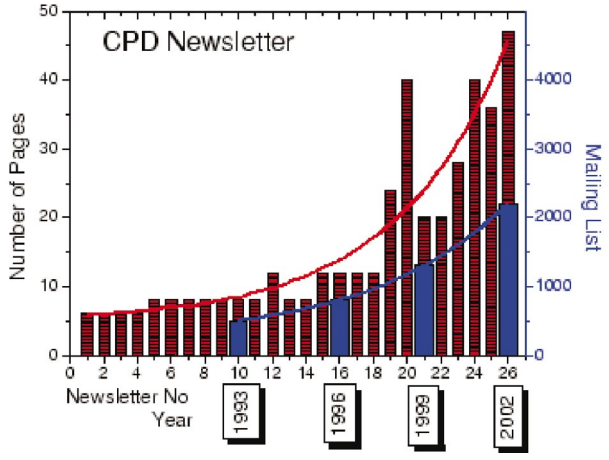

Figure 1
Number of pages in the CPD *Newsletter* and mailing list.

Software and the world wide web. The main interest in the CPD web site (http://www.iucr.org/iucr-top/comm/cpd/index.html) is in the opportunity of directly downloading the *Newsletter* (and annex publications), and in the round robin pages. The CPD web site has also been useful to direct interested parties to freely available software in powder diffraction. Links now exist to the CCP14 and program exchange banks. Further links on the CPD web site can easily lead the reader to all the most readily accessible crystallography sites in the world. Mirror sites have been set up in Australia and the USA.

IXAS. The CPD established a profitable collaboration with the recently constituted IXAS (International X-ray Analysis Society). The IXAS representative, R. L. Snyder, was invited to attend CPD meetings. The IXAS will provide useful support to the PD community, by publishing on the IXAS web site (http://www.ixas.org/) the Proceedings of several conferences related to applications of X-ray analytical methods. Concerning PD, of considerable interest is the availability of the Denver Conference Proceedings (formerly available through Plenum and ICDD) and the SS-III extended abstracts. Access to the IXAS web services is free, after submitting a request for registration.

P. Scardi, Chair

4.14. Commission on Small-Angle Scattering

The Commission's Annual Reports present the 'nuts and bolts' of the Commission's activities. This report will refer to some of those items, but it will mainly seek to provide an overview of the state of the Commission as it begins its third triennium of existence.

4.14.1. Meetings. The triennial Small-Angle Scattering (SAS) Congresses are perhaps the SAS community's most important single activity. The Commission needs to find effective means to promote the hosting of these Congresses and to assist organizers in establishing both sound technical content and a social environment that is conducive to strengthening ties between members of the community. The scheduling process that brings these Congresses into direct conflict with the IUCr Congresses is expected to be resolved so that community members will be able to support more effectively both the SAS Congresses and the IUCr Congresses.

The Commission should actively seek new interactions so that it can become more involved with meetings hosted by other organizations.

4.14.2. Education. As a unit of the IUCr, the Commission is obligated to support its parent body's activities in the diffusion of knowledge through meetings, educational activities, and publications. Three years ago, the Commission presented a session at the Glasgow Congress. In 2002, we expect to present two sessions and a tutorial workshop at the Geneva Congress.

Individual Commission members have contributed to various workshops and tutorials as described in our Annual Reports for the triennium.

4.14.3. Publication. Much credit is due to G. Kostorz for his concerted efforts to create a high-quality issue of *Journal of Applied Crystallography* out of the submissions from the SAS 99 Congress. This handsome volume of 868 pages is a credit to the community and especially to G. Kostorz, who gave it form and substance. We can hope that the Proceedings from the 2002 SAS Congress will be even better.

4.14.4. Technical issues. *Publication of errors*. The Commission needs to develop guidelines that reviewers of articles submitted to technical journals can use to determine whether uncertainties in the experimental data and in derived quantities are being properly reported.

Precision and accuracy of SAS measurements. Data from the Round Zero SAXS Round Robin should be studied and used to work out a better protocol for another round of testing. There are preliminary indications that a number of laboratories were not used to coping with the strongly scattering samples. They also did not appear to understand the sasCIF format well enough to employ it in reporting their results.

4.14.5. Software development. The Commission should seek to maintain well focused continued involvement with efforts like canSAS, NOBUGS and CCP13 in an effort to expand the availability of good software for analysing SAS data.

4.14.6. Community building. The existing SAS list server suffers from several problems. Traffic is sparse and there is little dialogue. The information presented consists mainly of meeting announcements and reminders. There are occasional pleas for help from scientists outside the main stream. The current 325 subscribers are only a small fraction of the community, although the base is very diverse.

The upcoming migration of the list from NIST to IUCr computers will provide a good opportunity to review the subscriber base and to seek better ways of generating new content. This move is driven by new NIST security procedures and a desire for an orderly succession when J. D. Barnes can no longer maintain the web site.

4.14.7. Prizes. There have been recent suggestions that appropriate prizes should be established to commemorate the work of pioneers in the SAS community. Because of the widespread impact and the sensitive nature of such prizes, these suggestions need to be developed further in appropriate open forums. Managing the processes for awarding prizes is certainly a valid role for the Commission, but broad community input is needed to establish criteria and funding mechanisms. This is a task for the Commission's next triennium.

4.14.8. Adding to the Commission's resource pool. The number of people who support the mission and processes of the Commission

needs to be increased significantly. The IUCr's guidelines mandate turnover in Commission membership, but this must be balanced against a strong need for 'institutional memory'. It is rare for a project to be completed in one three-year cycle and some projects require more than the eight or so participants that can be rounded up from the Commission on a good day.

The Commission therefore needs to broaden its base by adding more consultants, some of whom would be explicitly serving 'apprenticeships' in preparation for full membership.

4.14.9. Summary. The Commission's range of challenges and opportunities is very broad. The resources that individual active scientists have been able to devote to these challenges are very limited. The Commission should seek to increase its visibility and impact by focusing on the matter of organizing high-quality meetings and bellwether publications. The Commission also needs to promote closer collaboration with other IUCr Commissions whose interests overlap its own.

It has been an honour to work with this group of dedicated scientists throughout the formative period of the Commission. I look forward to continued interaction as others carry this very worthwhile cause forward.

J. D. Barnes, Chair

4.15. Commission on Structural Chemistry

The Commission met during the Glasgow Congress with both continuing and retiring members in attendance. Topics discussed at that meeting included a proposal put forth by J. D. Dunitz, R. E. Marsh and F. H. Herbstein that all journals require deposition of structure factors as well as coordinates for all published structures and that the information be stored electronically for easy retrieval. It was also suggested that structure factors from unpublished structures be collected as well. The reasoning behind the proposal was that such tables constitute the primary experimental information on which structural analyses are based and hence provide the only means of checking and extending their results. While all members of the Commission agreed in spirit with the proposal, it was felt that it would be an almost untenable task to collect and store all the structure-factor data. The issue was tabled pending further discussions with the Cambridge Crystallographic Data Centre (CCDC) and the IUCr editorial staff. Further discussions with the CCDC confirmed the opinion that this task, while scientifically valuable, would be daunting and most likely not economically feasible for them. This would be especially true if it was decided to attempt to collect structure factors for all compounds currently in the database. The IUCr, on the other hand, already has structure factors for the thousands of compounds published in *Acta Crystallographica* and they would be interested in recovering machine-readable files for older structures from authors' own archives. They suggest that scanning old hard-copy deposits is not practical, as the resultant files are essentially useless for generating machine-readable copy. They do find that harvesting of current files is very useful and feel that efforts should be made to encourage other journals and/or databases to archive them. It would appear from these follow-on discussions that archiving structure factors should remain on the Commission's agenda for the next triennium.

A continuing topic of interest to this Commission is how to reach out to colleagues in countries with small numbers of crystallographers and include them in our activities. Ways of using the *IUCr Newsletter* to help accomplish this have been discussed with the Editor, W. L. Duax. We feel that the Commission should act as a clearing house and conduit of information between the structural chemistry Special Interest Groups of the various IUCr Regional Associates and discussed the possibility of using the Commission web site and/or setting up a list server for exchange of ideas and information. As a follow-on to these discussions, a structural chemistry discussion group has been set up on the IUCr web site for the purposes of exchanging ideas and information within the community. The discussion group was established on an 'open' basis so that membership is not limited solely to members of the Commission. There has yet to be a large amount of 'discussion' among the members of the group and the Commission is exploring ways to make its existence more well known.

The Commission endorsed the NATO meeting on Data Mining organized by S. Fortier held in Erice, Italy, in May 1999. It also endorsed Indaba III 'Symmetry Breaking, Chirality and Disorder in Molecules and Crystals'. This very successful symposium was held in August 2000 in Skukuza, South Africa. Commission member D. Levendis served as Chair of the Organizing Committee and two Commission members, J. L. Flippen-Anderson and G. R. Desiraju, were among the invited speakers. J. L. Flippen-Anderson also served on the Programme Committee. Commission member V. Belsky was the Programme Chair for the second Russian National Conference on Crystal Chemistry that was held in May 2000 in Chernogolovka, near Moscow, Russia. There were about 300 posters and oral presentations divided into seven sections – organic, inorganic and coordination crystal chemistry, structure–properties correlation, chemical bonding, solid-state reactions, and dynamic crystal chemistry.

In 2000, the Commission endorsed three microsymposia to be held in 2001. The first was a Symposium on Organic Crystal Chemistry that was held in Poznan-Rydzyna, Poland, immediately preceding the ECM meeting in Krakow, Poland, in August 2001. The leading subject of the symposium was 'Weak Interactions in Crystals and their Implications'. The symposium was organized by T. Borowiak (Poland) and two Commission members, V. Belsky and J. L. Flippen-Anderson, were invited speakers. The second symposium endorsed by the Commission was entitled 'Horizons in Hydrogen Bond Research' and held in Torino, Italy, in September 2001, immediately following the ECM meeting in Krakow. A wide variety of topics relating to hydrogen bonding were discussed from both crystallographic and quantum-mechanical perspectives. Former Commission member G. Gilli (Italy) was one of the organizers of this symposium. Thirdly, the Commission endorsed 'Crystallography in Drug Design', which was held in Lodz, Poland, following the ECM meeting. The speakers at this symposium were mainly crystallographers. The audience, however, was heavily weighted towards medicinal chemists and pharmacologists so that researchers in these areas could become acquainted with crystallography and begin to understand the critical role it plays in the field of drug design. The Commission feels strongly that this sort of interdisciplinary interaction should be well supported.

Other activities involving members of the Commission in 2000 included reviewing the Notes for Authors for *Acta Crystallographica* Section E, serving as alpha and beta testers for the new ConQuest search engine for the Cambridge Structural Database, and keeping the Commission web site up-to-date.

2001 was a busy year for the Commission. Most Commission activities centred on assisting in programme preparations for the Geneva Congress. The Commission collected suggestions for microsymposia topics, potential session organizers and plenary lectures that were then submitted to the Programme Chair for consideration. The Commission Chair (J. L. Flippen-Anderson) served as a member of the International Programme Committee. In addition, two Commission members (G. Punte and L. Brammer) chaired the

organization of microsymposia and four others (V. Belsky, J. L. Flippen-Anderson, T. W. Hambley and D. Levendis) served as Co-Chairs for microsymposia. As a result of the Commission's input and involvement, there will be a very strong structural chemistry presence in Geneva. Overall there will be more than 20 microsymposia and a number of plenary lectures on topics related to structural chemistry, including such diverse topics as small-molecule drug design, nanomaterials, coordination chemistry, twins, disorders, solid-state reactions, zeolites, crystal growth, recent advances in supramolecular chemistry, molecular recognition and enantioselectivity, self-organization and self-assembly of biomaterials and biomimetics.

The Commission endorsed the XII International Symposium on Supramolecular Chemistry to be held in Eilat, Israel, in October 2002. This symposium will be organized by I. Goldberg and the scientific programme will include a wide variety of basic as well as applied topics in chemistry and materials science, such as nanostructures, chemistry at interfaces, self-assembly, crystal engineering, porous solids, molecular devices, supramolecular catalysis, polymers, dendrimers and biomaterials.

The Cambridge Structural Database passed 250,000 entries in 2001 and the rate of new entries continues to grow at a rapid pace. The Commission encouraged the CCDC to make incremental updates to the database available to be downloaded over the internet to registered users. This process went into beta test late in 2001 and will become available to all users with the April 2002 release of the database. As the database continues to grow at an ever-increasing rate, it becomes more and more important for coordinates to be 'automatically' deposited by the journals. Discussions were held with CCDC personnel on ways the Commission members might help convince more journals to send CIF files directly to the CCDC when papers containing X-ray structures are accepted for publication. The Commission also initiated a discussion on adding more terms to the small-molecule CIF dictionary to describe twinning and disorder so that information on these facets of a structure analysis could be easily captured by the database in a way that would facilitate searching. A number of issues addressed during this triennium, such as expansion of the CIF dictionary, automatic deposition of coordinates and structure factors by the journals, and expanding interactions between members of the structural chemistry community, are topics that will remain on the Commission's agenda as it moves forward into 2002.

J. L. Flippen-Anderson, Chair

4.16. Commission on Synchrotron Radiation

The Commission has been active in participating in the organization of various synchrotron-related conferences in connection with the upcoming Geneva Congress and other meetings. In particular, it is involved in the organization of the following two satellite meetings:

(1) Crystal Chemistry of Materials and Soft Matter Studied by Neutron Diffraction, 1–3 August 2002, at the ESRF–ILL site in Grenoble, France. This is a joint Neutron/Synchrotron Radiation Commission activity and the joint Commissions constitute the Programme Committee.

(2) Neutron and Synchrotron X-ray Scattering in Condensed Matter Research, 4–6 August 2002, to be held at the Paul Scherrer Institute, Villigen, Switzerland. C. Vettier is representing the Commission on the International Advisory Committee for this meeting and has also been heavily involved in the work of the Programme Committee for the Congress.

In addition, S. W. Wilkins was a member of the Programme Committee for the Third International Conference on Synchrotron Radiation in Materials Science (SRMS-3) held in Singapore, 21–24 January 2002. This meeting helped celebrate the recent commencement of operation of the Singapore Synchrotron Light Source (SSLS).

In the area of support for the establishment of new national synchrotron facilities, S. W. Wilkins has been actively involved in the establishment of the Australian Synchrotron Project. Funding of AUD 157M for this project was announced by the Victorian State Government in June 2001 and will be a national facility. The facility is to be located at Clayton adjacent to Monash University and a number of CSIRO Divisions. The design, yet to be finalized, will be for a third-generation 3 GeV ring with emittance of around 10 nm rad. Support and influence of the Commission has been helpful in getting this project established.

S. W. Wilkins, Chair

4.17. Commission on XAFS

No report was received from the Chair.

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

In the triennium 1999–2001, the Committee on Electronic Publishing, Dissemination and Storage of Information (CEP) constituted a small and very active working group. Following the unanimous proposition of the CEP, the IUCr's Executive Committee appointed S. Parsons, University of Edinburgh, UK, to the CEP on 9 May 2001. S. Parsons has accepted the responsibility of the day-to-day running of **Crystallography Online**, the IUCr's information service.

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

H. D. Flack visited the IUCr editorial office in Chester, UK, in November 1999, November 2000 and November 2001.

Y. Epelboin attended the ICSTI/ICSU Press interactive workshop on Digital Archiving: Bringing Issues and Stakeholders Together, Paris, France, 30–31 January 2000. H. D. Flack also attended as ICSTI representative.

B. McMahon and P. R. Strickland attended the annual ICSTI meeting and visited Chemical Abstracts Service (CAS) in Columbus, Ohio, USA, in May 2000. H. D. Flack also attended as ICSTI representative.

Y. Epelboin, H. D. Flack, B. McMahon and P. R. Strickland attended the UNESCO/ICSU Press Conference on Electronic Publishing in Science held at UNESCO, Paris, France, 20–23 February 2001. J. R. Helliwell also attended.

S. Parsons visited the IUCr editorial office in Chester, UK, in May 2001.

P. R. Strickland attended the presentation of the Ingenta study 'Research into the Relationship between Journal Subscriptions and Document Delivery and the Impact of Online Delivery on Article Distribution', London, UK, 25 September 2001.

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. Crystallography Journals Online

Until mid-March 1999, the IUCr editorial office continued the project with Munksgaard to provide an online version of *Acta Crystallographica* Section D on the Synergy server operated by Healthgate. As a consequence of these trials, it was decided to develop an entirely in-house system, which was successfully launched

for all six journals at the Glasgow Congress in August 1999. The development of this system was achieved in about three months, largely because of the substantial infrastructure already in place at the Chester office, and as a result of the systematic and thoughtful development of the computer-based workflow built on top of previous investment in equipment and personnel. Subsequently, an e-mail alerting service was put into operation and *Acta Crystallographica* Section C is now being prepared in SGML. From 1 September 2000, online access was limited to subscribers of the print journals. The IUCr has become a member of CrossRef enabling article cross referencing between journals of different publishers to be implemented. Individual online article sale was brought into service during 2000. During 2000, a policy document concerning the archiving of IUCr journals was drafted and after presentation and discussion by all the interested parties was approved by the Executive Committee on 18 July 2001. The participation of H. D. Flack and B. McMahon in an ICSTI review of the Open Archival Information System (OAIS) enabled both improvements in the archiving policy document during the discussion stage and improved understanding of the modelization and conceptualization of archiving and preservation. For the Glasgow Congress, experience had been gained in the scanning of documents for the preparation of a CD-ROM containing the Congress abstracts and other material. The Executive Committee approved the project to scan the back numbers of all IUCr journals. This project continued throughout the triennium and in November 2001 all back numbers were made available online to subscribers six weeks ahead of schedule. The CEP has also given attention to ways of improving the sales of IUCr journals to consortia of libraries. The IUCr's participation in an Ingenta study and developments in the field of crystalline phase descriptors are treated in the report of the representative to ICSTI. Attention has also been given, in collaboration with the Editor-in-Chief of the IUCr journals, to the questions concerning preprints and final publications, the acceptability of preprint manuscripts for journal publication, peer review (its operation and confidentiality), and the usefulness of a preprint service for crystallography. There appears to be only very modest interest in the establishment of a preprint server for crystallography.

5.2. Crystallography Online

The CEP holds the editorial powers for IUCr web services. Within the triennium, their information content has been regularly updated and this task is still perceived as being of high priority worthy of investment in time and resources. The rebranding and restructuring of the site, as a preliminary for the restyling of the existing pages, has been completed to be in tune with **Crystallography Journals Online**. The style and structure of **Crystallography Online** emphasizes the different aspects of crystallography and projects of the community rather than the IUCr as an institution. In May 2001, the task of day-to-day maintenance of **Crystallography Online** passed from H. D. Flack to S. Parsons. As part of the changeover, a set of detailed maintenance instructions was prepared for the incoming editor. The changeover proceeded very smoothly indeed. Some preparatory work and discussions on the restyling of **Crystallography Online** have taken place. As part of this activity, consideration has been given to the status and future role of the **Crystallography Online** mirror sites. A questionnaire was subsequently sent to those responsible for maintaining the mirror sites to obtain information and solicit opinion on matters such as advertising, perceived necessity of continuing with mirrors, and infrastructure at mirror sites. During the triennium, more efficient software for mirror-site updating was installed. As part of **Crystallography Online**, discussion forums are provided by means of list server software, but these are only very lightly used.

5.3. *World Directory of Crystallographers* (WDC)

A functional specification for a new implementation of WDC as a relational database using technology parallel to, but not directly integrated into, the IUCr editorial-office production database was completed. Owing to a heavy workload on the R&D staff in Chester, it was not possible to proceed to a working implementation immediately. The new online interface of WDC 11 was launched in mid-December 2001 leading to a temporary overload on the server, which was successfully reconfigured. The effort of the regional editors in verifying new entries is gratefully acknowledged. At present there is still a steady stream of new entries and over 5,000 people have logged in or created new entries. A printed version of the directory is planned to be produced in late 2002.

5.4. NeXus CD-ROM

Under the continued leadership of L. M. D. Cranswick, larger scale productions of the 'Xtal NeXus: Virtual Crystallographic Internet on CD-ROM' have been undertaken. These CD-ROMs are distributed free of charge to laboratories and scientists with an interest in crystallography but lacking adequate connection to the internet. The CD-ROMs contain public domain software and copies of web sites of interest to crystallographers. In both 2000 and 2001, 1,000 copies of the NeXus CD-ROM were produced and distributed through established distribution channels. Previously, these CD-ROMs had been produced on a one-by-one basis on request. In 2000, we received funding for this project from ICSU but this support was terminated owing to a major change in ICSU policy. The CEP wishes to thank the IUCr's Executive Committee for having provided all the finance for the NeXus CD-ROMs in 2001. The CEP intends to continue with the NeXus project in the coming triennium.

5.5. The future

It is evident that, over the past years in the field of electronic publishing, the IUCr has put a considerable effort into its journals and into its online news service provided by **Crystallography Online**. It would seem that the moment has come when thought and effort should be directed towards other aspects of the IUCr's publishing and information dissemination activities. Opportunities exist in the use of multimedia techniques that have been insufficiently exploited until now. The perenniality and adaptability of software is also another area of concern. It is also essential to continue to stay abreast of developments and opportunities in the preservation of digital information.

The CEP has hence a continuing role to play within the IUCr. All of its current members are prepared to continue to excercise their best efforts if this is required. 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. Purpose and membership

COMCIFS is the Committee appointed by the Executive Committee of the IUCr to oversee the Crystallographic Information File (CIF) project on behalf of the Union. It currently consists of six

voting members appointed by the Executive Committee of the IUCr and an unlimited number of non-voting members added at the discretion of the Chair. The non-voting members comprise those with an interest in the development of CIF who request to be placed on the COMCIFS list server. Both kinds of members are fully involved in the work of COMCIFS, but only voting members approve CIF policies and dictionaries. The voting membership during the current triennium comprises: I. D. Brown (Chair), B. McMahon (Secretary), H. M. Berman, H. J. Bernstein, S. R. Hall and G. Madariaga. P. Edgington was appointed to COMCIFS in 1999 but resigned during the course of the triennium.

6.2. Overview

It is now over a decade since *Acta Crystallographica* adopted the Crystallographic Information File (CIF) for the submission and archiving of crystal structures. When first adopted, CIF was intended as a medium for authors to submit structure reports electronically to the journals and, after publication, for the coordinates to be available to a user's program. Since then, CIF has evolved from a simple transfer and archiving format into a crystallographic language equipped with a dictionary that can be interpreted by computer. In the not too distant future, computer software will acquire its crystallographic knowledge from these dictionaries rather than have it hard-coded into the programs. A computer will transparently combine the knowledge in the CIF dictionaries with the numerical information in the crystallographic databases to generate answers to a user's queries. Two elements are needed to bring this vision to reality. The first is a set of dictionaries that capture the breadth of crystallographic knowledge and the second is a set of programs that can bring together the knowledge contained in the dictionaries with the structural information contained in the databases. No other discipline has such a comprehensive set of dictionaries, but we currently lack the software to exploit the potential that these dictionaries offer.

6.3. Dictionary definition languages

The names and properties of items that can appear in a CIF are defined in dictionaries that are themselves structured using the same STAR syntax as CIF. The Dictionary Definition Language (DDL) defines the names and properties of items that can appear in a dictionary. The approved CIF dictionaries are written in one of two versions of the DDL. DDL2, being more structured and less forgiving than DDL1, was designed to meet the requirements of the structural biology community where highly automated procedures are needed to handle the rapid increase in experimental information. These in turn require a highly structured dictionary.

Currently under development is a new dictionary language that will both simplify and extend the capabilities of CIF and should, in the longer term, remove the incompatibilities between existing dictionaries. It will include computer-readable definitions (algorithms) that will tell an application how to derive any item of crystallographic information from the basic experimental results contained in a CIF. When fully functional, this will revolutionize crystallographic computing since a single program will be able to calculate any item of crystallographic interest providing a dictionary definition exists. It will no longer be necessary to write crystallographic program code, testing a new algorithm will be as simple as adding a new definition to the dictionary.

6.4. CIF dictionaries

The strength of CIF lies in the extensive suite of dictionaries that COMCIFS has developed. Six dictionaries have now been approved and advanced drafts of three more are being tested in their communities.

The **Core CIF Dictionary** is used to describe crystal structures with small unit cells. Minor additions to the core dictionary were approved in March 1999 and January 2001 (version 2.2) but a major review of this dictionary is planned for the coming year in order to address the problems raised following a review of the archives held by *Acta Crystallographica* and the Cambridge Crystallographic Data Centre.

The **Powder Diffraction CIF Dictionary** is now routinely used for the submission of Rietveld refined structures to *Acta Crystallographica*. CIFs containing the powder patterns of these structures are forwarded to the International Centre for Diffraction Data for inclusion in the Powder Diffraction File.

The **Macromolecular CIF Dictionary** is being used for the archive of the Protein Data Bank (PDB) and software has been developed for manipulating these CIFs, but it will be some time before all the current macromolecular software is converted from the now obsolescent PDB format. Version 2.0 of the dictionary was approved in September 2000.

The **Image CIF/CBF Dictionary** is designed for the transmission and archiving of images, specifically from area detectors. Because these images can be very large, a Crystallographic Binary File (CBF) has been defined to provide a binary representation of an imageCIF. Version 1.0 of this dictionary was approved in January 2001.

The **Modulated Structure CIF Dictionary** will be used for the submission of incommensurate and modulated structure reports to *Acta Crystallographica*. Version 1.0 was approved in July 2001.

The **Symmetry CIF Dictionary** provides a structured description of crystallographic symmetry that will replace the symmetry items defined in the current core dictionary. The addition of advanced symmetry concepts is planned. Version 1.0 was approved in December 2001.

The **Electron Density Dictionary** will be used for reporting electron densities. A draft endorsed by the IUCr Commission on Charge, Spin and Momentum Densities has been circulated to members of the Commission for final evaluation before being presented to COMCIFS for approval.

The **Small-Angle Scattering Dictionary** is sponsored by the IUCr Commission on Small-Angle Scattering and a draft is in trial use prior to being presented to COMCIFS for approval.

The **Magnetic Structures Dictionary** is being prepared by the Database of Magnetic Structures Determined by Neutron Diffraction in Krakow, Poland. It should soon be presented to COMCIFS for approval.

After approval by COMCIFS, each dictionary is provided with a Dictionary Maintenance Group appointed from people within the discipline. It monitors the use of the dictionary and proposes revisions for COMCIFS approval. Requests for additions or changes to any of the dictionaries should be addressed to the appropriate dictionary maintenance group.

6.5. Software

CIF is a powerful crystallographic language with a well developed vocabulary, but such a language is of little use without the software to manipulate it. Many existing crystallographic programs have been modified to read and write CIFs, but so far few programs exploit CIF's full potential, namely the ability to extract their knowledge of crystallography directly from the dictionaries. While the writing of

such programs is essential to the future of crystallography, it is not yet considered a priority for those responsible for distributing crystallographic resources.

Among the programs that have been written are a generic CIF editor (one that obtains its crystallographic knowledge from the CIF dictionary) prepared by the Protein Data Bank for DDL2 dictionaries. A CIF editor for the core dictionary is soon to be released by the Cambridge Crystallographic Data Centre, and a number of CIF toolkits are available to help programmers interface their applications to CIF. A software list server on the IUCr web site encourages software developers to share their ideas and problems.

A possible short-term solution to the shortage of software is to interface CIF to XML (eXtensible Markup Language), a similar standard developed by the information technology community. Both CIF and XML store knowledge about a discipline in dictionaries (called DTDs in XML). CIF is further advanced in terms of its knowledge base (dictionaries) though XML currently has a wider range of software tools. A CIF to XML conversion program has been written.

6.6. Publicity

Because of the rapid pace at which information technology is advancing, and the expected benefits of CIF to the crystallographic community, education is an important aspect of COMCIFS work. All CIF dictionaries and COMCIFS discussions can be inspected on the IUCr web site and reports on the development of CIF appear in the *IUCr Newsletter*, but more work is needed to prepare the community for the changes ahead.

6.7. Interoperability

The rise of the World Wide Web and other Internet protocols has fuelled new developments in information interchange and it is important that CIF collaborate in these endeavours, particularly with neighbouring disciplines. Such initiatives include the Chemical Markup Language (CML – a DTD for describing chemical structures within SGML or XML documents), macromolecular structure descriptions in terms of the Common Object Request Broker Architecture (CORBA) objects and Resource Description Framework (RDF) schemas. Several other disciplines working with macromolecules are developing STAR DDL2 dictionaries that can be merged directly with CIF dictionaries, allowing CIF software to access information in related fields.

6.8. Intellectual property

Ownership of CIF is vested in the IUCr in order to prevent the development of incompatible CIF dialects. However, because the IUCr wishes to see the standard widely used without implied threats of legal action for software that inadvertently fails to follow the standard, COMCIFS is exploring friendly ways to ensure that the CIF standard is understood by its users and that archived CIFs properly conform to the standard.

6.9. Achieving the vision

The rapid development of CIF requires vigilance on several different fronts. The technical development of the standard is well advanced, and the dictionaries that support it are unequalled in their coverage, but software that can make use of the advanced features of CIF has not developed at the same rate. While the crystallographic community has accepted CIF as a convenient medium for the exchange of crystallographic information, it remains largely unaware how CIF will fundamentally alter the way in which we manage information and computing in crystallography. These are problems that we will try to address in the coming triennium.

6.10. Acknowledgements

It is a pleasure to extend thanks to the many people who have volunteered so much of their time and expertise to the work of COMCIFS. Particular thanks are extended to the IUCr staff in Chester for their unstinting support.

I. D. Brown, Chair

7. Appendix G: Committee on Crystallographic Databases

The IUCr Committee on Crystallographic Databases (CCD) has continued to provide a forum for discussion and information transfer between the major crystallographic databases. Information relating to the Committee, including current membership and links to crystallographic information sources, is now available *via* the IUCr web pages (http://www.iucr.org/).

Major issues arising during the triennium include:

(1) Consolidation of the Protein Data Bank (PDB) under the management of the Research Collaboratory for Structural Biology, with centres at Rutgers University, San Diego Supercomputer Centre and NIST, Washington, USA. H. D. Berman is Director of the RCSB–PDB.

(2) The release of new database access (ConQuest) and visualization (Mercury) software within the Cambridge Structural Database (CSD) System. The 250,000th structure was archived with the CSD in October 2001.

(3) The metals and alloys data file (CRYSTMET) was brought fully up to date in 1999, and Toth Inc. now offers search and visualization software that will also operate on data from the Inorganic Crystal Structure Database (ICSD).

(4) H. Behrens has retired as Head of the ICSD and is succeeded by P. Luksch. The ICSD continues to collaborate with NIST and new Windows-based software is due to be released.

(5) R. Jenkins has retired as Executive Director of the International Centre for Diffraction Data and is succeeded by T. Fawcett. ICDD has released its powder files (PDF-4) in relational format, and is collaborating with the Cambridge Crystallographic Data Centre to generate a database of calculated powder patterns from CSD contents.

During 2001 and 2002, the Committee has worked together to generate a Special Issue of *Acta Crystallographica* Sections B and D on Crystallographic Databases. The issue will be available at the Geneva Congress, and contains 18 papers covering database information content, access software and reviews of the research applications of the various systems. At the time of writing, the structural databases now contain data for more than 410,000 crystal structures, with the greatest rate of increase being seen in the PDB.

F. H. Allen, Chair

8. Appendix H: Promotion Committee

The triennium witnessed two major milestones for the IUCr journals: the launch of *Acta Crystallographica* Section E: *Structure Reports Online* in January 2001 (and its subsequent selection for inclusion in the ISI Web of Science®) and the completion of the back-issue digitization project later the same year. The Promotion Committee's Journals Working Group, enthusiastically and effectively chaired by

J. R. Helliwell, has been instrumental in publicising these events throughout the crystallographic community through the journals themselves, the *IUCr Newsletter* and the IUCr web site, promotional leaflets and exhibition posters, e-mail announcements, direct mail and press releases. The digitization of all back issues to 1948 has opened up the exciting prospect of 'themed CD-ROMs'; the Promotion Committee considered a long list of suggestions at ECM-20, and the first of these collections will be available at the Geneva Congress.

The full-colour IUCr Journals brochure is now a regular feature of the promotional campaign and has led to the publication of journal-specific leaflets, the first being for *Acta Crystallographica* Section D (in conjunction with *International Tables for Crystallography* Volume F) with a second in progress at the end of 2001 for the *Journal of Applied Crystallography*. Journal article reviews continue in a regular slot in the *IUCr Newsletter*, which also features an occasional 'journals bulletin' to promote specific issues, such as the Journal Grants Fund.

These three years also saw the publication of the second edition of *International Tables for Crystallography* Volume B and the first edition of *International Tables for Crystallography* Volume F, and work began on inviting non-IUCr journals to review these books. As a new publication, Volume F was extensively advertised in *Acta Crystallographica* Section D and the *IUCr Newsletter*, and promoted to the structural biology community through the above-mentioned leaflet. An *International Tables* order form downloadable from the IUCr web site has proved effective.

With a new edition of the *World Directory of Crystallographers* due to appear in 2002, entry-update notices have been published in the *IUCr Newsletter*. Mailing lists derived from the *World Directory* are a source of income for the IUCr, and new interest categories will allow purchasers to identify targets more specifically.

The IUCr's extensive range of publications and online services were exhibited at the major crystallographic meetings and at other meetings outside the community, and its profile was raised further by the presentation of prizes for posters that best promoted the understanding of crystallography. The Committee met annually and, in 2000, welcomed a new member, L. Nassimbeni of the University of Cape Town in South Africa.

A. M. Glazer, Chair

9. Appendix I: IUCr Newsletter

The *IUCr Newsletter* is a vehicle to broadcast and promote the interests and activities of the IUCr and its Commissions and Committees and to strengthen communication in the world community of crystallographers. An effort is made to promote meetings and publications sponsored by the IUCr. Highlights of the 12 issues published during the 1999–2001 triennium included extensive coverage of the Glasgow Congress, preliminary information concerning the Geneva Congress, cover stories on the 50th anniversary celebration of the IUCr held at the annual meetings of the three Regional Associates, the publication of *Crystallography Across the Sciences*, a collection of review articles based upon the 50th anniversary symposia, the development of **Crystallography Journals Online**, including the new all electronic *Acta Crystallographica* Section E: *Structure Reports Online*, and special issues on women in crystallography dedicated to Dorothy Hodgkin, on the role of crystallography in proteomics, and on the explosive growth of the Protein Data Bank.

Reports of 67 meetings on crystallographic topics in 27 countries were published:

Country	Number	Topics
Australia	1	Annual meeting (student views)
Belgium	2	General
Brazil	1	Materials
Cuba	1	Electronic materials
Egypt	1	Single crystal workshops
France	1	Annual meeting
India	7	General (three), Powder, Synchrotron, Weak interaction, Crystal and films
Israel	4	Chemical crystallography (Leiserowitz honoured),
Italy	5	Erice [Crystal engineering, Data mining, Crystal growth, Molecular biology (two)]
Japan	4	Annual meetings (three), Surface
Latvia	1	Chemical crystallography
Mexico	1	General
Moldova	1	Supramolecular chemistry
Morocco	1	Crystallography school
Poland	4	Drug design, Proteins, Crystal chemistry, Electron density (Sagamore)
Russia	1	Crystal chemistry
Serbia	1	General
Singapore	2	Crystal growth, Software
Slovenia, Croatia	3	Annual meetings (three)
South Africa	1	Symmetry and structure (Indaba)
Spain	3	Materials, Ferroelectrics, Crystal growth
Sweden	3	Electron diffraction, Aminoff prizes (Unwin and Henderson/Shecktman)
The Netherlands	1	Powder
Turkey	1	Materials
UK	5	General (two BCA, Birkbeck)
USA	10	General (two ACA, two Pittsburgh), Diffraction
Venezuela	1	Powder

Of these meetings, 21 were general in nature and covered a range of crystallographic topics. The 46 on specific topics concerned materials, powder diffraction, synchrotron applications, hydrogen bonding, chemical crystallography, electron diffraction, electron densities, crystal growth, engineering and chemistry, software, data collection, supramolecular structure, surfaces, strain, molecular biology and drug design. Announcements of future meetings throughout the world were published in every issue.

With the assistance of A. J. Sharpe (the IUCr Promotions Officer), summaries of selected papers from current IUCr journals became a regular feature in the *Newsletter*. 23 pages were devoted to summaries of 31 papers.

An effort is made to cover all areas of crystallography, both in the text and with the choice of cover illustrations. Cover illustrations in the 1999–2001 triennium included examples of small-molecule crystallography, macromolecular structures, polymorphism, electron densities and Geneva meeting sites. Some covers were composites combining small-molecule, materials and macromolecular applications to emphasize the broad range and remarkable power of crystallography. Sadly, obituaries of 24 prominent crystallographers were included in the issues of this triennium.

Each issue also contained a letter from the President, news of IUCr Commission activities, notices of elections, awards to crystallographers, and information on books, web sites, resources and activities of interest to crystallographers. Contributions from crystallographers everywhere are sought; material is gathered from newsletters of crystallographic associations and societies and from leading science news magazines. Reports were received from national crystallographic associations in Australia, Belgium, France, Germany, Israel, Japan, Mexico, Morocco, The Netherlands, Poland, Russia, Serbia, Switzerland, US, UK and Turkey. Photographs are provided by contributors or drawn from the personal collection of the Editor. Almost all submitted contributions are published and all material is edited to varying degrees.

The four issues of 1999 had 24 pages each. Since then, all issues have contained 32 pages. The inclusion of the 32 page Call for Papers

for the Geneva Congress resulted in a 52 page issue in 2001. This total of 372 pages is 60% greater than in the previous triennium during which only 11 issues with a total of 232 pages were printed.

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 rose from 12 in 1998 to 15.5 in 2001.

The staff of the editorial office in Buffalo, New York, is responsible for desktop preparation of all copy, all negotiations with the printer, postal authorities and distribution houses, correspondence with contributors, maintenance and production of the mailing list, and solicitation and handling of all advertising.

W. L. Duax, Editor

10. Appendix J: IUCr/Oxford University Press Book Series

Books by A. Authier (*Dynamical Theory of X-ray Diffraction*), I. D. Brown (*The Chemical Bond in Inorganic Chemistry*), J. Bernstein (*Polymorphism in Molecular Crystals*), W. Clegg, A. J. Blake, R. O. Gould and P. Main (*Crystal Structure Analysis*), W. I. F. David, K. Shankland, L. B. McCusker and Ch. Baerlocher (*Structure Determination from Powder Diffraction Data*) and C. Hammond (*The Basics of Crystallography and Diffraction*, Second Edition) were published in the reporting period. They all concern central topics in crystallographic science and are representative of the high professional standards adhered to in the IUCr/OUP Book Series.

Contacts with other potential authors are being maintained and are expected to lead to equally attractive titles in the coming triennium. Negotiations were pursued with several other authors, but were discontinued either because the material was already adequately covered in texts or because the topics were not considered compatible with the aims of the Series. Throughout, interaction with the Science Editor of OUP has been excellent.

P. Coppens, Chair

11. Appendix K: Sponsorship of meetings: Sub-committee on the Union Calendar

During the period since the last General Assembly, the Subcommittee has considered many requests for sponsorship and financial support by the IUCr and has made recommendations accordingly to the Executive Committee. The Executive Committee's policy, of giving financial support especially devoted to help young scientists, was successfully applied. An important aspect that must be guaranteed by the organizers of all meetings sponsored by the IUCr is the free circulation of *bona fide* scientists.

The following meetings on topics of crystallographic significance have received IUCr sponsorship, financial support for young scientists and, often, additional finance for general organizational expenses. The IUCr also provided substantial financial support to the Glasgow Congress and the Geneva Congress. The financial support given to assist young scientists totalled CHF 82,157 in 1999, CHF 112,200 in 2000 and CHF 127,092 in 2001. This support has helped several hundred young scientists attend a scientific meeting during the triennium.

Synchrotron Radiation, Daresbury, UK, 1–3 August 1999 (satellite meeting of Glasgow Congress)

Structural and Dynamical Aspects of Molecular and Ionic Solids Using Neutrons, Oxford, UK, 1–4 August 1999 (satellite meeting of Glasgow Congress)

Crystallographic Computing School, Cambridge, UK, 14–20 August 1999 (satellite meeting of Glasgow Congress)

Structural Characterisation of Amorphous and Nano Crystalline Materials, Suez Canal University, Egypt, 22–29 January 2000

Seventh European Powder Diffraction Conference, Barcelona, Spain, 20–23 May 2000

Crystallography of Molecular Biology (two meetings), Erice, Italy, 25 May–4 June 2000

Ninth Annual ACA Summer Course for Crystallographers, Athens, GA, USA, 7–19 July 2000

ACA Annual Meeting, St Paul, MN, USA, 22–27 July 2000

Eleventh International Conference on X-ray Absorption Fine Structure, Kyoto, Japan, 26–31 July 2000

Indaba 3, Skukuza, South Africa, 6–11 August 2000

Nineteenth European Crystallographic meeting (ECM-19), Nancy, France, 25–31 August 2000

Sagamore XIII, Jablonki, Poland, 3–9 September 2000

International Workshop on the Rietveld Method, Wisla, Poland, 7–10 September 2000

Workshop on Crystallography at High Pressure and High Temperature using X-rays and Neutrons, Hyogo, Japan, 30 September–3 October 2000

VII Workshop on Powder Diffraction: Structure Determination and Refinement from Powder Diffraction Data, Bayreuth, Germany, 4–8 October 2000

International Workshop on Preparation and Characterisation of Technologically Important Single Crystals, New Delhi, India, 26–28 February 2001

International School on Crystal Growth: Crystal Growth of Materials for Energy Production and Energy-Saving Applications, Trieste, Italy, 5–10 March 2001

BCA/CCG Eighth Intensive Course in X-ray Structure Analysis, Durham, UK, 30 March–6 April 2001

Accuracy in Powder Diffraction III, Gaithersburg, Maryland, USA, 22–25 April 2001

Strength from Weakness: Structural Consequences of Weak Interactions in Molecules, Supermolecules and Crystals, Erice, Italy, 23 May–3 June 2001

ACA Summer Course in Crystallography, Athens, Georgia, USA, 8–20 June 2001

Gordon Research Conference on Electron Distributions and Chemical Bonding, South Hadley, MA, USA, 8–13 July 2001

ACA Annual Meeting, Los Angeles, California, USA, 21–26 July 2001

11th International Summer School on Crystal Growth (ISSCG-11), Kyoto, Japan, 24–29 July 2001

11th Symposium on Organic Crystal Chemistry, Poznan, Poland, 20–24 August 2001

International Conference on Inelastic X-ray Scattering, Haikko, Finland, 22–26 August 2001

20th European Crystallographic Meeting (ECM-20), Krakow, Poland, 25–31 August 2001

Aperiodic Structures (satellite meeting of ECM-20), Krynica, Poland, 31 August–5 September 2001

Meeting on Crystallography and Drug Design, Lodz, Poland, 1–3 September 2001

XIV Conference on Horizons in Hydrogen Bond Research, Torino, Italy, 3–7 September 2001

International Workshop on Crystallography at High Pressures – 2001, Orsay, France, 4–8 September 2001

International Conference on Crystallogenesis and Mineralogy, St Petersburg, Russia, 17–21 September 2001

International School on Powder Diffraction, Jadavpur, Calcutta, India, 12–14 November 2001

International Symposium on Crystallography and Bioinformatics in Structural Biology, Bangalore, India, 22–25 November 2001

Size–Strain III, Analysis of Microstructure and Residual Stress by Diffraction Methods, Trento, Italy, 2–5 December 2001

School on Computer-Based Crystallographic Teaching Materials, Ismailia, Egypt, 20–23 January 2002

First Moroccan School of Crystallography, Marrakesh, Morocco, 29 January–1 February 2002

European Powder Diffraction Conference (EPDIC-8), Uppsala, Sweden, 23–26 May 2002

From Genes to Drugs *via* Crystallography, Erice, Italy, 23 May–2 June 2002

Organizers of meetings wishing to seek IUCr sponsorship should submit applications at least nine months in advance of the date of the meeting, writing to the Chair of the Sub-committee. The present Chair is H. Fuess. A new Chair will be appointed in Geneva.

12. Appendix L: Reports of Representatives on Regional and Scientific Associates

12.1. American Crystallographic Association (ACA)

The ACA held successful annual meetings, maintained its membership and provided its members with numerous services including four issues of the *ACA Newsletter* annually. The annual meetings are the principal function of the ACA.

The ACA annual meeting for 1999 was held in the spring to avoid conflict with the Glasgow Congress. Although attendance (709 scientific registrations) was lower than in recent years, the meeting in Buffalo was scientifically and financially successful. There were 400 abstracts and 30 oral sessions. Eight of the sessions were organized by the American Association for Crystal Growth. The A. L. Patterson Award was presented to G. Bricogne (MRC, Cambridge, UK) and the Elizabeth A. Wood Science Writing Award was presented to R. Weinberg (MIT) – author of *Racing to the Beginning of the Road: the Search for the Origin of Cancer* (1966). Student travel awards totalling USD 9,450 were presented to 24 participants.

The 50th anniversary meeting (2000) held in St Paul, Minnesota, was attended by 827 crystallographers including 16 past Presidents. The program of 440 abstracts, 30 oral sessions and three workshops was highlighted by two special sessions: The Transactions Symposium: Using Crystallography to Understand Enzyme Mechanism; and a session entitled Howard Hughes Medical Institute (HHMI) Contributions to Macromolecular Science.

ACA awards presented at the meeting included the Buerger Award to L. Jensen, the Warren Award to I. Robinson, ACA Service awards to *ACA Newsletter* Editors J. L. Flippen-Anderson and R. Stenkamp, and ACA's Public Service Award to P. Choppin, President Emeritus of the Howard Hughes Medical Institute. Memorial sessions were held for G. A. Jeffrey and P. Sigler. Student travel awards totalling USD 23,270 were presented to 44 participants, more than doubling the amount of support in 2000.

The ACA annual meeting for 2001 in Los Angeles, California, was attended by 931 crystallographers. The programme included 476 abstracts, 33 half-day oral sessions and 3 workshops. The workshops were on the topics of Interactive Single-Wavelength Anomalous-Scattering Methods, Real Space Pair Distribution Function Methods, Atomic Force Microscopy of Crystal Surfaces, and Neutron Diffraction. The Transactions Symposium was on High Throughput Crystallography. The Fankuchen Award was presented to J. Stewart, and an ACA Public Service Award was presented to J. Deschamps. A Memorial Session was held for H. Brumberger. Student Travel Awards totalled USD 23,900 and were presented to 55 participants.

Four volumes of the *ACA Transactions* were published during the triennium: Volume 32, Structural Informatics; Volume 33, Crystal Engineering; Volume 34, Two Decades of Synchrotron Radiation Research; and Volume 35, Using Crystallography to Understand Enzyme Mechanism.

The ACA contributed financial support annually to the ACA Summer School in Crystallography held in Athens, Georgia, and the Physics Olympiad. An effort to enhance participation by Central and South American crystallographers in ACA meetings and to support crystallography and crystallographers in Central and South America is a major topic of discussion in the ACA.

The ACA was accepted as a member of the American Association for the Advancement of Science (AAAS). The ACA By-Laws were changed by vote of the members. Beginning in 2001, there were three Committees of four members each: Continuing Education; Crystal Data; Standards and Computing; and Communications. The final total membership for 2000 was 1,860 (1,461 regular, 159 student, 211 retired and 29 corporate).

Scheduled future ACA meetings include San Antonio, Texas (25–30 May 2002), Cincinnati, Northern Kentucky (26–31 July 2003) and Chicago, Illinois (17–22 July 2004).

W. L. Duax, Representative

12.2. Asian Crystallographic Association (AsCA)

In 1999, the proposal to hold AsCA '01 in Bangalore, India, was endorsed. The Eighth Council Meeting of AsCA discussed a proposal to change item 3(a), Asian region, of the existing AsCA constitution and the new item was approved as follows: [Item 3(a): Membership shall be open to those countries and regions (which are hereafter referred to as 'countries') within the Asian region bounded by Japan, Korea, China, Pakistan, India, Australia and New Zealand and such other neighbouring countries as may be, from time to time, admitted by the Council].

Korea wished to be upgraded to the status of a Category II country in accordance with sections 4(a) and 5(a) of the constitution of the Association. The Council unanimously approved this proposal.

In 2000, the International Organizing Committee and Programme Committee for AsCA '01 were inaugurated (April). The Chairs of the Organizing and Programme Committees were appointed as Z. Rao (China) and C. Howard (Australia), respectively. The AsCA home page opened at http://neon.otago.ac.nz/chemistry/asca/2000/home.html. The *AsCA Newsletter* was published on this web site (October).

In 2001, the 4th AsCA Meeting was held at the Indian Institute of Science in Bangalore, India, 18–21 November. The IUCr President, H. Schenk, and the General Secretary and Treasurer, S. Larsen, kindly attended the meeting. A keynote lecture was given by H. Schenk, 4 plenary lectures and 10 microsymposia were held and 290 poster presentations were made. The participants from foreign countries were 151 from 18 countries: Australia, Bangladesh, China, Denmark, France, Germany, Hong Kong, Indonesia, Japan, Korea, New Zealand, Singapore, Sweden, Taiwan, Thailand, UK, USA and Vietnam. Among these, 37 were students. From the host country, India, there were 260 participants, including more than 100 students. Because of the events of 11 September, more than 50 participants from countries outside India cancelled their registrations. This also had an affect on the scientific programme as a number of scheduled speakers withdrew, requiring some alterations to the programme of

oral presentations. A satellite meeting on powder diffraction, which had been scheduled in Calcutta prior to AsCA'01, was also cancelled. The meeting on Crystallography and Bioinformatics in Structural Biology took place as scheduled in Bangalore following the main conference, with more than 370 registered participants.

The Council meeting was held in the afternoon of 19 November. Members from 11 of 17 countries attended the meeting. Although the final decision will be made at the ninth Council Meeting at the Geneva Congress, the following items were discussed.

(1) Future AsCA Meetings. The council discussed the proposal by the President, Y. Ohashi, that, in addition to the normal AsCA meetings, AsCA meetings also be held in conjunction with the meetings of the Society of Crystallographers in Australia and New Zealand (SCANZ) and the Crystallographic Society of Japan (CrSJ), such that AsCA members would have the opportunity to confer as a body twice in three years. S. R. Hall spoke in favour of the proposal and suggested that the upcoming Crystal-23 meeting of SCANZ, to be held in Broome, Western Australia, in August 2003, be the first such meeting to be jointly hosted with AsCA.

(2) Timing of AsCA Elections. A second proposal from the President's report concerned the timing of the election of officers and selection of venues for forthcoming AsCA meetings. There was general agreement that such important decisions would be more appropriately made in Council meetings held at AsCA conferences.

(3) Location of AsCA '04. It was proposed that the next AsCA meeting, AsCA '04, be held in Hong Kong, People's Republic of China. Representatives from Hong Kong indicated that they were still anxious to hold the meeting but that there would be logistical problems if the meeting were to be held at the traditional times of October–November. In discussion, it was agreed that the Association needed to be flexible over the meeting time, as it was clearly impossible to pick an ideal time that suited all participants.

(4) New AsCA Council Member. The application from crystallographers of Mongolia for their country to join the Association was approved unanimously. Mongolia became the 18th member country of AsCA.

The 4th AsCA meeting was very successful. The meeting attracted many more people than before in spite of the tragic events of 11 September. AsCA acquired a new Council Member (Mongolia) and is considering the joint hosting of a meeting with another meeting such as SCANZ, additional to the regular AsCA meetings, to raise the activity of the AsCA. It is good to report that AsCA is developing steadily.

M. Tanaka, Representative

12.3. European Crystallographic Association (ECA)

Since its establishment in 1997 and during the last three years, the ECA has launched some new initiatives, set up Special Interest Groups (SIGs), created the ECA Prize and established the procedure for adhesion and representation of Individual Members.

Ten SIG's are now formed and working within the ECA: Macromolecular Crystallography; Charge, Spin and Momentum Density; Aperiodic Crystallography; Electron Crystallography; Mineralogical Crystallography; Instrumentation and Experimental Techniques; Molecular Interaction and Recognition; Powder Diffraction; Crystallographic Computing; and Diffraction Physics and Optics.

ECA Prizes are presented at European Crystallographic Meetings and were established to recognize significant achievements or discoveries in the previous 5–10 years. The first Prize was awarded in 2000 during ECM-19 to A. Yonath from the Weizmann Institute of Science, Israel. The 2001 winner was J. Schneider from HASYLAB in Germany and the Prize was awarded during ECM-20 in Krakow, Poland.

ECA members are distributed between 30 National Members, 8 Corporate Affiliate Members and more than 500 Individual Members. Four Council members were elected to represent the Individual Members at the Council meeting in Nancy, France.

The second Executive Committee was elected during ECM-19 in Nancy, France, 2000. C. Lecomte is the President, P. T. Beurskens is Vice-President, G. Filippini Secretary, M. T. Duarte Treasurer, and E. Dodson, M. Jaskolski and D. Viterbo members.

Two very successful European Crystallographic Meetings were held, ECM-19 in Nancy, France, in 2000 and ECM-20 in Krakow, Poland, in 2001, attracting 1,020 and 720 participants, respectively. Forthcoming meetings will be held in Durban, South Africa, in 2003 (ECM-21) and in Budapest, Hungary, in 2004 (ECM-22).

M. A. Carrondo, Representative

12.4. International Centre for Diffraction Data (ICDD)

R. L. Snyder represented the ICDD at the meetings of the Commission on Powder Diffraction (CPD), reporting on a variety of activities, details of which can be found at http://www.icdd.com/. During the triennium (starting with the 1999 edition), the ICDD took over the organization of the Denver conference, an important event for the powder diffraction community. In addition, ICDD continued to organize clinics on powder diffraction methods, a valuable support for beginners.

Detailed reports on ICDD activity are constantly published in the CPD *Newsletter*. This forms part of the improved relationships between the CPD and the ICDD. This new course of collaboration includes the exchange of information, and permitted an important agreement concerning the dates of future Denver Conferences in relation to IUCr Congresses, so that the two events will not overlap.

P. Scardi, Representative

12.5. International Organization of Crystal Growth (IOCG)

During the triennium 1999–2001, the IOCG Executive Committee has taken several decisions regarding the life of the International Organisation of Crystal Growth: (i) it started exploring the possibility for IOCG to become an International Union to be affiliated to ICSU; (ii) it was decided that any National Association for Crystal Growth willing to organize ICCG must guarantee that the Proceedings will be published in *Journal of Crystal Growth*, along with a report on the Conference and the IOCG business meetings; (iii) the venues for the 2004 meetings of ICCG and ISSCG were selected – both will be held in Europe, the school in Berlin, Germany, and the conference in Grenoble, France.

The triennial reports (period 1998–2000) arranged by the individual National Crystal Growth Associations were collected by the President of IOCG, T. Nishinaga, and distributed to members of the Council and Executive Committee. It appears that National Associations for Crystal Growth are very active in promoting the crystal growth science in their own countries as well as in collaborating to organize international events. The International Conference on Crystal Growth (ICCG-13) took place in Kyoto, Doshisha University, Japan, 30 July–4 August 2001 in conjunction with the International Conference on Vapour Growth and Epitaxy (ICVGE-11).

The International Summer School on Crystal Growth (ISSCG-11) took place 24–29 July 2001. These are certainly the two events that more deeply characterize the life of IOCG and were both very successful. It is worth mentioning that ICCG-13 attracted over 1,200

delegates, which is approximately twice the number of participants at the previous meetings of the IOCG.

The Frank Prize for outstanding contributions to fundamental aspects of crystal growth was jointly assigned to D. Hurle and S. Coriell for their cooperative research leading to the quantitative understanding of the role of convective flows and electric fields in crystal growth and morphological stability. The Laudise Prize was awarded to G. Mueller for his contributions to the development of technological aspects and computer modelling of crystal growth processes.

The Officers and Executive Committee for the triennium 2001–2003, elected at the general meeting held during ICCG-13, are as follows: President: R. F. Sekerka (USA), Vice Presidents: K. W. Benz (Germany), J. P. Van der Eerden (The Netherlands), Secretary: T. F. Kuech (USA), Treasurer: T. Ohachi (Japan), Past President: T. Nishinaga (Japan), Honorary Principal Founder IOCG: M. Schieber (Israel). Executive Committee: T. Duffar (France), R. Fornari (Italy), Jiang Min-Hua (China), G. Mueller (Germany), V. V. Osiko (Russia), M. Roth (Israel), K. Sato (Japan), J. N. Sherwood (UK).

R. Fornari, Representative

13. Appendix M: Reports of Representatives on Bodies not belonging to the Union

13.1. Interdivisional Committee on Nomenclature and Symbols of the International Union of Pure and Applied Chemistry (IUPAC IDCNS)

The IUCr, together with the Bureau International des Poids et Mesures (BIPM), the International Organization for Standardization (ISO) and four other International Unions [of Biochemistry and Molecular Biology (IUBMB), Nutritional Sciences (IUNS), Pure and Applied Physics (IUPAP), and Pharmacology (IUPHAR)], is represented on IDCNS as the body charged by the International Union of Pure and Applied Chemistry (IUPAC) with the responsibility of ensuring that all recommendations concerned with terminology, nomenclature and symbols that are made in its name are consistent with its own and other international standards. IUPAC recommendations are published in *Pure and Applied Chemistry* following revision and final acceptance. A total of 163 such documents passed through IDCNS hands in the triennium under review.

IDCNS meets annually, usually in August and often at the same time as a major crystallographic meeting. The August 1999 meeting in Berlin, Germany, completely overlapped the triennial IUCr Congress in Glasgow and the August 2000 meeting in Sèvres, France, coincided with ECM-19, with the result that neither the IUCr Representative nor his Alternate were able to participate. The August 2001 meeting was held in Brisbane, Australia, in association with the 41st IUPAC General Assembly. In the interests of economy, D. C. Creagh, University of Canberra, kindly stood in for the IUCr Representative.

Matters of interest to crystallographers arising thereby include the International Standard (IEC 60027-2, January 1999) for binary multiple prefixes, which are to be distinguished from SI decimal multiple prefixes. In the former, for example, the prefix for 2^{10} is kibi, symbol Ki, that for 2^{60} is exbi, symbol Ei. Thus a kibibyte is 2^{10} = 1,024 bytes, a mebibyte is 2^{20} = 1,048,576 bytes; in SI, the common kilobyte = 10^3 bytes, the megabyte = 10^6 bytes. The corrected and revised version of the 2nd print edition of IUPAC's *Compendium of Chemical Technology* is now available online at http://www.iupac.org/publications/compendium/index.html for searching or browsing. A comprehensive online guide to IUPAC book publications is similarly available at http://www.iupac.org/publications/books/index.html. Online access to current values of the fundamental physical constants is accessible at http://www.physics.nist.gov/cuu/Constants/. Guidelines for the recommended use of italic and roman font for symbols in scientific text are given in http://www.iupac.org/standing/idcns/fonts_for_symbols.html. Additional guidelines on quantity calculus, the printing of numbers, and the use of terms such as % and p.p.m. have been proposed, consistent with *Quantities, Units and Symbols in Physical Chemistry*, 3rd edition. IDCNS reaffirmed the standard that dates should follow ISO 8601, in which the order is yyyy/mm/dd.

BIPM is working toward a redefinition of the kilogram linked to fundamental or atomic constants; toward an extension of the International Temperature scale below the present lower limit of 0.65 K; and approved katal (symbol 'kat') for the SI unit mole per second in the expression of catalytic activity. Biochemical nomenclature recommended by a joint IUPAC and IUBMB commission may be found at the web site http://www.chem.qmw.ac.uk/iupac/jcbn and other major biochemical nomenclature at http://www.chem.qmw.ac.uk. Useful online chemical naming services are given at http://www.iupac.org/nomenclature/index.html, http://www.acdlabs.com/ and http://www.beilstein.com/.

IUPAC has now restructured IDCNS, as part of a Strategic Plan for reorganizing its project management, to become the Interdivisional Committee on Terminology, Nomenclature, and Symbols (ICTNS). The change recognizes 'terminology' as part of the Committee's charge, adds titular and associate members, and provides a clear connection between the Committee and each Divisional Committee to ensure that all documents for publication are adequately reviewed.

S. C. Abrahams, Representative

13.2. International Council for Science (ICSU)

The election of a new Executive Board and a new Executive Director for ICSU has signalled a review of its activities. In particular, there is a desire to engage the Scientific Unions more fully. To this end, a meeting of International Union Presidents took place in Paris in February 2001. ICSU has also resolved to play an increased role in scientific debate on issues of significant scientific and public interest. During the past year, some 20 topics have been chosen for the preparation of position statements, including some of great public interest, such as GM foods, human cloning and gene therapies. Unions are invited to contribute on these topics. One that the IUCr is well placed to contribute to, through its Committee on Crystallographic Databases, is that of access to data and databases, and others that will be of particular interest include the issue of gene patenting and statements on the role and value of basic sciences. The next General Assembly of ICSU, and an opportunity for the IUCr to contribute, will be in September 2002, in Rio de Janeiro, Brazil.

E. N. Baker, Representative

13.2.1. 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, 14 international scientific unions, 5 co-opted delegates, and 21 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.

Following a review of Task Group and Commission activities in October 1999, the role of the Task Groups was revised to emphasize stronger planning and a clearer focus on deliverables. Current Task Groups cover a range of activities of interest, including: recommendation of standard values for the fundamental physical constants; data information and visualization; mathematical methodologies for data handling and knowledge interpretation; surveys of data sources in Asia/Oceania and in Africa; the establishment of a global species database; the construction of an information system on natural gas hydrates; and the creation of a standard file format for characterizing physicochemical properties. This last Task Group has interacted with the IUCr Commission on Crystallographic Nomenclature in a call for machine-readable identifiers suitable for locating and identifying information on phases stored across heterogeneous data banks.

Working Groups may also be formed to address particular areas of interest; among those currently in existence are one monitoring policy and legal issues of access to and ownership of databases and their content, and another concerned with the long-term archiving of electronic data collections.

In the last triennium, the major meeting was the CODATA 2000 conference at Lake Maggiore in Italy, subtitled 'Data and Information for the Coming Knowledge Millennium'. There were over 240 oral presentations and 20 posters in four parallel sessions, covering topics in geoscience, taxonomy and biological species data, genomics, chemistry, materials science, physical properties, astronomy and space sciences, and the environment. Interdisciplinary topics of interest to the IUCr included: interoperability between data representations and data collections; data access and intellectual property rights; access in perpetuity and the preservation of data sets over long time scales; and the usefulness and value of the World Wide Web in querying, retrieving and understanding data. A presentation by the IUCr representative on the IUCr's web-based services and its electronic journals programme was subsequently published in the inaugural issue of *Data Science*, a peer-reviewed journal long envisaged by CODATA as a valuable online publication covering the field of data and data systems.

Increasing overlap between electronic publishing and data handling initiatives have led to a greater synergy between the ICSU bodies concerned with publications and with data, and it is appropriate at this time that the IUCr representatives to ICSTI and CODATA are both members of the IUCr Committee on Electronic Publishing, Dissemination and Storage of Information.

B. McMahon, Representative

13.2.2. ICSU Committee on Science and Technology in Developing Countries – Incorporating International Biosciences and Other Scientific Networks (COSTED–IBN). COSTED–IBN is an advisory body to ICSU, whose goal it is to strengthen science in small states and developing countries. Its primary focus is on capacity building. At present, COSTED has few interactions with the ICSU Scientific Unions, or with their teaching commissions, and a review is currently under way in order to try to strengthen these links. Few communications have been received by the IUCr during the past three years, however.

E. N. Baker, Representative

13.2.3. ICSU Committee on Space Research (COSPAR). The 33rd COSPAR Scientific Assembly and Associated Events took place in Warsaw, Poland, 16–23 July 2000. This meeting included a plenary session entitled 'Space 2000' and another main session on 'Back to the Moon'. During the meeting, some distinguished scientists were awarded with the Space Science award (R. Bonnet, USA), the International Cooperation Medal (J. H. Carver, Australia), and the William Nordberg Medal (K. Ljiri, Japan).

As reported by the Chair, G. Haerendel, 2001 was a quiet year from both administrative and scientific points of view. In the administration, the major change was in January 2001 when a new Executive Director was appointed by COSPAR. The new Director is I. Revah, formerly at the French Centre National d'Etudes Spatiales. As regards space science, there were few major launch events but nevertheless the harvest of new scientific insights was rich: the discovery of what lies beneath a sunspot and the new information on the Earth's magnetosphere, for example.

Recently, the COSPAR Bureau focused its activity on the 34th COSPAR Scientific Assembly, which will be held in conjunction with the 2nd World Space Congress, 10–19 October 2002, Houston, TX, USA. The preliminary programme of the Congress and all relevant information (deadlines, applications for travel support *etc*.) may be found in COSPAR Bulletin 151 (August 2001) or at the web site http://www.copernicus.org/COSPAR/COSPAR.html.

A survey of the most important space missions and relevant results may be found in COSPAR Bulletin Nos. 146–152 published by Elsevier. Other important information is available at the new COSPAR web site http://www.cosparhq.org/.

A list of the main meetings sponsored/organized by COSPAR during the last triennium follows:

Joint URSI–COSPAR 99, Lowell, MA, USA, 9–12 August 1999

IAU–COSPAR–UN Workshop on Education in Astronomy and Space Science, Vienna, Austria, 20–22 July 1999

Magnetospheres of the Outer Planets (MOP 99), Paris, France, 9–14 August 1999

5th Asia–Pacific Conference on Cooperation in Space Technology and Applications, Teheran, Iran, 2–7 May 1999

Long Term Changes in Atmosphere, Puni, India, 15–19 February 1999

Chapman Conference on Space Weather, Florida, USA, February 2000

IAU–COSPAR Colloquium on Dust in Solar System, Kent, UK, April 2000

NATO–ASI Space Storms and Space Weather Hazards, Crete, June 2000

1st International Solar Cycle Symposium, Tatranska Lomnica, Slovakia, July 2000

COSPAR Colloquium on the Outer Heliosphere, Potsdam, Germany, July 2000

COSPAR Colloquium on Space Weather Study using Multi-Point Techniques, Taiwan, September 2000

1st S-RAMP Conference, Sapporo, Japan, October 2000

MARISY, Rabat, Morocco, November 2000

2nd SPARC General Assembly, Mar del Plata, Argentina, November 2000

R. Fornari, Representative

13.2.4. ICSU Programme on Capacity Building in Science (PCBS). At the 26th General Assembly of ICSU, Cairo, Egypt, 27–30 September 1999, it was noted that:

(i) one of ICSU's seven principal objectives as stated in its Statutes is 'to encourage the strengthening of human and physical scientific resources world wide';

(ii) ICSU and its Scientific Unions are engaged in a wide variety of educational activities from the primary through the tertiary level;

(iii) the Scientific Unions have suggested that ICSU's and the Unions' educational objectives would benefit greatly from better

communication and coordination of the several educational goals and activities.

A compendium on ICSU activities in capacity building is being prepared by the ICSU Secretariat.

The IUCr's Visiting Professorship Programme, which received support from the ICSU/UNESCO subvention in 1999 and 2000, continues.

K. El-Sayed, Representative

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

The IUCr representative attended the following ICSTI meetings in the triennium 1999–2001:

Winter committee and discussion meeting held at ICSU, Paris, France, 29–30 January 2000.

An interactive workshop on Digital Archiving: Bringing Issues and Stakeholders Together at UNESCO, Paris, France, 30–31 January 2000; this workshop was organized jointly by ICSTI/ICSU Press. Y. Epelboin also attended.

Annual ICSTI meeting held in Columbus, Ohio, USA, 19–22 May 2000. This meeting was hosted by Chemical Abstracts Service (CAS). The IUCr's Managing Editor, P. R. Strickland, and the IUCr's Research and Development Officer, B. McMahon, also attended. The main discussion session was entitled 'Economic Impacts of Electronic Publishing'. A working visit was paid to CAS after the ICSTI meeting.

Winter ICSTI committee and discussion meeting held at ICSU, Paris, France, 13–14 January 2001.

Annual ICSTI meeting held in the European Patent Office, Munich, Germany, 3–7 May 2001. This included a one-day public conference entitled 'Scientific Information and Intellectual Property: Problems and Opportunities'.

No representative of the IUCr was present at the annual meeting in Taipei, 6–10 May 1999.

ICSTI, in conjunction with CODATA and ICSU Press, organized a symposium devoted to 'Sharing Information Knowledge' in the framework of the World Conference on Science organized by ICSU in Budapest, Hungary, in June 1999. The ICSTI President expressed the concern of the scientific information community regarding digital electronic archiving and continued preservation and access to scientific literature.

On the administrative side, an important task concerned the policy to adopt for the replacement of the ICSTI Executive Secretary who retired in September 2000. In the event, the secretariat was put out to tender and from the offers received the ICSTI bureau selected the offer of Information International Associates (IIA), a specialized consultancy established in the USA with whom ICSTI has had contacts for a considerable number of years. The arrangement consists in the services of a part-time Executive Director experienced in STM publishing and a part-time Secretary in Paris, France.

Through ICSTI, the IUCr participated in the Ingenta study on 'Research into the Relationship between Journal Subscriptions and Document Delivery and the Impact of Online Delivery on Article Distribution'. Data were provided to Ingenta on some of the IUCr journals. Detailed analyses on these were made available at the conclusion of the study and the IUCr's Managing Editor, P. R. Strickland, attended the public presentation of the whole study in London, UK, on 25 September 2001.

The IUPAC–CODATA–ICSTI project on the 'Standardisation of Physico-Chemical Property Electronic Datafiles' (IUCODIX) seeks to bring to the world of physical chemistry the advantages that CIF has brought to crystallography. The project brought to light a problem in the current nomenclature of phase identifiers for crystals, showing this to be unsuitable as an identifier in electronic databases. Interaction with the IUCr's Commission on Crystallographic Nomenclature has led to the formation of a working group with a mandate to seek a solution to this problem.

ICSTI is not alone in maintaining a watch on developments in copyright law and practice. Of special concern, the EU copyright directive gives much power and freedom to database generators. CODATA programmed a one-day workshop on this topic at its 2001 annual meeting. ICSU itself is concerned about the implications of the EU directive on copyright and ICSU's President has corresponded with its associated organizations on this matter.

A major preoccupation of ICSTI is the archiving and preservation of digital information. Presentations at various workshops and meetings have had tangible effects on the IUCr's activity in electronic publishing. One example is the policy on archiving for journals in electronic form presented by the American Institute of Physics. This document was used as the basis for drafting an archive policy for the IUCr undertaken by the Committee on Electronic Publishing, Dissemination and Storage of Information (CEP). A second example is the participation of the IUCr's representative to ICSTI and the IUCr's Research and Development Officer in studying the OAIS (Open Archive Information System) draft. This study enabled, nay forced, these two people to comprehend the immense value of OAIS as a conceptual and practical model in the archiving and preservation of the IUCr's electronic journals. Mention should also be made to the report of an international working group convened by the International Association of STM Publishers (IASTMP) concerned with 'defining and certifying electronic publication in science'. ICSTI is now committed to providing advocacy for the preservation of digital scientific and technical information and of the record of science. The intention is to facilitate the provision of resources for preservation.

At their annual meetings, ICSTI invites short presentations from member organizations. The undersigned presented the IUCr, and especially its publishing activities, using the excellent slide presentation prepared in Chester. As the IUCr provides a nice example of a knowledge management organization in the scientific sphere, the representative has been solicited several times to contribute a detailed article to the ICSTI newsletter *Forum*.

ICSTI maintains both a public web site at http://www.icsti.org/, where the ICSTI newsletter *Forum* and other general information are made available. A private section is available only to members, the IUCr representative sharing this opportunity with the IUCr's 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. During this triennium, ICSTI has maintained its principal mission as directed towards strategy in the scientific and technical information industry as a whole. IUCr membership of ICSTI continues to fulfil its expectations by providing a source of current documentation and personal contacts.

H. D. Flack, Representative

14. Appendix N: Budget estimates for period to Twentieth General Assembly: determination of unit contribution

14.1. Budget estimates

The estimated budget for the General Fund (GF) 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 2002–31 December 2004.

	CHF	CHF
Income		
Subscriptions from Adhering Bodies	450,000	
Yield from investments and banking accounts	750,000	1,200,000
Expenditure		
Administration	940,000	
Subscriptions to ICSU and bodies of ICSU	33,000	
Administrative meetings	272,500	
Scientific meetings	110,500	1,356,500
Estimated profit or deficit		−156,500

14.2. 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 for the years 2003–2005.